Lecture Notes on Group Theory in Physics
(A Work in Progress)

Daniel Arovas
Department of Physics
University of California, San Diego

August 12, 2022

Contents

Contents i

List of Figures ix

List of Tables xiii

0.1 Preface . . . xviii

0 Reference Materials 1

0.1 General Texts . . . 1

0.2 Specific Applications . . . 2

0.3 Group Theory for Solid State Physics . . . 2

0.4 Lie Groups and Lie Algebras . . . 3

0.5 Other . . . 4

1 Introduction to Groups 5

1.1 Disclaimer . . . 5

1.2 Why Study Group Theory? . . . 5

1.2.1 Discrete and continuous symmetries . . . 5

1.2.2 Symmetries in quantum mechanics . . . 6

1.3 Formal definition of a discrete group . . . 7

1.3.1 Group properties . . . 7

1.3.2 The Cayley table . . . 8

1.3.3 Loops and groups . . . 8

1.3.4 The equilateral triangle : C_{3v} and C_3 . . . 9
1.3.5 Symmetry breaking . . . 11
1.3.6 The dihedral group D_n . . . 13
1.3.7 The permutation group S_n . . . 14
1.3.8 Our friend, SU(2) . . . 16
1.4 Aspects of Discrete Groups . . . 18
1.4.1 Basic features of discrete groups . . . 18
1.4.2 Other math stuff . . . 22
1.4.3 More about permutations . . . 23
1.4.4 Conjugacy classes of the dihedral group . . . 25
1.4.5 Quaternion group . . . 25
1.4.6 Group presentations . . . 27
1.5 Lie Groups . . . 28
1.5.1 Definition of a Lie group . . . 28
1.5.2 The big happy family of matrix Lie groups . . . 29
1.5.3 More on semidirect products . . . 34
1.5.4 Topology of the happy family . . . 35
1.5.5 Matrix exponentials and the Lie algebra . . . 37
1.5.6 Structure constants . . . 40
1.6 Appendix : Ideal Bose Gas Condensation . . . 41

2 Theory of Group Representation **45**
2.1 Basic Definitions . . . 45
2.1.1 Group elements cry out for representation . . . 45
2.1.2 Equivalent and reducible representations . . . 46
2.1.3 Conjugate and adjoint representations . . . 47
2.1.4 Unitary representations of finite groups . . . 47
2.1.5 Projective representations . . . 48
2.2 The Great Orthogonality Theorem . . . 51

2.2.1 Schur's first lemma . . . 51
2.2.2 Schur's second lemma . . . 52
2.2.3 Great Orthogonality Theorem . . . 53
2.3 Group Characters . . . 54
2.3.1 Example : D_3 . . . 55
2.3.2 Orthogonality theorem for characters . . . 56
2.3.3 Dirac characters . . . 57
2.4 Decomposition of Representations . . . 58
2.4.1 Reducible representations . . . 58
2.4.2 Projection onto a particular representation . . . 59
2.4.3 The regular representation . . . 61
2.4.4 Induced and subduced representations . . . 61
2.4.5 Summary of key results . . . 63
2.4.6 Example character tables . . . 63
2.4.7 Character table for $\mathbb{Z}_2 \times G$ . . . 65
2.4.8 Direct product representations . . . 65
2.5 Real Representations . . . 67
2.6 Representations of the Symmetric Group . . . 69
2.6.1 Partitions, Young diagrams and Young tableaux . . . 69
2.6.2 S_3 and S_4 . . . 70
2.6.3 IRREPs of S_n . . . 72
2.7 Application of Projection onto IRREPs : Triatomic Molecule . . . 73
2.8 Jokes for Chapter Two . . . 77

3 Group Theory and Quantum Mechanics 79
3.1 Hilbert Space and Group Symmetries . . . 79
3.1.1 Classification of the basis states . . . 79
3.1.2 Accidental degeneracies . . . 81
3.1.3 Operators and wavefunctions . . . 86

3.1.4 Projection operators . . . 87
3.1.5 Projecting arbitrary functions onto IRREPs . . . 88
3.1.6 Partial diagonalization of H . . . 91
3.2 Product Representations . . . 92
3.2.1 Direct product of two representations . . . 92
3.2.2 Products of identical representations . . . 92
3.2.3 Clebsch-Gordan Coefficients . . . 94
3.2.4 Simply reducible groups . . . 95
3.2.5 Wigner-Eckart theorem . . . 97
3.2.6 Level repulsion and degeneracies . . . 100
3.2.7 Example: C_{4v} . . . 101
3.3 Appendix : Random True Facts About Linear Algebra . . . 103
3.4 Jokes for Chapter Three . . . 106

4 Continuous Translations and Rotations **109**
4.1 Translations and their Representations . . . 109
4.1.1 Discrete translations and their continuum limit . . . 109
4.1.2 The cyclic group and its continuum limit . . . 110
4.1.3 Consequences of parity symmetry on the eigenspectrum . . . 111
4.1.4 Invariant measure for SO(2) . . . 112
4.2 Remarks about SO(N) and SU(N) . . . 113
4.2.1 How SO(N) acts on vectors, matrices, and tensors . . . 113
4.2.2 Invariant symbols, dual tensors, and up/down index notation . . . 114
4.2.3 Tensor representations of SU(N) . . . 115
4.3 SO(3) and SU(2) . . . 116
4.3.1 Irreducible representations of SO(3) . . . 119
4.3.2 Rotation matrices . . . 120
4.3.3 Guide for the perplexed . . . 123
4.3.4 Invariant measure for Lie groups . . . 124

4.3.5 Peter-Weyl theorem . . . 127
4.3.6 Projection operators . . . 127
4.3.7 Product representations for SU(2) . . . 128
4.3.8 Spherical harmonics . . . 130
4.3.9 Tensor operators and the Wigner-Eckart theorem for SU(2) . . . 132
4.4 Joke for Chapter Four . . . 133

5 Crystal Math **135**
5.1 Classification of Crystalline Structures . . . 135
5.1.1 Bravais Lattices . . . 135
5.1.2 Miller indices . . . 138
5.1.3 Crystallographic restriction theorem . . . 139
5.1.4 Enumeration of two and three-dimensional Bravais lattices . . . 140
5.1.5 Crystals . . . 142
5.1.6 Trigonal crystal system . . . 146
5.1.7 Point groups, space groups and site groups . . . 147
5.2 More on Point Groups . . . 149
5.2.1 Standard notation for point group operations . . . 149
5.2.2 Proper point groups . . . 150
5.2.3 Commuting operations . . . 151
5.2.4 Improper point groups . . . 152
5.2.5 The ten two-dimensional point groups . . . 155
5.2.6 The achiral tetrahedral group, T_d . . . 156
5.2.7 Tetrahedral *vs.* octahedral symmetry . . . 158
5.2.8 The 32 crystallographic point groups . . . 159
5.2.9 Hermann-Mauguin (international) notation . . . 159
5.2.10 Double groups . . . 164
5.2.11 The three amigos : D_4 , C_{4v} , D_{2d} . . . 167
5.3 Space Groups . . . 171

5.3.1 Space group elements and their properties . . . 171
5.3.2 Factor groups . . . 174
5.3.3 How to make a symmorphic space group . . . 177
5.3.4 Nonsymmorphic space groups . . . 178
5.3.5 Translations and their representations . . . 179
5.3.6 Space group representations . . . 181
5.4 Fourier Space Crystallography . . . 183
5.4.1 Space group symmetries . . . 184
5.4.2 Extinctions . . . 185
5.4.3 Sticky bands . . . 186

6 Consequences of Crystallographic Symmetry 191
6.1 Atomic Physics and the Periodic Table . . . 191
6.1.1 Aufbau principle . . . 191
6.1.2 Splitting of configurations: Hund's rules . . . 192
6.2 Crystal Field Theory . . . 194
6.2.1 Decomposing IRREPs of O(3) . . . 195
6.2.2 Atomic levels in a tetragonal environment . . . 197
6.2.3 Point charge model . . . 197
6.2.4 Cubic and octahedral environments . . . 199
6.2.5 Matrix elements and selection rules . . . 201
6.2.6 Crystal field theory with spin . . . 205
6.3 Macroscopic Symmetry . . . 211
6.3.1 Ferroelectrics and ferromagnets . . . 211
6.3.2 Spontaneous symmetry breaking . . . 213
6.3.3 Pyroelectrics, thermoelectrics, ferroelectrics, and piezoelectrics . . . 214
6.3.4 Second rank tensors : conductivity . . . 218
6.3.5 Third rank tensors : piezoelectricity . . . 220
6.3.6 Fourth rank tensors : elasticity . . . 222

6.3.7 Summary of tensor properties of the crystallographic point groups 227
6.4 Vibrational and Electronic States of Molecules 227
6.4.1 Small oscillations of molecules 227
6.4.2 Group theory and the dynamical matrix 229
6.4.3 Selection rules for infrared and Raman spectroscopy 233
6.4.4 Electronic spectra of molecules 238
6.5 Phonons in Crystals 239
6.5.1 Translation and rotation invariance 243
6.5.2 Phonons in an fcc lattice 243
6.5.3 Elasticity theory redux : Bravais lattices 244
6.5.4 Elasticity theory in cases with bases 247
6.6 Appendix : O(3) Characters of Point Group Operations 248
6.7 Appendix : Construction of Group Invariants 248
6.7.1 Polar and axial vectors 248
6.7.2 Invariant tensors 249
6.7.3 Shell theorem 250
6.8 Appendix : Quasi-degenerate Perturbation Theory 251
6.8.1 Type A and type B operators 251
6.8.2 Unitary transformation for block diagonalization 252
6.9 Jokes for Chapter Six 254

7 Time Reversal **257**
7.1 The Poincaré Group 257
7.1.1 Space inversion and time-reversal 257
7.1.2 Representations of the Poincaré Lie algebra 258
7.1.3 Whither time-reversal? 259
7.2 Antilinearity : The Solution to All Our Problems 260
7.2.1 Properties of antilinear operators 260
7.2.2 Position and momentum eigenstates 262

7.2.3 Change of basis for time-reversal . . . 263
7.2.4 Time reversal with spin . . . 264
7.2.5 Kramers degeneracy . . . 265
7.2.6 External fields . . . 265
7.3 Time Reversal and Point Group Symmetries . . . 266
7.3.1 Complex conjugate representations . . . 267
7.3.2 Generalized time-reversal . . . 268
7.4 Consequences of Time-Reversal . . . 269
7.4.1 Selection rules and time-reversal . . . 269
7.4.2 Onsager reciprocity . . . 270
7.5 Color groups . . . 272
7.5.1 Magnetic Bravais lattices and magnetic space groups . . . 275
7.5.2 Corepresentations of color groups . . . 279
7.6 Appendix : The Foldy-Wouthuysen Transformation . . . 279
7.6.1 Derivation of the Spin-Orbit Interaction . . . 280

8 Lie Groups and Lie Algebras, and their Representations 283
8.1 Mathematical Preliminaries . . . 283
8.1.1 Why Lie groups are special smooth manifolds . . . 284
8.1.2 Structure constants . . . 285
8.1.3 Exponential map . . . 286
8.1.4 Baker-Campbell-Hausdorff formula . . . 287
8.2 Vector fields and the Lie algebra . . . 288
8.2.1 Smooth vector fields . . . 288
8.2.2 Integral curves and the exponential map . . . 291
8.3 Representations of Lie Algebras . . . 292
8.3.1 Properties of the structure constants . . . 292
8.3.2 Representations . . . 293
8.3.3 Matrix Lie groups and their Lie algebras . . . 293

8.3.4 Some examples 294
8.3.5 SU(3) 295
8.4 Classification of Semisimple Lie Algebras 298
8.4.1 Real, complex, simple, and semisimple 298
8.4.2 The Killing form and Cartan's criterion 300
8.4.3 Casimirs 301
8.5 The Cartan Subalgebra 303

List of Figures

1 Henry (2000 - 2015) xviii

1.1 Examples of beauty and symmetry 6
1.2 C_{3v} and C_3 10
1.3 Injective, surjective, and bijective functions 11
1.4 The double torus and its fundamental group generators 36
1.5 The fundamental group of $\mathsf{SO}(3)$ is $\mathbb{Z}_2$. 37

2.1 Equilateral triangular planar molecule 74

3.1 Six site cluster with D_{3h} symmetry 81
3.2 Electronic structure of the C_{60} molecule 85
3.3 A projector from the early days of group theory 88
3.4 Eugene P. Wigner 98

4.1 Definition of Euler angles and their order of operations 118

5.1 Brillouin zones 136
5.2 Simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices 137
5.3 Examples of Miller planes 138
5.4 Fivefold symmetry 140
5.5 The five two-dimensional Bravais lattices 141
5.6 Cubic, trigonal, and hexagonal Bravais lattices 142
5.7 Orthorhombic Bravais lattices 143

5.8 Tetragonal, monoclinic, and triclinic Bravais lattices . . . 143
5.9 Tetrahedral, cubic, and icosahedral group symmetry operations . . . 144
5.10 Unit cells of four high temperature cuprate superconductors . . . 145
5.11 Two nonsymmorphic crystal lattices . . . 149
5.12 The symmetry operations of T and O . . . 152
5.13 Stereograms of point groups (I) . . . 153
5.14 Stereograms of point groups (II) . . . 154
5.15 Stereograms of point groups (III) . . . 155
5.16 The zincblende structure and the group T_d . . . 156
5.17 Subgroup relations among the 32 crystallographic point groups . . . 160
5.18 Schematic diagram of (common axis) double group rotation generators . . . 165
5.19 Structure of hexagonal H_2O ice . . . 172
5.20 Unit cells for the 17 two-dimensional space groups . . . 175
5.21 Some common AB crystal structures and their space groups . . . 178
5.22 Stickiness of tight binding energy bands in an hcp crystal . . . 187
5.23 Examples of one-dimensional symmorphic and nonsymmorphic lattices . . . 189
5.24 Examples of space groups and their nonsymmorphic ranks . . . 190

6.1 The *Aufbau* principle and the diagonal rule . . . 192
6.2 Title from Bethe's original article on term splitting in crystals . . . 195
6.3 Atomic p orbital in a tetragonal environment with D_{4h} symmetry . . . 196
6.4 Trigonal and rhombic distortions of an octahedral environment . . . 199
6.5 Splitting of an atomic d-level in different crystalline environments . . . 200
6.6 Decomposition of the ^{5}D states of Cr^{++} into IRREPs of O . . . 206
6.7 Decomposition of the ^{4}F states of Co^{++} into IRREPs of the double group O' . . . 208
6.8 High spin and low spin states of the Co^{4+} ion in a cubic environment . . . 210
6.9 High temperature cubic perovskite crystal structure of $BaTiO_3$ . . . 215
6.10 Mixed ferroelectric and antiferroelectric order in $BaTiO_3$ . . . 217
6.11 Small molecules with low symmetry . . . 230

6.12 Normal modes of the H_2O molecule and their C_{2v} IRREP labels 232
6.13 The buckyball C_{60} and its IRREPs 233
6.14 Rayleigh and Raman spectral lines in crystalline sulfur 237
6.15 Phonons in elemental rhodium and in gallium arsenide 241
6.16 Type-A and type-B operators 253

7.1 Colored squares and their magnetic point group symmetries 273
7.2 The two magnetic point groups deriving from $C_{2v} = mm2$ 274
7.3 The five new black and white Bravais lattices in two dimensions 275

8.1 A manifold and two overlapping charts 284
8.2 A smooth curve $\gamma(t)$ on a manifold M 290
8.3 SU(3) root vectors 297

List of Tables

1.1 Convention for group multiplication tables . . . 8
1.2 A non-associative loop of order 5 . . . 9
1.3 A non-associative loop of order 6 . . . 9
1.4 Multiplication table for the group C_{3v} . . . 10
1.5 Table of discrete groups up to order $|G| = 15$ . . . 27
1.6 Examples of discrete group presentations. . . . 28
1.7 Topological properties of matrix Lie groups . . . 37

2.1 Character table for C_{3v} . . . 55
2.2 Character table for C_3 . . . 63
2.3 Character table for the quaternion group Q . . . 64
2.4 Character table for the dihedral group D_4 . . . 64
2.5 Character table for $\mathbb{Z}_2 \times G$ . . . 65
2.6 Character table for the symmetric group S_3 . . . 71
2.7 Partial character table for the symmetric group S_4 . . . 71

3.1 Character table for the group D_{3h} . . . 83
3.2 Character table for the group C_{4v} . . . 102

5.1 True Facts about two and three-dimensional crystallography . . . 147
5.2 Standard notation for point group operations . . . 150
5.3 The ten two-dimensional point groups . . . 155
5.4 Character table for the group T_d . . . 156

5.5 Elements and classes for T_d . . . 157
5.6 Irreducible representations and basis functions for T_d and O . . . 158
5.7 The 32 three-dimensional crystallographic point groups . . . 159
5.8 Two element point group notation . . . 160
5.9 Notations for simple crystallographic point groups . . . 162
5.10 Notations for multi-axis point groups . . . 162
5.11 HM and Schoenflies notation for the 32 crystallographic point groups . . . 163
5.12 Character table for the double group of T_d . . . 167
5.13 Character table for the point groups D_4, C_{4v}, and D_{2d} . . . 168
5.14 Character table for the double groups of D_4 , C_{4v} , and D_{2d} . . . 170
5.15 The 17 wallpaper groups and their short notation . . . 174
5.16 The 73 symmorphic three-dimensional space groups . . . 176
5.17 The 157 nonsymmorphic three-dimensional space groups . . . 180

6.1 Order in which atomic shells are filled . . . 192
6.2 Electronic configuration of 3d-series metals . . . 193
6.3 Hund's rules applied to p, d, and f shells . . . 194
6.4 Character table of D_4 and decomposition of atomic p- and d- levels in a D_4 environment . . . 197
6.5 Character table of O and decomposition of $\mathsf{O}(3)$ IRREPs in terms of O IRREPs . . . 198
6.6 Splitting of one-electron levels in crystal fields of different symmetry . . . 202
6.7 Characters for the electric and magnetic dipole operators . . . 203
6.8 Character table for D_{3d} . . . 204
6.9 Decomposition of products of IRREPs in C_{3v} and D_{3d} . . . 205
6.10 Character table for the double groups O' and T_d' . . . 207
6.11 Character tables for C_3 and C_{3v} and decomposition of $\boldsymbol{P}$ and $\boldsymbol{M}$ . . . 211
6.12 Point groups supporting ferroelectricity and ferromagnetism . . . 212
6.13 Phases of $BaTiO_3$ and their space and point groups . . . 217
6.14 Allowed nonzero entries of symmetric rank two tensors by crystal system . . . 219
6.15 Composite indices for symmetric rank two tensors . . . 220

6.16 Tensor properties of the 32 crystallographic point groups 228
6.17 Character and representation product tables for C_{2v} 231
6.18 Character table for the icosahedral group $I_{\rm h}$ 234
6.19 Partial character table for O_h 239
6.20 Composite indices for symmetric rank two tensors 245
6.21 Composite indices for symmetric rank two tensors 245
6.22 $\mathsf{O}(3)$ characters of crystallographic point group operations 249
6.23 Characters for improper $\mathsf{O}(3)$ operations 249
6.24 Commutators and their types 252
6.25 Multiple commutators and their types 254

7.1 Representations and degeneracies for generalized time reversal $\check{\Theta} = \hat{r}\,\check{T}$ 269
7.2 The 58 colored three-dimensional magnetic point groups 277
7.3 True Facts about magnetic lattices, point groups, and space groups 278

8.1 Nonzero structure constants for $\mathsf{su}(3)$ 295

0.1 Preface

This is a proto-preface. A more complete preface will be written after these notes are completed. Which may not be for some time.

These lecture notes are intended to supplement a graduate level course in group theory applied to condensed matter physics. Or one can skip all the math and just read the jokes.

These notes are dedicated to the memory of my dog, Henry.



Figure 1: Henry (2000 - 2015)

Chapter 0

Reference Materials

No one book contains all the relevant material. Here I list several resources, arranged by topic. My personal favorites are marked with a diamond (⋄).

0.1 General Texts

⋄ B. Simon, *Representations of Finite and Compact Groups* (AMS, 1995)

⋄ A. Zee, *Group Theory in a Nutshell for Physicists* (Princeton, 2016)

⋄ W.-K. Tung, *Group Theory in Physics* (World Scientific, 1985)

⋄ M. Hamermesh, *Group Theory and its Application to Physical Problems* (Dover, 1962)

⋄ J. P. Elliott and P. G. Dawber, *Symmetry in Physics*, 2 vols. (Oxford, 1985)

- M. Tinkham, *Group Theory and Quantum Mechanics* (Dover, 2003)

- V. Heine, *Group Theory in Quantum Mechanics* (Dover, 2007)

- Z.-Q. Ma, *Group Theory for Physicists* (World Scientific, 2007)

- Z.-Q. Ma and X.-Y. Gu, *Problems & Solutions in Group Theory for Physicists* (World Scientific, 2007)

- R. Mirman, *Group Theory: An Intuitive Approach* (World Scientific, 1997)

- M. Stone and P. Goldbart, *Mathematical Physics* (Cambridge, 2009)

0.2 Specific Applications

- W. Ledermann, *Introduction to Group Characters* (Cambridge, 1987)

- B. E. Sagan, *The Symmetric Group: Representations, Combinatorial Algorithms, and Symmetric Functions* (Springer, 2001)

- W. Fulton, *Young Tableaux: With Applications to Representation Theory and Geometry* (Cambridge, 1996)

0.3 Group Theory for Solid State Physics

◇ M. Lax, *Symmetry Principles in Solid State and Molecular Physics* (Dover, 2012)

◇ B. S. Tsukerblat, *Group Theory in Chemistry and Spectroscopy* (Dover, 2006)

◇ T. Wolfram and Ş. Elliatioğlu, *Applications of Group Theory to Atoms, Molecules, and Solids* (Cambridge, 2014)

◇ R. C. Powell, *Symmetry, Group Theory, and the Physical Properties of Crystals* (Springer, 2010)

- R. A. Evarestov and V. P. Smirnov, *Site Symmetry in Crystals* (Springer, 1997)

- M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory : Application to the Physics of Condensed Matter* (Springer, 2008)

- S. H. Kim, *Group Theoretical Methods and Applications to Molecules and Crystals* (Cambridge, 2005)

- U. Müller, *Symmetry Relations between Crystal Structures* (Oxford, 2013)
- G. F. Koster, J. O Dimmock, R. C. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (MIT Press, 1963)
- M. El-Batanouny and F. Wooten, *Symmetry and Condensed Matter Physics* (Cambridge, 2008)
- T. Inui, Y. Tanabe, and Y. Onodera, *Group Theory and its Applications in Physics* (Springer, 1996)
- R. Mirman, *Point Groups, Space Groups, Crystals, and Molecules* (World Scientific, 1999)
- J. L. Birman, *Theory of Crystal Space Groups and Lattice Dynamics* (Springer, 1984)
- A. V. Shubnikov and N. V. Belov, *Colored Symmetry* (Pergamon, 1964)
- S. J. Joshua, *Symmetry Principles and Magnetic Symmetry in Solid State Physics* (Adam Hilger, 1991)

0.4 Lie Groups and Lie Algebras

◇ A. Das and S. Okubo, *Lie Groups and Lie Algebras for Physicists*, 2nd. ed. (World Scientific, 2014)

◇ B. C. Hall, *Lie Groups, Lie Algebras, and Representations*, 2nd. ed. (Springer, 2015)

◇ J. Fuchs and C. Schweigert, *Symmetries, Lie Algebras, and Representations* (Cambridge, 1997)

◇ W. Fulton and J. Harris, *Representation Theory: A First Course* (Springer, 2004)

◇ T. Kemp, *Introduction to Smooth Manifolds & Lie Groups* (unpublished)

- H. Georgi, *Lie Algebras in Particle Physics*, 2nd ed. (Westview Press, 1999)
- R. Gilmore, *Lie Groups, Physics, and Geometry* (Cambridge, 2008)

- R. Gilmore, *Lie Groups, Lie Algebras, and Some of their Applications* (Dover, 2006)
- R. Campoamor-Stursberg and M. R. de Traubenberg, *Group Theory in Physics* (World Scientific, 2019)
- A. O. Barut, and R. Rączka, *Theory of Group Representations and Applications*, (World Scientific, 1986)
- C. Procesi, *Lie Groups : An Approach through Invariants and Representations*, (Springer, 2007)
- P. Ramond, *Group Theory : A Physicist's Survey* (Cambridge, 2010)
- H. J. Lipkin, *Lie Groups for Pedestrians* (Dover, 2002)
- J. G. F. Belinfante and B. Kolman, *A Survey of Lie Groups and Lie Algebras with Applications and Computational Methods* (SIAM, 1987)
- M. Varadarajan, *Lie Groups, Lie Algebras, and their Representations* (Springer, 1984)
- F. W. Warner, *Foundations of Differentiable Manifolds and Lie Groups* (Springer, 1983)

0.5 Other

◇ J. H. Conway, H. Burgiel, and C. Goodman-Strauss, *The Symmetries of Things* (A. K. Peters, 2008)

◇ T. Weller, *Science Made Stupid* (Mariner, 1985)

◇ T. Weller, *Culture Made Stupid* (Houghton Mifflin, 1987)

◇ H. Beard, *Latin for All Occasions* (Villard, 1990)

Chapter 1

Introduction to Groups

1.1 Disclaimer

This is a course on applications of group theory to physics, with a strong bias toward condensed matter physics, which, after all, is the very best kind of physics. Abstract group theory is a province of mathematics, and math books on the subject are filled with formal proofs, often rendered opaque due to the efficient use of mathematical notation, replete with symbols such as $\cap$, $\rtimes$, $\exists$, $\oplus$, $\triangleleft$, $\flat$, ©, ♠, ♡, ♢, ♣, *etc.* In this course I will keep the formal proofs to a minimum, invoking them only when they are particularly simple or instructive. I will try to make up for it by including some good jokes. If you want to see the formal proofs, check out some of the texts listed in Chapter 0.

1.2 Why Study Group Theory?

1.2.1 Discrete and continuous symmetries

Group theory – big subject! Our concern here lies in its applications to physics (see §1.1).

Why is group theory important? Because many physical systems possess *symmetries*, which can be broadly classified as either *continuous* or *discrete*. Examples of continuous symmetries include space translations and rotations in homogeneous and isotropic systems, Lorentz transformations, internal rotations of quantum mechanical spin and other multicomponent quantum fields such as color in QCD, *etc.* Examples of discrete symmetries include parity, charge conjugation, time reversal, permutation symmetry in many-body systems, and the discrete remnants of space translations and rotations applicable to crystalline systems.

In each case, the symmetry operations are represented by individual group elements. Discrete symmetries entail discrete groups, which may contain a finite or infinite number of elements[1]. Continuous

[1] An example of a finite discrete group is the two-element group consisting of the identity I and space inversion (parity) P, otherwise known as $\mathbb{Z}_2$. An example of a discrete group containing an infinite number of elements is the integers $\mathbb{Z}$ under

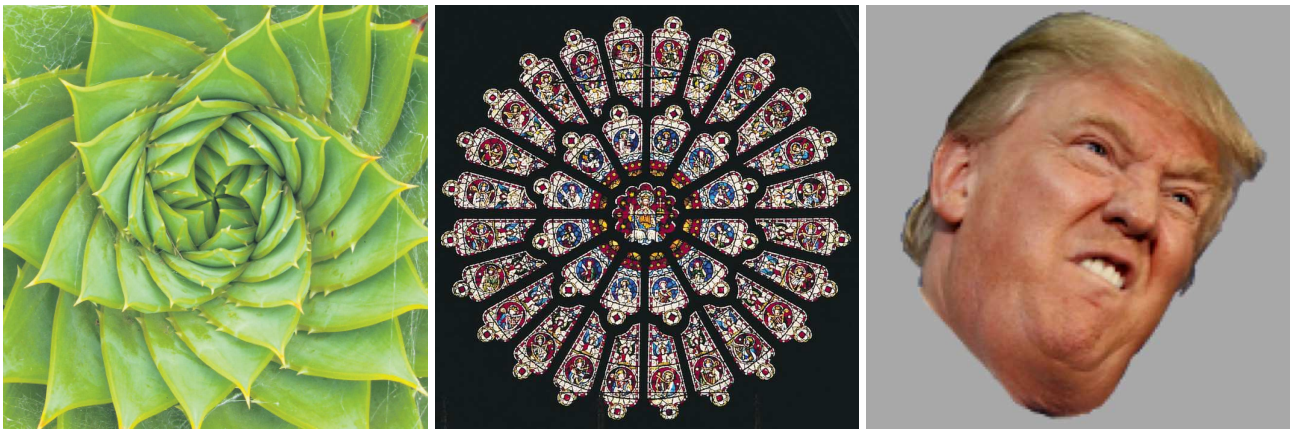


Figure 1.1: Western theories of beauty date to the pre-Socratic Greek philosophers (6th - 5th c. BCE), such as the Pythagoreans, who posited a connection between aesthetic beauty and mathematical properties of symmetry and proportion. Left: Symmetry in the natural world (aloe vera plant). Center: The beautiful Rose Window at the Durham Cathedral (originally 15th c.). Right: A non-symmetric image.

symmetries entail continuous (Lie) groups. Lie groups are themselves *smooth manifolds* endowed with a group structure. Necessarily, they contain an infinite number (continuum) of elements, and they can be either compact or noncompact[2].

1.2.2 Symmetries in quantum mechanics

In quantum mechanics, symmetries manifest themselves as *unitary operators* U which commute with the system Hamiltonian, H. (An important exception which we shall study later is the case of *anti-unitary* symmetries, such as time-reversal.) Any operator Θ transforms under the symmetry as $\Theta' = U^\dagger \, \Theta \, U$. The simplest example is space inversion, also known as *parity*, and denoted by the symbol P. One then has $\mathsf{P}^\dagger \boldsymbol{r} \, \mathsf{P} = -\boldsymbol{r}$ and $\mathsf{P}^\dagger \boldsymbol{p} \, \mathsf{P} = -\boldsymbol{p}$. Clearly $\mathsf{P}^2 = 1$, so $\mathsf{P}^\dagger = \mathsf{P}^{-1} = \mathsf{P}$, *i.e.* P is Hermitian as well as unitary. For a single particle Hamiltonian of the form $H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$, we have $[H, \mathsf{P}] = 0$ if $V(\boldsymbol{r}) = V(-\boldsymbol{r})$. This means that H and P are simultaneously diagonalizable, which means that energy eigenstates may be chosen to be parity eigenstates. Clearly the eigenvalues of P are ± 1.

Now let $|\, n \,\rangle$ denote any one-body quantum state, *i.e.* a vector in Hilbert space. The position space wavefunction is $\psi_n(\boldsymbol{r}) = \langle\, \boldsymbol{r} \,|\, n \,\rangle$. Since $\mathsf{P} \,|\, \boldsymbol{r} \,\rangle = |\, -\boldsymbol{r} \,\rangle$, we have that the parity-flipped wavefunction is given by[3] $\tilde{\psi}_n(\boldsymbol{r}) = \langle\, \boldsymbol{r} \,|\, \mathsf{P} \,|\, n \,\rangle = \psi_n(-\boldsymbol{r})$. If $|\, n \,\rangle$ is a parity eigenstate, *i.e.* if $\mathsf{P} \,|\, n \,\rangle = \pm |\, n \,\rangle$, then we have $\tilde{\psi}_n(\boldsymbol{r}) = \psi_n(-\boldsymbol{r}) = \pm \psi_n(\boldsymbol{r})$. Furthermore, if $|\, n \,\rangle$ and $|\, n' \,\rangle$ are parity eigenstates with eigenvalues σ and σ', respectively, then for any even parity (parity-invariant) operator $\Theta_{\rm e} = \mathsf{P}^\dagger \, \Theta_{\rm e} \, \mathsf{P}$, we have

$$\langle\, n \,|\, \Theta_{\rm e} \,|\, n' \,\rangle = \langle\, n \,|\, \mathsf{P}^\dagger \, \Theta_{\rm e} \, \mathsf{P} \,|\, n' \,\rangle = \sigma\sigma' \langle\, n \,|\, \Theta_{\rm e} \,|\, n' \,\rangle \quad , \tag{1.1}$$

addition.

[2] In mathematical parlance, compact means 'closed and bounded'. An example of a compact Lie group is SU(2), which describes spin rotation in quantum mechanics. An example of a noncompact Lie group is the Lorentz group, O(3,1).

[3] Note $\langle\, \boldsymbol{r} \,|\, \mathsf{P} \,|\, n \,\rangle = \langle\, -\boldsymbol{r} \,|\, n \,\rangle$.

and therefore if $\sigma\sigma' = -1$, meaning that $|\, n \,\rangle$ and $|\, n' \,\rangle$ are states of opposite parity, then $\langle\, n \,|\, \Theta_{\rm e} \,|\, n' \,\rangle = 0$. This is an example of a *selection rule* : operators which preserve a symmetry cannot mix states which transform differently under that symmetry. Another consequence of this analysis is that any *odd*-parity operator, for which $\mathtt{P}^\dagger\, \Theta_{\rm o}\, \mathtt{P} = -\Theta_{\rm o}$, will *only* have nonzero matrix elements between opposite parity states. Thus, if $[H, \mathtt{P}] = 0$, and the eigenstates are all chosen to have definite parity, any perturbation $V = \lambda\, \Theta_{\rm o}$ will result in no energy shifts within first order perturbation theory.

1.3 Formal definition of a discrete group

1.3.1 Group properties

What is a group? A discrete group G consists of distinct *elements* g_a and a group operation called multiplication, satisfying the following conditions:

(i) **Closure** : The product of two group elements is also a group element.

(ii) **Associativity** : In taking the product of three group elements, it doesn't matter if you first multiply the two left ones and then the right one, or first the two right ones and then the left one.

(iii) **Identity** : There exists a unique identity element, which is the same for both left and right multiplication.

(iv) **Inverse** : Each group element has its own unique inverse, which is both a left and a right inverse[4].

Mathy McMathstein says it this way:

(i′) $\forall\ g_a,\ g_b \in G$, $\exists\ g_c \in G$ s.t. $g_a\, g_b = g_c$.

(ii′) $g_a\, g_b\, g_c = (g_a\, g_b)\, g_c = g_a\, (g_b\, g_c)\ \forall\ a, b, c$.

(iii′) $\exists!\ E \in G$ s.t. $g_a\, E = E g_a = g_a\ \forall\ a$.

(iv′) $\forall\ g_a \in G$, $\exists\ g_a^{-1} \in G$ s.t. $g_a\, g_a^{-1} = g_a^{-1}\, g_a = E$.

These properties hold for continuous groups as well, in which case the group elements $g(\lambda)$ are labeled by a continuous parameter. Some remarks:

- If $g_a\, g_b = g_b\, g_a$ for all a, b, the group is said to be *abelian*. Otherwise, it is *nonabelian*.
- For discrete groups, $|G| \equiv N_G$ denotes the number of elements in G, which is the *order* of G. This may be finite $\big(|S_3| = 6\big)$, finite but ridiculously large $\big(|M| \sim 8 \times 10^{53}$ for the *Monster group*$\big)$, or infinite $\big(\mathbb{Z}$ under addition$\big)$.

[4] Tony Zee pithily summarizes this property as "there's nothing you can do that can't be undone". Real life is not like this! There is no inverse operation applicable to late homework, for example.

1.3.2 The Cayley table

All the information about any discrete group is provided by its multiplication table (also called a *Cayley table*). Our convention for group multiplication tables is given in Tab. 1.1 We shall write the group elements as $\{g_1, g_2, \ldots, g_{N_G}\}$, where $g_1 \equiv E$ is always taken to be the identity, and where N_G is the number of elements in the group. Note the following salient features of the Cayley table:

- The rows and columns range over all the symmetry operations (*i.e.* group elements) g, so that the entry for row g_a and column g_b is the result of the combined operation $g_a \cdot g_b \equiv g_a\, g_b$.
- The identity occurs once in each row and in each column; furthermore $g_a\, g_b = E$ means $g_b\, g_a = E$ as well. Thus, each element g has a unique inverse g^{-1}, which is both a left and a right inverse.
- Indeed, each group element occurs precisely once in each row and in each column. If the same element h were to appear more than once in the $g^{\rm th}$ row, it would mean that there would exist two distinct elements, g_a and g_b such that $gg_a = gg_b = h$. But applying the inverse g^{-1} on the left says $g_a = g_b$, which contradicts our assumption that these elements are distinct. Such a table is called a *Latin square*, *i.e.* an $n \times n$ array of n different symbols, each of which appears exactly once in each row and column.

If the Cayley table is symmetric, the multiplication operation is commutative. Alas, there is no simple test to check, from a given Cayley table, whether the multiplication operation is associative, which is necessary in order for G to be a group. In principle, one must test whether $g \cdot (h \cdot k) = (g \cdot h) \cdot k$ for all $g, h, k \in G$, which involves verifying $|G|^3$ equalities[5].

G	g_1	g_2	g_3	g_4	$\cdots$
g_1	g_1	g_2	g_3	g_4	$\cdots$
g_2	g_2	g_2^2	$g_2\, g_3$	$g_2\, g_4$	$\cdots$
g_3	g_3	$g_3\, g_2$	g_3^2	$g_3\, g_4$	$\cdots$
g_4	g_4	$g_4\, g_2$	$g_4\, g_3$	g_4^2	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

Table 1.1: Convention for group multiplication tables. The identity element is $E \equiv g_1$.

1.3.3 Loops and groups

A finite *loop*[6] is a set L consisting of $|L| \equiv N_L$ elements plus a binary operation (*i.e.* multiplication) such that if $\ell, \ell' \in L$, then each of the equations $\ell \cdot x = \ell'$ and $y \cdot \ell = \ell'$ has a unique solution in L. Furthermore, the loop possesses a unique identity element E such that $E \cdot \ell = \ell \cdot E = \ell$ for all $\ell \in L$. If we order

[5] A procedure known as *Light's associativity test* can sometimes simplify this tedious task.

[6] See *"Non-Associative Loops for Holger Bech Nielsen"*, https://arxiv.org/pdf/hep-th/0111292.pdf.

the loop elements as $\{\ell_1, \ell_2, \ldots, \ell_{N_L}\}$, with $\ell_1 = E$, then the multiplication table for L is a Latin square whose first row and first column are identical. If the multiplication operation is associative, then the loop is a group!

It turns out that all loops with $|L| \leq 4$ are associative, *i.e.* they are groups. At order $N = 5$ there is one discrete group, $\mathbb{Z}_5$, corresponding to clock arithmetic *modulo* 5. There are also four non-associative loops. At order $|L| = 6$ there are two groups: $\mathbb{Z}_2 \times \mathbb{Z}_3$, which is abelian, and $C_{3v} \cong D_3$, which is nonabelian and which we shall discuss in detail in §1.3.4 below. There are also 107 non-associative loops. A non-associative loop may nevertheless be abelian! A particularly interesting and beautiful non-associative loop is that of the eight element *octonions*[7]. In Tabs. 1.2 and 1.3, we present the Cayley tables for two non-associative loops, one (L_5) of order 5 and one (L_6) of order 6. In each case the identity element is denoted as a. Note that within L_5 we have $(c \cdot d) \cdot e = b \cdot e = c$, but $c \cdot (d \cdot e) = c \cdot b = e$. The Cayley table for L_6 is symmetric, hence the loop L_6 is abelian, but $(b \cdot c) \cdot d = f \cdot d = c$ while $b \cdot (c \cdot d) = b \cdot b = a$, so it is non-associative.

L_5	a	b	c	d	e
a	a	b	c	d	e
b	b	a	d	e	c
c	c	e	a	b	d
d	d	c	e	a	b
e	e	d	b	c	a

Table 1.2: A non-associative loop of order 5.

L_6	a	b	c	d	e	f
a	a	b	c	d	e	f
b	b	a	f	e	c	d
c	c	f	a	b	d	e
d	d	e	b	a	f	c
e	e	c	d	f	a	b
f	f	d	e	c	b	a

Table 1.3: A non-associative loop of order 6.

1.3.4 The equilateral triangle : C_{3v} and C_3

Contemplating the symmetries of the lowly equilateral triangle is an instructive introductory exercise. Consider the left panel of Fig. 1.2. The equilateral triangle has the following six symmetries:

(i) identity E (ii) rotation by $\frac{2\pi}{3}$, R (iii) rotation by $-\frac{2\pi}{3}$, W
(iv) reflection σ (v) reflection σ' (vi) reflection σ''

Taken together, these symmetry operations constitute a discrete group known as C_{3v}[8]. Note that R and W commute, since they are rotations about the same axis. Indeed, $W = R^{-1} = R^2$. However, staring at the figure for a little while, one can deduce that $R\sigma = \sigma''$ while $\sigma R = \sigma'$, so R and σ do not commute! Thus, the group C_{3v} is *nonabelian*.

To construct the Cayley table of C_{3v} , we must evaluate the binary products of various group operations. Clearly $R^2 = W$ since two 120° rotations combine to give a 240° rotation. Similarly, $W^2 = R$, since rotating twice by 240° yields a 480° $\cong$ 120° rotation. More attention is required when working out the

[7] See http://math.ucr.edu/home/baez/octonions/.

[8] In the group C_{nv}, the C stands for "cyclic", the subscript n refers to the n-fold symmetry axis, and the subscript v signifies the presence of n reflection planes, each containing that axis.

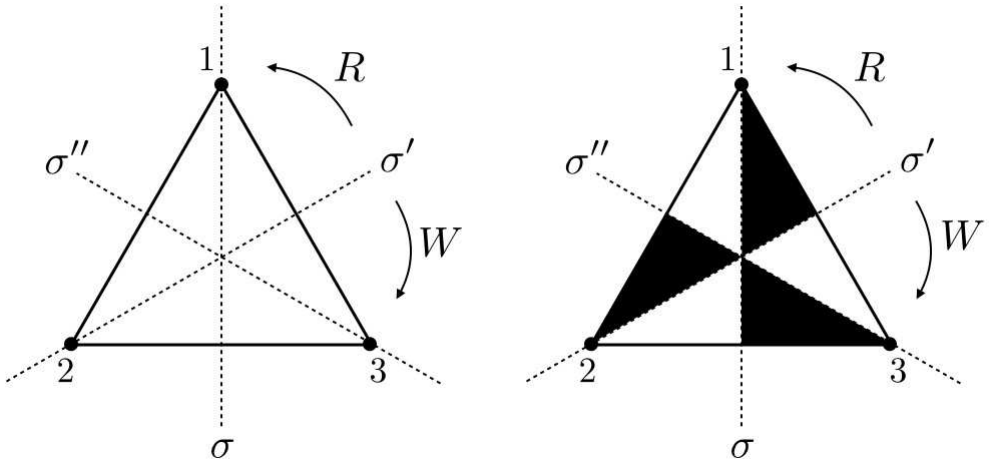


Figure 1.2: Left: The symmetry group C_{3v} of the equilateral triangle contains six elements, which are the identity E, counterclockwise and clockwise 120° rotations R and W, and three reflections σ, σ', and σ''. Right: The black regions break the reflection symmetries, resulting in a lower symmetry group C_3, which contains only the two rotations and the identity.

products of the rotations $\{R, W\}$ and the mirrors $\{\sigma, \sigma', \sigma''\}$. For example, consider the product $R\sigma$. First applying the σ operation, the labels of the vertices are permuted from $\{1, 2, 3\}$, starting at the top and proceeding counterclockwise, to $\{1, 3, 2\}$. Rotating by 120° results in the labeling $\{2, 1, 3\}$, which is also obtained by applying the σ'' operation to the labels $\{1, 2, 3\}$. Reasoning thusly, one obtains the full Cayley table for C_{3v} , given in Tab. 1.4 below.

C_{3v}	E	R	W	σ	σ'	σ''
E	E	R	W	σ	σ'	σ''
R	R	W	E	σ''	σ	σ'
W	W	E	R	σ'	σ''	σ
σ	σ	σ'	σ''	E	R	W
σ'	σ'	σ''	σ	W	E	R
σ''	σ''	σ	σ'	R	W	E

Table 1.4: Multiplication table for the group C_{3v}.

Group representations : first encounter

We can *represent* the various symmetry operations via a map $D^{(2)} : C_{3v} \to \mathsf{O}(2)$ from C_{3v} to the space of 2×2 orthogonal matrices:

$$D^{(2)}(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^{(2)}(R) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \qquad D^{(2)}(W) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \tag{1.2}$$

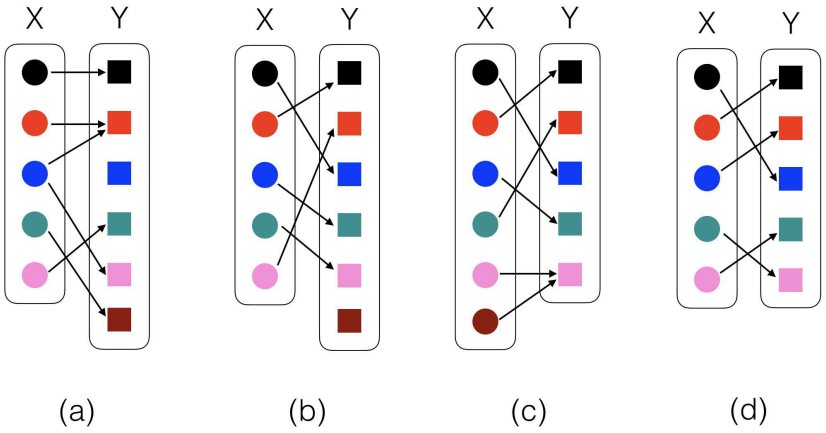


Figure 1.3: A function $f : X \to Y$ maps a set X (the *domain*) to a set Y (the *codomain*). The *range* of a function f is the set $f(X)$. (a) Are you f'ing kidding me?! This is not a function. (b) This function is *injective* (one-to-one), *i.e.* $f(x) \neq f(x')$ whenever $x \neq x'$. (c) This function is *surjective* (onto), *i.e.* $f(X) = Y$. (d) This function is *bijective* (one-to-one and onto).

and

$$D^{(2)}(\sigma) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^{(2)}(\sigma') = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \qquad D^{(2)}(\sigma'') = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \quad . \tag{1.3}$$

Here the superscript $^{(2)}$ denotes the fact that our *representation* is in terms of two-dimensional matrices. One can check that $D^{(2)}(g)\, D^{(2)}(g') = D^{(2)}(gg')$ for all g and g'. Restricted to this subset of $\mathsf{O}(2)$, the mapping $D^{(2)}$ is *bijective* (*i.e.* one-to-one and onto), which means that $D^{(2)}(C_{3v})$ is a *faithful representation* of our group C_{3v}. See Fig. 1.3 for a reminder of the meanings of the terms *injective*, *surjective*, and *bijective*.

Formally, a representation of a group G on a vector space $\mathcal{V}$ over a field $\mathbb{F}$ is a group homomorphism ρ from G to $\mathsf{GL}(\mathcal{V})$, the general linear group on $\mathcal{V}$, *i.e.*

$$\varphi \;:\; G \to \mathsf{GL}(\mathcal{V}) \tag{1.4}$$

such that $\varphi(g_a\, g_b) = \varphi(g_a)\, \varphi(g_b)$. The vector space $\mathcal{V}$ is then called a *G-module*. If the module $\mathcal{V}$ has a nontrivial invariant proper subspace, the representation is said to be *reducible*. When $\mathcal{V}$ is of finite dimension $n \in \mathbb{Z}_+$, we may identify $\mathsf{GL}(\mathcal{V})$ with $\mathsf{GL}(n, \mathbb{F})$, which is the group of invertible $n \times n$ matrices on $\mathbb{F}$. Typically the field $\mathbb{F}$ is the real or complex numbers under addition and multiplication. In the case of $D^{(2)}(C_{3v})$, the vector space is $\mathcal{V} = \mathbb{R}^2$, the field is $\mathbb{R}$, and $n = 2$.

1.3.5 Symmetry breaking

Breaking C_{3v} to C_3

Consider now the right panel of Fig. 1.2. The figure is still fully symmetric under the operations $\{E, R, W\}$, but no longer is symmetric under any of the reflections $\{\sigma, \sigma', \sigma''\}$. The remaining symmetry group is denoted C_3, and consists only of the identity and the two rotations, since the reflection

symmetries are broken. This corresponds to restricting ourselves to the upper left 3×3 block of Tab. 1.4, which satisfies all the desiderata for a multiplication table of a group with three elements. One says that C_{3v} has been broken down to its *subgroup* C_3. Note that the cyclic group C_3 is equivalent to modulo 3 arithmetic, *i.e.* $C_3 \cong \mathbb{Z}_3$.

Upon inspection of Tab. 1.4, it is apparent that C_{3v} has other subgroups. For example, the elements $\{E, \sigma\}$ form a closed set under multiplication, with $E^2 = \sigma^2 = E$ and $E\sigma = \sigma E = \sigma$. This corresponds to the group $\mathbb{Z}_2$ (equivalent to C_2). What is special about the C_3 subgroup $\{E, R, W\}$ is that it is a *normal* (or *invariant*) subgroup. More on this in §1.4 below.

Spontaneous symmetry breaking

In quantum mechanics, as we shall see, the eigenstates of a Hamiltonian H_0 which commutes with all the *generators* of a symmetry group G may be classified according to the *representations* of that group. Typically this entails the appearance of degeneracies in the eigenspectrum, with degenerate states transforming into each other under the group operations. Adding a perturbation V to the Hamiltonian which breaks G down to a subgroup H will accordingly split these degeneracies, and the new multiplets of $H = H_0 + V$ are characterized by representations of the lower symmetry group H.

In quantum field theory, as a consequence of the infinite number of degrees of freedom, symmetries may be *spontaneously broken*. This means that even if the Hamiltonian H (or action S) for the field theory is invariant under a group G of symmetry transformations, the ground state may not be invariant under the full symmetry group G. The presence or absence of spontaneous symmetry breaking (SSB), and its detailed manifestations, will in general depend on the couplings, or the temperature in the case of quantum statistical mechanics. SSB is usually associated with the presence of a local *order parameter* which transforms nontrivially under some group operations, and whose whose quantum statistical average vanishes in a fully symmetric phase, but takes nonzero values in symmetry-broken phase[9]. The parade example is the Ising model, $H = -\sum_{i<j} J_{ij}\,\sigma_i\,\sigma_j$, where each $\sigma_i = \pm 1$, the subscript i indexes a physical location in space, such as a site $\boldsymbol{R}_i$ on a particular lattice. The model is explicitly $\mathbb{Z}_2$ symmetric under $\sigma_i \to \varepsilon\sigma_i$ for all i, where $\varepsilon \in \{+1, -1\}$, yet if the interaction matrix $J_{ij} = J(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is short-ranged and the space dimension d is greater than one, there is a *critical temperature* $T_{\rm c}$ below which SSB sets in, and the system develops a spontaneous magnetization $\phi = \langle\sigma_i\rangle$. You know how in quantum mechanics, the eigenstates of a particle moving in one-dimensional double-well potential $V(x) = V(-x)$ can be classified by their parity eigenvalues, and the lowest two energy states are respectively symmetric ($\mathsf{P} = +1$) and antisymmetric ($\mathsf{P} = -1$), and are delocalized among both wells. For a quantum field theory, however, with (Euclidean) Lagrangian density $\mathcal{L}_{\rm E} = \frac{1}{2}(\boldsymbol{\nabla}\phi)^2 + V(\phi)$, for $d > 1$ and $T < T_{\rm c}$, the system actually picks the left or the right well, so that $\langle\phi(\boldsymbol{r})\rangle \neq 0$. Another example is the spontaneously broken $\mathsf{O}(2)$ invariance of superfluids, where the boson annihilation operator $\psi(\boldsymbol{r})$ develops a spontaneous average $\big\langle\psi(\boldsymbol{r})\big\rangle = \sqrt{n_0}\,e^{i\theta}$, where n_0 is the condensate density and θ the condensate phase.

Truth be told, the above description is a bit of a swindle. In the ferromagnetic ($J_{ij} > 0$) Ising model, for example, at $T = 0$, there are still two ground states, $|\Uparrow\rangle \equiv |\uparrow\uparrow\uparrow\cdots\rangle$ and $|\Downarrow\rangle \equiv |\downarrow\downarrow\downarrow\cdots\rangle$. The (ergodic) zero temperature density matrix is $\rho_0 = \frac{1}{2}|\Uparrow\rangle\langle\Uparrow| + \frac{1}{2}|\Downarrow\rangle\langle\Downarrow|$, and therefore $\langle\sigma_i\rangle = \mathsf{Tr}\big(\rho_0\,\sigma_i\big) = 0$. The

[9] While SSB is generally associated with the existence of a phase transition, not all phase transitions involve SSB. Exceptions include topological phases, which have no local order parameter.

order parameter apparently has vanished. WTF?! There are at least two compelling ways to resolve this seeming conundrum:

(a) First, rather than defining the order parameter of the Ising model, for example, to be the expected value $m = \langle \sigma_i \rangle$ of the local spin[10], consider instead the behavior of the *correlation function* $C_{ij} = \langle \sigma_i \, \sigma_j \rangle$ in the limit $d_{ij} = |\boldsymbol{R}_i - \boldsymbol{R}_j| \to \infty$. In a disordered phase, there is no correlation between infinitely far separated spins, hence $\lim_{d_{ij}\to\infty} C_{ij} = 0$. In the ordered phase, this is no longer true, and we define the *spontaneous magnetization* m from the long distance correlator: $m^2 \equiv \lim_{d_{ij}\to\infty} \langle \sigma_i \, \sigma_j \rangle$. In this formulation, SSB is associated with the emergence of *long-ranged order* in the correlators of operators which transform nontrivially under the symmetry group.

(ii) Second, we could impose an external field which *explicitly* breaks the symmetry, such as a Zeeman term $H' = -h \sum_i \sigma_i$ in the Ising model. We now compute the magnetization (per site) $m(T, h, V) = \langle \sigma_i \rangle$ as a function of temperature T, the external field h, *and* the volume V of our system. The order parameter $m(T)$ in zero field is then defined as

$$m(T) = \lim_{h\to 0} \lim_{V\to\infty} m(T, h, V) \quad . \tag{1.5}$$

The order of limits here is crucially important. The thermodynamic limit $V \to \infty$ is taken first, which means that the energy difference between $|\Uparrow\rangle$ and $|\Downarrow\rangle$, being proportional to hV, diverges, thus infinitely suppressing the $|\Downarrow\rangle$ state if $h > 0$ (and the $|\Uparrow\rangle$ state if $h < 0$). The magnitude of the order parameter will be independent on the way in which we take $h \to 0$, but its sign will depend on whether $h \to 0^+$ or $h \to 0^-$, with $\mathsf{sgn}(m) = \mathsf{sgn}(h)$. Physically, the direction in which a system orders can be decided by the presence of small stray fields or impurities. An illustration of how this works in the case of ideal Bose gas condensation is provided in the appendix §1.6 below.

Note that in both formulations, SSB is necessarily associated with the existence of a local operator $\mathcal{O}_i$ which is identified as the order parameter field. In (i) the correlations $\langle \mathcal{O}_i \, \mathcal{O}_j \rangle$ exhibit long-ranged order in the symmetry-broken phase. In (ii) $\mathcal{O}_i$ is the operator to which the external field h_i couples.

1.3.6 The dihedral group D_n

In the mathematics literature, the symmetry group of the planar n-gon is called the *dihedral group*[11], D_n. Elements of D_n act on two-dimensional space as (i) rotations about a central point by multiples of $2\pi/n$ and (ii) reflections in any of n lines each containing the central point, and oriented at multiples of π/n from some fiducial axis. D_n thus contains $2n$ elements. If we denote by r the group element which rotates (counterclockwise, say) by $2\pi/n$, and we denote by σ any one of the mirror symmetries of the n-gon, then the following are True Facts: (i) $r^n = 1$, (ii) $\sigma^2 = 1$, and (iii) $\sigma r \sigma = r^{-1}$. The first two are obvious. The third is also obvious after a moment's thought: by reflecting, rotating, and reflecting again, the sense of rotation is reversed. One says that r and σ are the *generators* of D_n, and the three True Facts are *relations* satisfied by the generators. Below in §1.4.6, we shall discuss how the full group multiplication table, which can be quite unwieldy for groups with many elements, can be replaced by a

[10] We assume translational invariance, which means $\langle \sigma_i \rangle$ is independent of the site index i.

[11] The word *dihedral* means "two faces" and probably has its origins in Greek political rhetoric.

group presentation, denoted $\langle\, \mathcal{G} \,|\, \mathfrak{R} \,\rangle$, where $\mathcal{G}$ are the generators and $\mathfrak{R}$ the relations. Thus, the presentation for D_n is $\langle\, r\,,\, \sigma \,|\, r^n = 1\,,\, \sigma^2 = 1\,,\, \sigma r \sigma = r^{-1} \,\rangle$. D_n's $2n$ elements then nicely divide into two subsets: $\{E\,,\, r\,,\, \ldots\,,\, r^{n-1}\}$ and $\{\sigma\,,\, \sigma r\,,\, \ldots\,,\, \sigma r^{n-1}\}$. The first of these is itself the group $C_n \cong \mathbb{Z}_n$.

Apologia pro vita mea : D_n *versus* C_{nv}

What is the difference between D_n and C_{nv}? As we've just defined D_n above, it is identical to C_{nv}. Each of the reflections is an *improper rotation*, *i.e.* it is represented by a 2×2 orthogonal matrix whose determinant is -1. According to crystallographers, however, the definition of D_n is the group of symmetry operations consisting of a single n-fold axis plus n equally splayed *twofold axes* each perpendicular to the n-fold axis. In other words, D_n in *three* space dimensions is a subgroup of $\mathsf{SO}(3)$, and as such it involves only *proper rotations*. Could anything be more awful?[12] We will revisit the distinction when we discuss crystallographic point groups, but at the level of group theory this is all a tempest in a teapot, because D_n and C_{nv} are *isomorphic* – their elements may be placed in one-to-one correspondence, and their multiplication tables are the same. One way to think about it is to take the six 2×2 matrices $D^{(2)}(g)$ faithfully representing the elements of C_{3v} and add a third row and column, padding the additional entries with zeroes except in the lower right $(3,3)$ corner, where we place a 1. Clearly the multiplication table is the same. But we could also choose to place a 1 in the $(3,3)$ slot for $g \in \{E, R, W\}$, and a (-1) there for $g \in \{\sigma, \sigma', \sigma''\}$. The multiplication table remains the same! The representation is still faithful! And now each of our six 3×3 matrices has determinant $+1$. So let's all just chill and accept that C_{nv} is a perfectly acceptable notation for the symmetries of the planar n-gon, as our crystallographer forebears have wisely decreed[13].

1.3.7 The permutation group S_n

A permutation of the symbols $\{1, 2, \ldots, n\}$ is a rearrangement $\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$ of those same symbols, commonly denoted by

$$\sigma \equiv \begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \sigma(1) & \sigma(2) & \sigma(3) & \cdots & \sigma(n) \end{pmatrix} \quad . \tag{1.6}$$

The meaning of the above notation is the following. We are to imagine an ordered set of n boxes, each of which contains an object[14]. Applying the operation σ means that the contents of box 1 are placed in box $\sigma(1)$, the contents of box 2 are placed in box $\sigma(2)$, *etc.* The inverse operation is given by

$$\sigma^{-1} = \begin{pmatrix} \sigma(1) & \sigma(2) & \sigma(3) & \cdots & \sigma(n) \\ 1 & 2 & 3 & \cdots & n \end{pmatrix} \quad , \tag{1.7}$$

[12] Well, of course it could. Cancer, for example.

[13] Crystallography is a subset of solid state physics, and solid state physics is a subset of condensed matter physics. And condensed matter physics is the very best kind of physics, as we pointed out in §1.1.

[14] The objects are arbitrary, and don't necessarily have to be distinct themselves. Some boxes could contain nothing at all. Others might contain a magnificent present for your group theory instructor.

and the rule for composition (multiplication) of permutations is then

$$\begin{aligned}\mu\sigma &= \begin{pmatrix} 1 & 2 & \cdots & n \\ \mu(1) & \mu(2) & \cdots & \mu(n) \end{pmatrix} \begin{pmatrix} 1 & 2 & \cdots & n \\ \sigma(1) & \sigma(2) & \cdots & \sigma(n) \end{pmatrix} \\ &= \begin{pmatrix} 1 & 2 & \cdots & n \\ \mu\big(\sigma(1)\big) & \mu\big(\sigma(2)\big) & \cdots & \mu\big(\sigma(n)\big) \end{pmatrix} \quad ,\end{aligned} \tag{1.8}$$

and thus the initial contents of box k wind up in box $\mu\big(\sigma(k)\big)$. These operations form a discrete group, since the composition of two rearrangements is another rearrangement, and since, as anyone who has rearranged furniture to satisfy the whims of a fussy spouse can attest, you can always "just put it back the way it was", *i.e.* each element has its inverse. This group of operations is known as the *permutation group* (or *symmetric group*), and is abbreviated S_n.

Clearly S_n has $n!$ elements, so the size of the multiplication table is $n! \times n!$. Furthermore, we can represent each element $\sigma \in S_n$ as an $n \times n$ matrix consisting of zeros and ones, such that $\big[D^{(n)}(\sigma)\big]_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. This generates the desired permutation when acting on the column vector $\boldsymbol{v}$ whose transpose is $\boldsymbol{v}^{\rm T} = (1\ 2\ 3\ \cdots\ n)$.

We will study S_n in more detail below (see §1.4.3), but for now let's consider the case $n = 3$, which is the permutation group for three objects. Consulting the left panel of Fig. 1.2 once more, we see to each element of C_{3v} there corresponds a unique element of S_3:

$$\begin{aligned} E &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} \qquad R = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \qquad W = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} \\ \sigma &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} \qquad \sigma' = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \qquad \sigma'' = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \quad .\end{aligned} \tag{1.9}$$

Note we can write $R = (123)$, $W = (132)$, $\sigma = (23)$, $\sigma' = (13)$, and $\sigma'' = (12)$, using the cycle notation. The above relations constitute a bijection between elements of C_{3v} and elements of S_3. The multiplication tables therefore are the same. Thus, in essence, S_3 *is* C_{3v}. In mathematical notation, we write $S_3 \cong C_{3v}$, where the symbol $\cong$ denotes *group isomorphism*.

We mentioned above how S_n has a representation in terms of $n \times n$ matrices. We may write the 3×3 matrices $D^{(3)}(g)$ for S_3 as

$$\begin{aligned} D^{(3)}(E) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad D^{(3)}(R) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad D^{(3)}(W) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \\ D^{(3)}(\sigma) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad D^{(3)}(\sigma') = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad D^{(3)}(\sigma'') = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad .\end{aligned} \tag{1.10}$$

One can check that these matrices yield the same multiplication table as for $S_3 \cong C_{3v}$. Thus, we have thus far obtained two faithful representations of this group, one two-dimensional and one three-dimensional.

Remember the interpretation that the permutation σ places the former contents of box j into box $\sigma(j)$ for all j. We can arrange these boxes in a column vector of length n. If in our $n = 3$ case we start with ♣ in box 1, ⋈ in box 2, and ☋ in box 3, application of the element R results in

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \clubsuit \\ \bowtie \\ \upsilon \end{pmatrix} = \begin{pmatrix} \upsilon \\ \clubsuit \\ \bowtie \end{pmatrix} \quad , \tag{1.11}$$

and now we have ♣ in box 2, ⋈ in box 3, and ☋ in box 1.

1.3.8 Our friend, SU(2)

SU(2) is an example of a continuous group known as a *Lie group*. We shall introduce Lie groups more thoroughly in §1.5 below. For the moment, recall that a matrix $U \in \mathsf{U}(2)$ is a 2×2 complex-valued matrix which satisfies $U^\dagger = U^{-1}$, *i.e.* $U^\dagger U = E$, where E is the identity matrix. This entails $|\det U| = 1$, and requiring $U \in \mathsf{SU}(2)$ imposes the additional constraint $\det U = 1$. Now let us parameterize U, initially in terms of four complex numbers, and examine the matrices $U^\dagger$ and U^{-1}:

$$U = \begin{pmatrix} w & x \\ y & z \end{pmatrix} \quad \Rightarrow \quad U^\dagger = \begin{pmatrix} w^* & y^* \\ x^* & z^* \end{pmatrix} \quad , \quad U^{-1} = \frac{1}{\det U} \begin{pmatrix} z & -x \\ -y & w \end{pmatrix} \quad . \tag{1.12}$$

Since $\det U = 1$, we conclude $z = w^*$ and $y = -x^*$, hence we may parameterize all matrices in SU(2) in terms of two complex numbers, $w \in \mathbb{C}$ and $x \in \mathbb{C}$, *viz.*

$$U = \begin{pmatrix} w & x \\ -x^* & w^* \end{pmatrix} \quad , \quad U^{-1} = U^\dagger = \begin{pmatrix} w^* & -x \\ x^* & w \end{pmatrix} \tag{1.13}$$

and subject to the constraint

$$\det U = |w|^2 + |x|^2 = 1 \quad . \tag{1.14}$$

Thus, SU(2) is topologically equivalent to the 3-sphere S^3 sitting inside $\mathbb{C}^2 \cong \mathbb{R}^4$.

We can check the closure:

$$U_1 U_2 = \begin{pmatrix} w_1 & x_1 \\ -x_1^* & w_1^* \end{pmatrix} \begin{pmatrix} w_2 & x_2 \\ -x_2^* & w_2^* \end{pmatrix} = \begin{pmatrix} w_1 w_2 - x_1 x_2^* & w_1 x_2 + x_1 w_2^* \\ -w_1^* x_2^* - x_1^* w_2 & w_1^* w_2^* - x_1^* x_2 \end{pmatrix} \quad . \tag{1.15}$$

Thus, $U_1 U_2$ is of the appropriate form, provided its determinant is indeed unity. We have

$$\begin{aligned} \det(U_1 U_2) &= |w_1 w_2 - x_1 x_2^*|^2 + |w_1 x_2 + x_1 w_2^*|^2 \\ &= |w_1|^2 |w_2|^2 + |x_1|^2 |x_2|^2 + |w_1|^2 |x_2|^2 + |x_1|^2 |w_2|^2 \\ &= \big(|w_1|^2 + |x_1|^2\big)\big(|w_2|^2 + |x_2|^2\big) = \det U_1 \det U_2 = 1 \quad , \end{aligned} \tag{1.16}$$

and so closure is verified. Of course, we knew in advance this would work out, *i.e.* that determinant of a product is the product of the determinants.

Another useful parameterization of SU(2) is in terms of the Pauli matrices:

$$g(\alpha, \hat{\boldsymbol{n}}) \equiv \exp\big(-\tfrac{i}{2}\,\alpha\,\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\big) = \cos\tfrac{\alpha}{2} - i \sin\tfrac{\alpha}{2}\,\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma} \quad , \tag{1.17}$$

where $\hat{\boldsymbol{n}}$ is a three-dimensional unit vector and where $\alpha \in [0, 2\pi)$. The inverse operation is given by $g^{-1}(\alpha, \hat{\boldsymbol{n}}) = \exp\big(\frac{i}{2}\,\alpha\,\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\big)$. Recall that $g(\alpha, \hat{\boldsymbol{n}})$ rotates a spinor by an angle α about the $\hat{\boldsymbol{n}}$ axis in internal spin space. Note that $g(2\pi, \hat{\boldsymbol{n}}) = -1$, so rotation by 2π about any axis is equivalent to multiplication by -1. We shall comment more fully on this in future chapters. Writing the unit vector $\hat{\boldsymbol{n}}$ in terms of a polar angle θ and azimuthal angle ϕ, note that

$$w = \cos\tfrac{\alpha}{2} - i \sin\tfrac{\alpha}{2} \cos\theta \qquad , \qquad x = -i \sin\tfrac{\alpha}{2} \sin\theta\, e^{-i\phi} \quad . \tag{1.18}$$

and thus $\big(\mathsf{Re}\,\omega, \mathsf{Im}\,\omega, \mathsf{Re}\,x, \mathsf{Im}\,x\big)$ is a real four-component unit vector lying on S^3.

We already know that it must work out, but it is somewhat instructive to verify closure in this parameterization. This means that $g(\alpha, \hat{\boldsymbol{n}})\, g(\beta, \hat{\boldsymbol{m}}) = g(\gamma, \hat{\boldsymbol{k}})$ for some angle γ and unit vector $\hat{\boldsymbol{k}}$. We can evaluate the product explicitly:

$$\begin{aligned} g(\alpha, \hat{\boldsymbol{n}})\, g(\beta, \hat{\boldsymbol{m}}) &= \Big(\cos\tfrac{\alpha}{2} - i \sin\tfrac{\alpha}{2}\, \hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\Big)\Big(\cos\tfrac{\beta}{2} - i \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{m}} \cdot \boldsymbol{\sigma}\Big) \\ &= \cos\tfrac{\alpha}{2} \cos\tfrac{\beta}{2} - i \Big(\sin\tfrac{\alpha}{2} \cos\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} + \cos\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{m}}\Big) \cdot \boldsymbol{\sigma} - \sin\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, (\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})(\hat{\boldsymbol{m}} \cdot \boldsymbol{\sigma}) \\ &= \Big(\cos\tfrac{\alpha}{2} \cos\tfrac{\beta}{2} - \sin\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{m}}\Big) \\ &\qquad - i \Big(\sin\tfrac{\alpha}{2} \cos\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} + \cos\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{m}} + \sin\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} \times \hat{\boldsymbol{m}}\Big) \cdot \boldsymbol{\sigma} \quad , \end{aligned} \tag{1.19}$$

where we have invoked $\sigma^\alpha \sigma^\beta = \delta^{\alpha\beta} + i\,\epsilon_{\alpha\beta\gamma}\,\sigma^\gamma$. We therefore have

$$\begin{aligned} \cos\tfrac{\gamma}{2} &= \cos\tfrac{\alpha}{2} \cos\tfrac{\beta}{2} - \sin\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{m}} \\ \sin\tfrac{\gamma}{2} &= \Big| \sin\tfrac{\alpha}{2} \cos\tfrac{\beta}{2}\, \hat{\boldsymbol{m}} + \cos\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} + \sin\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} \times \hat{\boldsymbol{m}} \Big| \\ &= \sqrt{\tfrac{1}{2}(1 - \cos\alpha\cos\beta) + \tfrac{1}{2}\sin\alpha\sin\beta\, \hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{m}} + \tfrac{1}{4}(1 - \cos\alpha)(1 - \cos\beta)\big[1 - (\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{m}})^2\big]} \quad , \end{aligned} \tag{1.20}$$

from which one verifies $\cos^2\big(\frac{\gamma}{2}\big) + \sin^2\big(\frac{\gamma}{2}\big) = 1$. The vector $\hat{\boldsymbol{k}}$ is then given by

$$\hat{\boldsymbol{k}} = \frac{\sin\frac{\alpha}{2} \cos\frac{\beta}{2}\, \hat{\boldsymbol{m}} + \cos\frac{\alpha}{2} \sin\frac{\beta}{2}\, \hat{\boldsymbol{n}} + \sin\frac{\alpha}{2} \sin\frac{\beta}{2}\, \hat{\boldsymbol{n}} \times \hat{\boldsymbol{m}}}{\Big| \sin\frac{\alpha}{2} \cos\frac{\beta}{2}\, \hat{\boldsymbol{m}} + \cos\frac{\alpha}{2} \sin\frac{\beta}{2}\, \hat{\boldsymbol{n}} + \sin\frac{\alpha}{2} \sin\frac{\beta}{2}\, \hat{\boldsymbol{n}} \times \hat{\boldsymbol{m}} \Big|} \tag{1.21}$$

and the angle γ by

$$\gamma = 2 \cos^{-1}\Big(\cos\tfrac{\alpha}{2} \cos\tfrac{\beta}{2} - \sin\tfrac{\alpha}{2} \sin\tfrac{\beta}{2}\, \hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{m}}\Big) \tag{1.22}$$

with $\gamma \in [0, 2\pi)$. We see that $\big[g(\alpha, \hat{\boldsymbol{n}})\,,\, g(\beta, \hat{\boldsymbol{m}})\big] = 0$ if $\hat{\boldsymbol{n}} \times \hat{\boldsymbol{m}} = 0$, *i.e.* if the two rotations are about the same axis.

1.4 Aspects of Discrete Groups

1.4.1 Basic features of discrete groups

Here we articulate a number of key concepts in the theory of discrete groups.

GROUP HOMOMORPHISM : A *group homomorphism* is a map $\phi : G \mapsto G'$ which respects multiplication, *i.e.* $\phi(g_a)\,\phi(g_b) = \phi(g_a\,g_b)$, where $g_{a,b} \in G$ and $\phi(g_{a,b}) \in G'$. If ϕ is *bijective* (one-to-one and onto), it is an *isomorphism*, and we write $G \cong G'$. This means that *G and G' are the same group*. The maps $D^{(2)}(C_{3v})$ and $D^{(3)}(C_{3v})$ discussed above in §1.3.4 and §1.3.7 are isomorphisms.

The *kernel* of a homomorphism ϕ is the set of elements in G which get mapped to the identity in G', whereas the *image* of ϕ is the set of elements in G' which have a pre-image in G. Thus[15],

$$\mathsf{ker}(\phi) = \big\{g \in G \,\big|\, \phi(g) = E'\big\} \qquad , \qquad \mathsf{im}(\phi) = \big\{\phi(g) \,\big|\, g \in G\big\} \quad . \tag{1.23}$$

As an example, consider the homomorphism which maps C_{3v} to $\mathbb{Z}_2$, where $\phi(E) = \phi(R) = \phi(W) = +1$ and $\phi(\sigma) = \phi(\sigma') = \phi(\sigma'') = -1$. Then $\mathsf{ker}(\phi) = \big\{E, R, W\big\}$. Consider next the map $D^{(2)} : C_{3v} \mapsto \mathsf{O}(2)$ in Eqn. 2.123. Clearly, not every element in $\mathsf{O}(2)$ has a preimage in C_{3v}, as $\mathsf{O}(2)$ is a continuous group with an infinite number of elements! $\mathsf{im}\big(D^{(2)}\big)$ is then the six matrices defined in Eqn. 2.123.

REARRANGEMENT THEOREM : Let the set of group elements be $\big\{E, g_2, g_3\,, \ldots\,, g_N\big\}$, where $N = |G|$. Call this particular ordering the *sequence* $\mathcal{S}_1$. Then for any $g_a \in G$, the sequence $\mathcal{S}_2 = \big\{g_aE, g_a\,g_2\,, \ldots\,, g_a\,g_N\big\}$ contains every element in G.

The proof is elementary. First note that each element occurs in $\mathcal{S}_2$ at least once, since for any b one has $g_a^{-1}g_b \in G$, hence $g_a\big(g_a^{-1}g_b\big) = g_b$ is a member of $\mathcal{S}_2$. This is all we need to show, since $\mathcal{S}_1$ and $\mathcal{S}_2$ contain the same number N of elements, and every element in $\mathcal{S}_1$ is contained in $\mathcal{S}_2$. Therefore $\mathcal{S}_2$ is merely a *rearrangement* of $\mathcal{S}_1$.[16]

SUBGROUPS : A collection H of elements $\{h_j\}$ is called a *subgroup* of G if each $h_j \in G$ and if H itself forms a group under the same multiplication law. One expresses this as $H \subset G$. Some examples: $C_3 \subset C_{3v}$, $\mathsf{SO}(2) \subset \mathsf{SO}(3)$, $S_n \subset S_{n'}$ if $n < n'$. Note $\mathbb{Z}_2 \subset \mathbb{Z}_4$ but $\mathbb{Z}_2 \not\subset \mathbb{Z}_5$ (more on this below)[17]. The identity element $\{E\}$ always forms its own (trivial) subgroup[18].

COSETS AND LAGRANGE'S THEOREM : If G is of finite order, and $H \subset G$, then $M \equiv |H|$ is a divisor of $N \equiv |G|$. The proof is somewhat instructive. Consider some ordering $\big\{E, g_2, g_2\,, \ldots\,, g_N\big\}$ of all the elements of G and pick the first element in this set which is not a member of H. Call this element g. Then form the *left coset* $gH \equiv \big\{gE, g\,h_2\,, \ldots\,,\ g\,h_M\big\}$. Note that gH is not a group because it cannot contain the identity[19]. Note also that gH contains M unique elements, none of which is a member of H. To see this,

[15] Be aware, in my notation, that im means 'image', whereas Im means 'imaginary part'.

[16] Just to put a fine point on it, suppose there is a repeating element in $\mathcal{S}_2$, *i.e.* suppose $g_a\,g_b = g_a\,g_c$ for $b \neq c$. Then applying g_a^{-1} on the left, we have $g_b = g_c$, which is a contradiction.

[17] Recall $\mathbb{Z}_n$, the group of "clock arithmetic base n", is the same group as C_n, *i.e.* n-fold rotations about a single axis, or the set $\big\{e^{2\pi ij/n} \,\big|\, j \in \{0, 1, \ldots, n-1\}\big\}$ under complex multiplication.

[18] If you do not understand why, please *kill yourself*.

[19] By assumption $g \notin H$, so $g \neq h_j^{-1}$ for all j, meaning $gh_j \neq E$ for all j.

first assume $gh_j = gh_k$ for some distinct j and k (with $h_0 = E$). Applying g^{-1} on the left yields $h_j = h_k$, which is a contradiction. Next, assume $gh_j = h_k$. This means $g = h_j^{-1} h_k$, which is again a contradiction since H is a group and therefore $h_j^{-1} h_k \in H$, but by assumption $g \notin H$. Now take the first element from G which is neither a member of H nor of gH, and call this g'. We form the corresponding coset $g'H$. By the same arguments, $g'H$ contains M distinct elements, none of which appears in H. But is $g'H$ distinct from gH? Indeed it is, for if $gh_j = g'h_k$ for some j and k, then $g' = gh_j h_k^{-1} \in gH$, since $h_j h_k^{-1} \in H$. But this contradicts our assumption that $g' \notin gH$. We iterate this procedure, forming $g''H$, *etc.* Since G is of finite order, this business must eventually end, say after the construction of l such cosets. But then we have managed to divide the entire N elements of G into $l+1$ sets, each of size M (H plus its l iteratively constructed cosets). We then say that H is a subgroup of *index* $l+1$. QED

Thus, $\mathbb{Z}_2 \not\subset \mathbb{Z}_5$, and furthermore no group of prime order can have a nontrivial subgroup.

ABELIAN SUBGROUPS : Let G be a finite discrete group. Then for any $g \in G$, there exists $n > 0$ such that $g^n = E$ (prove it!). The smallest such n is called the *order of the element* g. Therefore the set $\{E, g, g^2 , \ldots , g^{n-1}\}$ constitutes an *abelian subgroup* of G, itself of order n. For example, $\{E, \sigma\} \subset C_{3v}$ is the abelian subgroup $\mathbb{Z}_2$. $\{E, R, W = R^2\} \subset C_{3v}$ is the abelian subgroup C_3.

CENTER OF A GROUP : The *center* $Z(G)$ of a group G is the set of elements which commute with all other elements. *I.e.*

$$Z(G) = \{z \in G \,|\, zg = gz \quad \forall g \in G\} \quad . \tag{1.24}$$

Clearly $Z(G) \subset G$. The center of any abelian group G is G itself. For the dihedral groups D_n, the content of the center depends on whether n is even or odd. One has $Z(D_{2k+1}) \cong \{E\}$ and $Z(D_{2k}) \cong \{E, R^k\}$, where R rotates by π/k about the central axis. *I.e.* $Z(D_{2k}) \cong \mathbb{Z}_2$.

CENTRALIZER AND NORMALIZER : The *centralizer* $C_G(z)$ of a group element $z \in G$ is the set of all elements of G which commute with z , *i.e.* $C_G(z) = \{g \in G \,|\, gz = zg\}$. The centralizer of a subgroup $H \subset G$ is the set of all elements of G which commute with every element of H. Clearly the centralizer of any element or of any subgroup will contain $Z(G)$, the center of the group.

The *normalizer* of a subgroup $H \subset G$, denoted $N_G(H)$, is the set of all $g \in G$ such that $g^{-1}Hg = H$, which is equivalent to $gH = Hg$. Note that $C_G(H) \subseteq N_G(H)$, because $g \in C_G(H)$ requires $gh = hg$ for all $h \in H$, but $g \in N(G)$ satisfies the weaker requirement that for all $h \in H$, there exists $h' \in H$ with $gh = h'g$.

DIRECT PRODUCTS : Given two groups G and H, one may construct the *product group* $F = G \times H$, whose elements are ordered pairs (g, h) where $g \in G$ and $h \in H$. Multiplication in the product group is given by the natural extension $(g, h)(g', h') = (gg', hh')$. Note $|F| = |G| \cdot |H|$.

CONJUGACY : Two elements g and g' are said to be *conjugate* to each other if $\exists\, f \in G$ such that $g' = f^{-1}gf$. This has odors of the similarity transformation from linear algebra. Note that if g is conjugate to g' and g' is conjugate to g'', then $\exists\ f, h$ such that $g' = f^{-1}gf$ and $g'' = h^{-1}g'h$, from which we derive $g'' = (hf)^{-1}g(fh)$, *i.e.* g and g'' are also conjugate. Thus, conjugacy is transitive.

The set of distinct elements $\{f^{-1}gf \mid f \in G\}$ is called the *conjugacy class* (or *equivalency class*) of the element g. Note that $g_0 \equiv E$ is always in its own conjugacy class, with no other elements. Similarly, in abelian groups, each element is its own class. For C_{3v} there are three conjugacy classes: $\{E\}$, $\{R, W\}$,

and $\{\sigma, \sigma', \sigma''\}$. All elements in a given conjugacy class have the same order, for if $g^n = E$, then clearly $\left(f^{-1}gf\right)^n = f^{-1}Ef = E$.

NORMAL (INVARIANT) SUBGROUPS : A subgroup $H \subset G$ is called a *normal* (or *invariant*) *subgroup* if $g^{-1}Hg = H$ for all $g \in G$. Thus, any normal subgroup must be expressible as the union of some conjugacy classes. For example, $C_3 \subset C_{3v}$ is a normal subgroup, and the union of conjugacy classes $\{E\}$ and $\{R, W\}$. But $\mathbb{Z}_2 \subset C_{3v}$ consisting of (E, σ) is not, because $W^{-1}\sigma W = \sigma'$. Instead of writing "H is an invariant subgroup of G," Mathy McMathstein writes $H \triangleleft G$. Note that if $F = G \times H$, then $G \triangleleft F$ and $H \triangleleft F$.

SIMPLE GROUP : Any group G which contains no invariant subgroups is said to be *simple*. Tony Zee explains this beautifully. He says that we'd like to be able to articulate a notion of simplicity, meaning that a group can't be broken up into smaller groups. One might think we should then demand that G have no nontrivial subgroups[20] at all in order for it to be simple. Alas, as Zee points out, "subgroups are a dime a dozen". Indeed, as we've already seen, one can form an abelian subgroup $\left\{E, g, g^2, \ldots, g^{n-1}\right\}$, where n is the order of g, starting with *any* group element. But while you find subgroups everywhere, *invariant* subgroups are quite special. Clearly any group of prime order is simple. So are the alternating groups[21] A_n for $n > 4$. The classification of all finite simple groups has been a relatively recent triumph in mathematics[22]. Other examples of finite simple groups include the classical and exceptional Chevalley groups, the Mathieu groups, the McLaughlin group[23], the Baby Monster group, with $4154781481226426191177580544000000$ elements, and the Monster group[24], which has $808017424794512875886459904961710757005754368000000000$ elements[25].

COSETS AND FACTOR GROUPS : We have already introduced the concept of a *left coset*, gH, formed by multiplying each element of a subgroup $H \subset G$ on the left by a given element $g \in G$. (Of course, one can just as well define the right cosets of H, *i.e.* $\{Hg\}$.) Consider now the left cosets of an invariant subgroup $H \triangleleft G$. Now here's something cool and mathy: cosets can be multiplied. The result is rather simple:

$$(g_a h_m)(g_b h_n) = g_a\, g_b\, (g_b^{-1} h_m\, g_b)\, h_n \equiv g_a\, g_b\, h_l\, h_n \quad , \tag{1.25}$$

where $h_l \equiv g_b^{-1} h_m\, g_b \in H$, since H is an invariant subgroup. Thus, $(g_a H)(g_b H) = (g_a\, g_b)H$. This means the left cosets $\{gH\}$ themselves form a group under multiplication. This group is called the *quotient group*, G/H. Note that $|G/H| = |G|/|H|$, because there are $|H|$ elements in each coset, and therefore there must be $|G|/|H|$ cosets in total. In general, the quotient group is not a normal subgroup of G. Example: $C_{3v}/C_3 = \mathbb{Z}_2$.

COMMUTATOR SUBGROUP : Recall the algebraic notion of the commutator $[X, Y] = XY - YX$. For group operations, the commutator $\langle \bullet, \bullet \rangle$ is defined as

$$\langle g, h \rangle = g^{-1} h^{-1} g h \quad . \tag{1.26}$$

[20] *I.e.* no subgroups other than the identity and G itself.

[21] In §1.4.3 we will learn that A_n is the subgroup consisting of all even permutations in S_n.

[22] See https://en.wikipedia.org/wiki/List_of_finite_simple_groups

[23] See *e.g.* https://www.youtube.com/watch?v=mx9Ue9XLGW8. I always thought the McLaughlin group had five members, but Wikipedia says it has 898128000.

[24] The Monster group is the largest of the sporadic simple groups.

[25] If, as a summer student project, one endeavored to associate each atom contained in planet earth with a unique element of the Monster group, one would eventually run out of atoms.

The inverse of this operation is $\langle g,h\rangle^{-1} = \langle h,g\rangle$. Note that if $gh = hg$, then $\langle g,h\rangle = E$. Also note that upon conjugation,

$$s^{-1}\langle g,h\rangle s = \langle s^{-1}gs, s^{-1}hs\rangle \quad . \tag{1.27}$$

Now the product of two commutators under group multiplication is not in general another commutator. However, we can use the commutators $\langle g_a, g_b\rangle$ to *generate* a closed set under group multiplication, *i.e.*

$$\langle G,G\rangle = \left\{ \langle g_{a_1}, g_{a_2}\rangle\langle g_{a_3}, g_{a_4}\rangle \cdots \langle g_{a_{2n-1}}, g_{a_{2n}}\rangle \,\middle|\, n\in\mathbb{N},\ g_{a_k}\in G\ \forall\, k \right\} \tag{1.28}$$

Clearly $\langle G,G\rangle$ satisfies all the axioms for a group, and is a subgroup of G. We call $\langle G,G\rangle$ the *commutator* (or *derived*) subgroup of G. And because the set of commutators is closed under conjugation, $\langle G,G\rangle$ is an invariant subgroup of G: $\langle G,G\rangle \triangleleft G$. Some examples:

(i) $\langle S_n, S_n\rangle \cong A_n$, the group of even permutations (see §1.4.3 below).

(ii) $\langle A_n, A_n\rangle \cong A_n$ for $n > 4$, but $\langle A_4, A_4\rangle \cong \mathbb{Z}_2 \times \mathbb{Z}_2$.

(iii) $\langle Q, Q\rangle \cong \mathbb{Z}_2$, where Q is the quaternionic group (see §1.4.5 below).

As Zee explains, the size of the commutator subgroup tells us roughly how nonabelian the group itself is. For abelian groups, $\langle G,G\rangle \cong \{E\}$. When $\langle G,G\rangle \cong G$, the group is maximally nonabelian in some sense. The quotient group $G^{\rm ab} \equiv G/\langle G,G\rangle$ is called the *abelianization* of G. A group is called *perfect* if it is isomorphic to its own commutator subgroup. The smallest nontrivial perfect group is A_5.

GROUP ALGEBRA : The *group algebra* $\mathcal{G}$ for any finite discrete group G is defined to be the set of linear combinations of the form $\boldsymbol{x} = \sum_{g\in G} x_g\, g$, where each $x_g \in \mathbb{C}$ is a complex number. Note that both addition and multiplication are defined for elements of $\mathbb{G}$, for if $\boldsymbol{y} = \sum_{g\in G} y_g\, g$, then

$$\boldsymbol{x}+\boldsymbol{y} = \sum_{g\in G}(x_g+y_g)\,g \qquad , \qquad \boldsymbol{x}\cdot\boldsymbol{y} = \sum_{g\in G}\sum_{h\in G} x_g\, y_h\, hg = \sum_{g\in G} \overbrace{\left(\sum_{h\in G} x_{h^{-1}g}\, y_h\right)}^{(xy)_g} g \equiv \sum_g (xy)_g\, g \quad . \tag{1.29}$$

We can think of the group elements as basis elements of a vector space $\mathcal{A}$ which acts on itself by multiplication as well as addition[26]. This structure we have just described is known in mathematical parlance as an *algebra*. An (associative) algebra is a linear vector space which is closed under some multiplication law. Thus there are two types of multiplication in an algebra. As a vector space over a field $\mathbb{F}$, one has ordinary multiplication by scalars in $\mathbb{F}$, *e.g.* real or complex numbers. But the individual basis elements, which in our case are group elements, have their own multiplication rule, specified by the Cayley table for the group. Another example which will be relevant to us is that of a *Lie algebra*, which, for our purposes, is also a vector space over $\mathbb{R}$ or $\mathbb{C}$, but where multiplication of two elements X and Y in the algebra is defined by the *Lie bracket*, $\big[X,Y\big]$. We will mainly be concerned with matrix Lie groups, in which case the Lie bracket is the familiar commutator.

[26]The vector space spanned by $g \in G$ is not necessarily normed.

The concept of an algebra is very close to that of another mathematical structure known as a *ring*. A ring $\mathcal{R}$ is a set endowed with the binary operations of addition and multiplication which is an abelian group under addition, a *monoid* under multiplication[27], and where multiplication distributes over addition[28].

1.4.2 Other math stuff

Here are some other math definitions which may be useful to clarify before going forward. They don't really belong in this section on discrete groups, but I thought it would be fun to hide them here anyway.

MONOID : A *monoid* is a triple $(M\,,\,\cdot\,,\,1)$ where M is a set which is closed under the associative binary product $\cdot$, and where 1 is the multiplicative identity (*i.e.*$m\cdot 1 = 1\cdot m = m$ for all $m\in M$).

RING : A *ring* is a set R where $(R\,,\,+\,,\,0)$ is an abelian group under addition, $(R\,,\,\cdot\,,\,1)$ is a monoid, and multiplication distributes over addition, *viz.*

$$\begin{aligned} a\cdot(b+c) &= a\cdot b + a\cdot c \\ (a+b)\cdot c &= a\cdot c + b\cdot c \quad . \end{aligned} \tag{1.30}$$

Examples of rings include $\mathbb{Z}$, $\mathbb{R}$, $\mathbb{C}$, the set $\left\{m+n\sqrt{2}\,|\,m,n\in\mathbb{Z}\right\}$, real continuous functions $f:[0,1]\to\mathbb{R}$ with $f(x)=0$ the additive identity and $f(x)=1$ the multiplicative identity, *etc.*

IDEAL : A *left ideal* I is a subset of a ring $I\subset R$ where $(I\,,\,+\,,\,0)$ is an abelian group, and where $ri\in I$ for all $r\in R$ and $i\in I$. For a *right ideal* the requirement is that $ir\in I$. If we require both $ir\in I$ and $ri\in I$, this defines an *ideal* (*i.e.* no need to specify left or right). Example: $I=2\mathbb{Z}\subset\mathbb{Z}$, *i.e.* the set of even integers, is an ideal in the ring $\mathbb{Z}$.

QUOTIENT RING : If $I\subset R$ is an ideal in R, the *quotient ring* $\overline{R}\equiv R/I$ is the set of elements of R modulo I, any of which we can write in the form $a+I$ where $a\in R$. Thus, two elements a and a' in the quotient ring $\overline{R}$ are equivalent if their difference lies in I (*i.e.* $a\equiv a'\;\Leftrightarrow\;a-a'\in I$). Within $\overline{R}$ we then have

$$\begin{aligned} (a+I)+(b+I) &= a+b+I \\ (a+I)\cdot(b+I) &= a\cdot b+I \quad . \end{aligned} \tag{1.31}$$

Thus, $\mathbb{Z}/2\mathbb{Z}=\{0,1\}$.

DOMAIN : Let R be a ring and $R^*=R-0$ the set of its nonzero elements (using $-$ for set subtraction). If $(R^*\,,\,\cdot\,,\,1)$ is a monoid then R is a domain. How on earth could $(R^*\,,\,\cdot\,,\,1)$ fail to form a monoid, I hear you thinking. Well, let R be the ring of real smooth functions[29] and define $f(x)=\left(\frac{1}{2}-x\right)\Theta\left(\frac{1}{2}-x\right)$ and

[27] A monoid is a set with a closed, associative binary operation and with an identity element. The difference between a monoid and a group is that each element of the monoid needn't have an inverse. In physics, the "renormalization group" should more appropriately be called the "renormalization monoid" since RG processes have no inverse.

[28] The formal difference between a ring $\mathcal{R}$ an an algebra $\mathcal{A}$ is that in a ring, the algebraic structure is entirely internal, but in an algebra there is additional structure because it allows for multiplication by an external ring $\mathcal{R}'$ in such a way that the two multiplication properties are compatible. So an algebra is actually two compatible rings. If this is confusing, take comfort in the fact that for our purposes, the external ring $\mathcal{R}'$ is just the complex numbers.

[29] Parsing disambiguation: by "real smooth functions" I mean functions $f(x)$ which are both real and in the class C^∞, as opposed to functions which are somehow like Luther Vandross.

$g(x) = \big(x - \frac{1}{2}\big)\,\Theta\big(x - \frac{1}{2}\big)$, where $\Theta(u)$ is the step function. Then both $f(x)$ and $g(x)$ lie within R^*, but their product $f(x) \cdot g(x) = 0 \notin R^*$. So R is not a domain.

DIVISION RING : Let R be a ring and again let $R^* = R - 0$. If $(R^*, \cdot, 1)$ is a group, we say that R is a *division ring*. A commutative division ring is a *field*.

VECTOR SPACE : A *vector space* $\mathcal{V}$ over a scalar field $\mathbb{F}$ consists of a set $\mathcal{V}$ and operations $+$ and $\cdot$ such that (i) $(\mathcal{V}\,,\,+\,,\,0)$ is an abelian group, (ii) $\mathcal{V}$ is closed under scalar multiplication by any $c \in \mathbb{F}$, (iii) scalars and vectors may be multiplied, and the $\cdot$ operation is, commutative, associative, and distributes over addition, and (iv) for all $\boldsymbol{v} \in \mathcal{V}$, $1 \cdot \boldsymbol{v} = \boldsymbol{v} \cdot 1 = \boldsymbol{v}$.

ASSOCIATIVE ALGEBRA : As mentioned above, an *associative algebra* is a vector space which is closed under some multiplication law. Thus there are two types of multiplication in an algebra.

1.4.3 More about permutations

Recall the general form of a permutation of n elements:

$$\sigma \equiv \begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \sigma(1) & \sigma(2) & \sigma(3) & \cdots & \sigma(n) \end{pmatrix} \quad . \tag{1.32}$$

Each such permutation can be factorized as a product of disjoint *cycles*, a process known as *cycle decomposition*. A k-cycle involves cyclic permutation of k elements, so $(i_1\, i_2\, \cdots\, i_k)$ means $\sigma(i_1) = i_2$, $\sigma(i_2) = i_3$, *etc.*, and finally $\sigma(i_k) = i_1$. Consider, for example, the following element from S_7 :

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 7 & 2 & 6 & 8 & 1 & 3 & 5 & 4 \end{pmatrix} = (1\,7\,5)\,(2)\,(3\,6)\,(4\,8) \quad . \tag{1.33}$$

Thus σ is written as a product of one three-cycle, two two-cycles, and two one-cycles. The one-cycles of course do nothing. Written in this way, the cycle decomposition obeys the following sum rule: the sum of the lengths of all the cycles is the index n of S_n. Denoting all the one-cycles is kind of pointless, though, and typically we omit them in the cycle decomposition; in this case we'd just write $\sigma = (1\,7\,5)\,(3\,6)\,(4\,8)$. Alas, by virtue of suppressing the one-cycles, the sum rule no longer holds.

In fact, any k-cycle may be represented as a product of $k - 1$ two-cycles (also called *transpositions*):

$$(i_1\, i_2\, \cdots\, i_k) = (i_1\, i_2)(i_2\, i_3) \cdots (i_{k-1}\, i_k) \quad . \tag{1.34}$$

Note that the two-cycles here are not disjoint. The decomposition of a given k-cycle into transpositions is not unique, save for the following important feature: the total number of transpositions is preserved *modulo* 2. This feature allows us to associate a sign $\mathsf{sgn}(\sigma)$ with each permutation σ, given by $(-1)^r$, where r is the number of transpositions in any complete decomposition of σ into two-cycles. An equivalent definition: $\mathsf{sgn}(\sigma) = \epsilon_{\sigma(1)\,\sigma(2)\,\cdots\,\sigma(n)}$, where $\epsilon_{\alpha_1\,\alpha_2\,\cdots\,\alpha_n}$ is the completely antisymmetric tensor of rank n , with $\epsilon_{1\,2\,3\,\cdots\,n} = +1$. Note that $\mathsf{sgn}(\sigma\sigma') = \mathsf{sgn}(\sigma)\,\mathsf{sgn}(\sigma')$. This distinction allows us to define a subgroup of S_n known as A_n , the *alternating group*, consisting of all the *even* permutations in S_n. Clearly A_n contains the identity, and since the product of two even permutations is itself an even permutation, we may conclude that A_n is itself a group. Indeed, since $\mathsf{sgn}(\tilde{\sigma}^{-1}\sigma\tilde{\sigma}) = \mathsf{sgn}(\sigma)$, conjugacy preserves the

sign of any element of S_n , and we conclude $A_n \triangleleft S_n$, *i.e.* the alternating group is a normal subgroup of the symmetric group.

Let me conclude with a few other details about the symmetric group. First, the mapping $\mathsf{sgn} : S_n \mapsto \mathbb{Z}_2$ is a group homomorphism. This means that $D^{(1)}(\sigma) = \mathsf{sgn}(\sigma)$ is a one-dimensional representation of S_n, called the *sign representation*. Of course it is not a faithful representation, but fidelity is so 1990s[30]. Second, recall from §1.3.7 the representation $D^{(n)}(S_n)$ in terms of $n \times n$ matrices, where $\big[D^{(n)}(\sigma)\big]_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. This is called the *defining representation*, and it is faithful. One then has that $\mathsf{sgn}(\sigma) = \det\big[D^{(n)}(\sigma)\big]$. Finally, we consider a cyclic decomposition of any permutation σ into ν_1 1-cycles, ν_2 2-cycles, *etc.* The sum rule is then $\sum_{k=1}^{n} k\,\nu_k = n$. Now any such decomposition is invariant under (i) permuting any of the k-cycles, and (ii) cyclic permutation within a k-cycle. Consider our friend $\sigma = (1\,7\,5)\,(2)\,(3\,6)\,(4\,8)$ from Eqn. 1.33. Clearly $n_1 = 1$, $n_2 = 2$, and $n_3 = 1$ with $1\cdot n_1 + 2\cdot n_2 + 3\cdot n_3 = 8$. Furthermore, we could equally well write $\sigma = (1\,7\,5)\,(2)\,(4\,8)\,(3\,6)$, permuting the two 2-cycles, or as $\sigma = (7\,5\,1)\,(2)\,(4\,8)\,(6\,3)$, cyclically permuting within the 3-cycle and one of the 2-cycles. This leads us to the following expression for the number $N(\nu_1, \nu_2, \ldots, \nu_n)$ of possible decompositions into ν_1 1-cycles, ν_2 2-cycles, *etc.* :

$$N(\nu_1, \nu_2, \ldots, \nu_n) = \frac{n!}{1^{\nu_1}\,\nu_1!\,2^{\nu_2}\,\nu_2!\,\cdots\,n^{\nu_n}\,\nu_n!} \quad . \tag{1.35}$$

The sign of each permutation is then uniquely given by its cyclic decomposition:

$$\mathsf{sgn}(\sigma) = (+1)^{\nu_1}(-1)^{\nu_2}(+1)^{\nu_3}(-1)^{\nu_4}\cdots = (-1)^{\#\text{ of cycles of even length}} \quad . \tag{1.36}$$

Finally, let's check that the sum over all possible decompositions gives the order of the group, *i.e.* that

$$\sum_{\nu_1=0}^{\infty}\cdots\sum_{\nu_n=0}^{\infty} N(\nu_1, \nu_2, \ldots, \nu_n)\,\delta_{\nu_1+2\nu_2+\ldots+n\nu_n\,,\,n} = n! \quad , \tag{1.37}$$

or, equivalently,

$$F_n \equiv \sum_{\nu_1=0}^{\infty}\cdots\sum_{\nu_n=0}^{\infty} \frac{\delta_{\nu_1+2\nu_2+\ldots+n\nu_n\,,\,n}}{1^{\nu_1}\,\nu_1!\,2^{\nu_2}\,\nu_2!\,\cdots\,n^{\nu_n}\,\nu_n!} = 1 \quad . \tag{1.38}$$

This must be true for all nonnegative integers n, with $F_0 \equiv 1$. In dealing with the constraint, recall the treatment of the grand canonical ensemble in statistical physics. We write the generating function

$$F(z) \equiv \sum_{n=0}^{\infty} F_n z^n = \prod_{k=0}^{\infty}\sum_{\nu_k=0}^{\infty} \frac{z^{k\nu_k}}{k^{\nu_k}\,\nu_k!} \quad , \tag{1.39}$$

in which case

$$F_n = \oint\limits_{|z|=1} \frac{dz}{2\pi i z}\,\frac{F(z)}{z^n} \quad . \tag{1.40}$$

[30] Please don't tell my wife I wrote that.

Thus, F_n is simply the coefficient of z^n in the Taylor expansion of $F(z)$. But now,

$$\begin{aligned} F(z) &= \prod_{k=0}^{\infty} \sum_{\nu_k=0}^{\infty} \frac{1}{\nu_k!} \left(\frac{z^k}{k} \right)^{\nu_k} = \prod_{k=0}^{\infty} \exp\left(z^k/k\right) \\ &= \exp\left(\sum_{k=0}^{\infty} \frac{z^k}{k} \right) = e^{-\ln(1-z)} = \frac{1}{1-z} = 1 + z + z^2 + \dots \quad , \end{aligned} \tag{1.41}$$

and so indeed $F_n = 1$ for all $n \geq 0$. Ta da!

1.4.4 Conjugacy classes of the dihedral group

Let's count the conjugacy classes of D_n. First, we note that $D_n = \mathbb{Z}_n \cup \sigma\mathbb{Z}_n$, where $\mathbb{Z}_n \cong C_n$ is the cyclic group of order n, which is abelian, and σ is any one of the n twofold axes. Let r denote the primitive rotation by $2\pi/n$, and consider any of the elements $r^k \in \mathbb{Z}_n$, with $k \in \{1, \dots, n-1\}$.[31] If we conjugate $r^k \to g^{-1} r^k g$ by any $g \in \mathbb{Z}_n$, we recover r^k because $\mathbb{Z}_n$ is abelian. So consider $g = \sigma r^l \in \sigma\mathbb{Z}_n$. Using $\sigma r \sigma = r^{-1}$, we readily obtain $g^{-1} r^k g = r^{-k}$. We conclude that for n odd, there are $\frac{1}{2}(n+1)$ two element conjugacy classes of the form $\{r, r^{n-1}\}$ through $\{r^{(n-1)/2}, r^{(n+1)/2}\}$, to which we add the one element class $\{E\}$. For n even, though, there are $\frac{1}{2}(n+2)$ such classes: two element classes $\{r, r^{n-1}\}$ through $\{r^{(n-2)/2}, r^{(n+2)/2}\}$ plus one element classes $\{E\}$ and $\{r^{n/2}\}$.

Next, we start with a general element $\sigma r^k \in \sigma\mathbb{Z}_n$ and generate its conjugates. If $g = r^l$, we have $g^{-1}\sigma r^k g = \sigma r^{2l+k}$, whereas if $g = \sigma r^l$, we have $g^{-1}\sigma r^k g = \sigma r^{2l-k}$. Thus if n is odd, we obtain one more conjugacy class, which is $\sigma\mathbb{Z}_n$ itself, with n elements. If, on the other hand, n is even, then $\sigma\mathbb{Z}_n$ splits into two conjugacy classes: $\{\sigma r^{2j}\}$ and $\sigma r^{2j+1}\}$, each with $j \in \{0, \dots, \frac{1}{2}n - 1\}$, each of which has $\frac{1}{2}n$ elements. In the latter case, the two classes consist of all twofold axes which preserve a pair of vertices, and all twofold axes which preserve a pair of edges.

Putting it all together, we conclude that for n odd, D_n has $\frac{1}{2}(n+5)$ conjugacy classes, while for n even D_n has $\frac{1}{2}(n+6)$ conjugacy classes.

1.4.5 Quaternion group

The group Q is a nonabelian group consisting of eight elements, $\{\pm 1, \pm \mathtt{i}, \pm \mathtt{j}, \pm \mathtt{k}\}$, where $E = 1$. Its multiplication table is defined by the relations

$$\mathtt{i}^2 = \mathtt{j}^2 = \mathtt{k}^2 = -1 \quad , \quad \mathtt{ij} = -\mathtt{ji} = \mathtt{k} \quad , \quad \mathtt{jk} = -\mathtt{kj} = \mathtt{i} \quad , \quad \mathtt{ki} = -\mathtt{ik} = \mathtt{j} \quad . \tag{1.42}$$

Note that Q has the same rank as C_{4v} ($\cong D_4$), but has a different overall structure, *i.e.* Q is not isomorphic to D_4. Indeed, D_4 and Q are the only two non-Abelian groups of order eight[32]. Q has five conjugacy classes: $\{1\}$, $\{-1\}$, $\{\mathtt{i}, -\mathtt{i}\}$, $\{\mathtt{j}, -\mathtt{j}\}$, and $\{\mathtt{k}, -\mathtt{k}\}$. It has six subgroups, all of which are invariant subgroups:

$$\{1\} \quad , \quad \{1, -1\} \quad , \quad \{1, -1, \mathtt{i}, -\mathtt{i}\} \quad , \quad \{1, -1, \mathtt{j}, -\mathtt{j}\} \quad , \quad \{1, -1, \mathtt{k}, -\mathtt{k}\} \quad , \tag{1.43}$$

[31] Recall that the identity E is always its own conjugacy class.

[32] Hence if G is a nonabelian group of order eight, then either $G \cong D_4$ or $G \cong Q$.

as well as Q itself. The quaternion group can be faithfully represented in terms of the Pauli matrices, with $\mathtt{i} \to -i\sigma^x$, $\mathtt{j} \to -i\sigma^y$, and $\mathtt{k} \to -i\sigma^z$.

Incidentally, how do we know that $Q \ncong D_4$? Both groups have eight elements and both have five conjugacy classes! However, upon further inspection, Q has one element of order two (-1) and six of order four $(\pm\mathtt{i}, \pm\mathtt{j}, \pm\mathtt{k})$. D_4, on the other hand, has five elements of order two $(r^2, \sigma, \sigma r, \sigma r^2, \sigma r^3\}$ and two of order four (r, r^3). So the groups cannot have identical multiplication tables.

When we speak of *quaternions*, or of *quaternionic numbers*, we refer to an extension of complex numbers $z = x + iy$ to $h = a + \mathtt{i}b + \mathtt{j}c + \mathtt{k}d$, with $a, b, c, d \in \mathbb{R}$, and the set of quaternionic numbers is denoted $\mathbb{H}$. The quaternion algebra is not commutative! If $u = u_0 + \mathtt{i}u_1 + \mathtt{j}u_2 + \mathtt{k}u_3$ and $v = v_0 + \mathtt{i}v_1 + \mathtt{j}v_2 + \mathtt{k}v_3$, then representing these in terms of the Pauli matrices, $u = u_0 - i\boldsymbol{u}\cdot\boldsymbol{\sigma}$ and $v = v_0 - i\boldsymbol{v}\cdot\boldsymbol{\sigma}$, and therefore

$$\begin{aligned} uv &= (u_0 - i\boldsymbol{u}\cdot\boldsymbol{\sigma})(v_0 - i\boldsymbol{v}\cdot\boldsymbol{\sigma}) \\ &= u_0\, v_0 - \boldsymbol{u}\cdot\boldsymbol{v} - i(u_0\,\boldsymbol{v} + v_0\,\boldsymbol{u} - \boldsymbol{u}\times\boldsymbol{v})\cdot\boldsymbol{\sigma} \quad , \end{aligned} \tag{1.44}$$

which differs from vu whenever $\boldsymbol{u}\times\boldsymbol{v} \neq 0$. Hence multiplication is not commutative for quaternions. Complex conjugation of quaternions is defined as $h^* = a - \mathtt{i}b - \mathtt{j}c - \mathtt{k}d$. Note that $h^{**} = h$, which says that conjugation is its own inverse operation, as in the case of complex numbers (Mathy McMathstein says it this way: conjugation is an *involution*.) Note however that $(h_1 h_2)^* = h_2^*\, h_1^*$, *i.e.* the conjugate of a product of quaternions is the product of their conjugates, but in the reverse order. The norm of a quaternion is defined as

$$|h| = \sqrt{h^* h} = \sqrt{a^2 + b^2 + c^2 + d^2} \quad , \tag{1.45}$$

and the distance between two quaternions is accordingly $d(h_1, h_2) = |h_1 - h_2|$. The inverse of the quaterion $h = a + \mathtt{i}b + \mathtt{j}c + \mathtt{k}d$ is

$$h^{-1} = \frac{a - \mathtt{i}b - \mathtt{j}c - \mathtt{k}d}{a^2 + b^2 + c^2 + d^2} = \frac{h^*}{|h|^2} \quad . \tag{1.46}$$

Recall that the real numbers $\mathbb{R}$ and complex numbers $\mathbb{C}$ are *fields*. A field is a set together with the operations of addition and multiplication such that both operations are individually commutative (*i.e.* $a + b = b + a$ and $ab = ba$), both operations are associative, both operations have identities and inverses, and that multiplication distributes over addition. Since multiplication within $\mathbb{H}$ is not commutative, $\mathbb{H}$ is not a field. Rather, Mathy McMathstein tells us, $\mathbb{H}$ is an *associative division algebra* over the real numbers.

A *unit quaternion* $u = \exp(-i\,\xi\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}/2) = \cos(\xi/2) - i\sin(\xi/2)\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}$ may be used to effect rotations. Define the quaternion $R = -i\boldsymbol{R}\cdot\boldsymbol{\sigma}$ with no constant component. Then one can show directly that

$$\begin{aligned} R' &= u\,R\,u^{-1} = -i\boldsymbol{R}'\cdot\boldsymbol{\sigma} \\ \boldsymbol{R}' &= \cos\xi\,\boldsymbol{R} + (1 - \cos\xi)\,(\hat{\boldsymbol{n}}\cdot\boldsymbol{R})\,\hat{\boldsymbol{n}} - \sin\xi\,\hat{\boldsymbol{n}}\times\boldsymbol{R} \end{aligned} \tag{1.47}$$

which is the rotation of $\boldsymbol{R}$ about $\hat{\boldsymbol{n}}$ by θ. Thus the algebra of $\mathsf{SO}(3)$ rotations is simply the algebra of unit quaternions!

True story: Alexander Hamilton invented quaternions while he was Treasury Secretary of the United States, and his quaternionic arithmetic proved so useful in reducing the computational effort involved in overseeing the Treasury Department that he was honored by having his portrait on the \$10 bill[33].

[33] This is not a true story.

order	abelian G	nonabelian G	order	abelian G	nonabelian G
2	$\mathbb{Z}_2 \cong S_2 \cong D_1$	none	9	$\mathbb{Z}_3^2$, $\mathbb{Z}_9$	none
3	$\mathbb{Z}_3 \cong A_3$	none	10	$\mathbb{Z}_2 \times \mathbb{Z}_5$	D_5
4	$\mathbb{Z}_2 \times \mathbb{Z}_2 \cong V$, $\mathbb{Z}_4$	none	11	$\mathbb{Z}_{11}$	none
5	$\mathbb{Z}_5$	none	12	$\mathbb{Z}_2^2 \times \mathbb{Z}_3$, $\mathbb{Z}_3 \times \mathbb{Z}_4$	D_6 , A_4
6	$\mathbb{Z}_2 \times \mathbb{Z}_3$	S_3	13	$\mathbb{Z}_{13}$	none
7	$\mathbb{Z}_7$	none	14	$\mathbb{Z}_2 \times \mathbb{Z}_7$	D_7
8	$\mathbb{Z}_2^3$, $\mathbb{Z}_2 \times \mathbb{Z}_4$, $\mathbb{Z}_8$	D_4 ; Q	15	$\mathbb{Z}_3 \times \mathbb{Z}_5$	none

Table 1.5: Table of discrete groups up to order $|G| = 15$. Note that $Z_n \cong C_n$ and that $\mathbb{Z}_p \times \mathbb{Z}_q \cong \mathbb{Z}_{pq}$ when p and q are relatively prime.

1.4.6 Group presentations

Tab. 1.5 lists all discrete groups up to order 15. Note that at order $|G| = 4$ there are two distinct groups, $\mathbb{Z}_4$ and $\mathbb{Z}_2 \times \mathbb{Z}_2$; the latter is also called the *Klein group*, V. Both are abelian, but $\mathbb{Z}_4$ is *not* the same group as $\mathbb{Z}_2 \times \mathbb{Z}_2$. These two groups have different multiplication tables. $\mathbb{Z}_4$ is generated by a single element r which satisfies $r^4 = 1$. $\mathbb{Z}_2 \times \mathbb{Z}_2$ is generated by two elements σ and τ such that $\sigma^2 = \tau^2 = 1$ and $\sigma\tau = \tau\sigma$.

While $\mathbb{Z}_4 \ncong \mathbb{Z}_2 \times \mathbb{Z}_2$, it *is* the case that $\mathbb{Z}_6 \cong \mathbb{Z}_2 \times \mathbb{Z}_3$. Let's understand why this is the case. The group $\mathbb{Z}_2 \times \mathbb{Z}_3$ is generated by two elements, σ and ω, where $\sigma^2 = \omega^3 = 1$ and $\sigma\omega = \omega\sigma$. Now define $r \equiv \sigma\omega$. Clearly the order of the element r is six, *i.e.* $r^6 = 1$. One can write $\sigma = r^3$ and $\omega = r^4$, as well as $\omega^2 = r^2$ and $\sigma\omega^2 = r^5$. That accounts for all the elements once we include the identity E. Similarly, $\mathbb{Z}_{10} \cong \mathbb{Z}_2 \times \mathbb{Z}_5$ and $\mathbb{Z}_{15} \cong \mathbb{Z}_3 \times \mathbb{Z}_5$. Can you see a generalization to cyclic groups whose order is a product of unique prime factors?

At order eight, there are three inequivalent abelian groups: $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ (*i.e.* $\mathbb{Z}_2^3$), $\mathbb{Z}_2 \times \mathbb{Z}_4$, and $\mathbb{Z}_8$. $\mathbb{Z}_2^3$ is generated by elements (σ, τ, ρ) which all mutually commute and for which $\sigma^2 = \tau^2 = \rho^2 = 1$. $\mathbb{Z}_2 \times \mathbb{Z}_4$ is generated by (σ, δ) which mutually commute and which satisfy $\sigma^2 = \delta^4 = 1$. Finally, $\mathbb{Z}_8$ has a single generator r satisfying $r^8 = 1$.

Indeed, more economically than providing the full group multiplication table with its $|G|^2$ entries, a group can be defined by a *presentation* in which one specifies a set $\mathcal{G}$ of *generators* and a set $\mathfrak{R}$ of *relations* which the generators satisfy. We then say that the group G has the presentation $\langle\, \mathcal{G} \,|\, \mathfrak{R} \,\rangle$. The group elements are then given by all possible products of the generators, subject to the relations $\mathfrak{R}$. For example, the presentation for $C_n \cong \mathbb{Z}_n$ would be $\langle\, r \,|\, r^n = 1 \,\rangle$, which is usually abbreviated simply as $\langle\, r \,|\, r^n \,\rangle$. The dihedral group D_n has the presentation $\langle\, r, \sigma \,|\, r^n, \sigma^2, (r\sigma)^2 \,\rangle$. $\mathbb{Z}_2 \times \mathbb{Z}_4$ has the presentation $\langle\, \sigma, \delta \,|\, \sigma^2, \delta^4, \sigma\delta = \delta\sigma \,\rangle$. Note how in the last example we had to specify in $\mathfrak{R}$ that σ and δ commute.

While every group has a presentation, presentations are not necessarily unique. More examples are presented (hah!) in Tab. 1.6. The *free group* $F_{\mathcal{G}}$ on the set $\mathcal{G}$ of generators is simply all possible products. For example, if $\mathcal{G} = \{a, b\}$, $F_{\mathcal{G}}$ would be an infinite nonabelian group with elements

$$F_{\mathcal{G}} = \left\{ E, a, b, a^{-1}, b^{-1}, a^2, ab, ba, b^2, a^3, a^2b, aba, ba^2, \ldots \right\} \quad . \tag{1.48}$$

group	order	presentation	group	order	presentation
$\mathbb{Z}_n$	n	$\left\langle\, r \,\middle|\, r^n \,\right\rangle$	S_3	6	$\left\langle\, a,b \,\middle|\, a^2, b^3, (ab)^2 \,\right\rangle$
$\mathbb{Z}_m \times \mathbb{Z}_n$	mn	$\left\langle\, r,s \,\middle|\, r^m, s^n, rs=sr \,\right\rangle$	$T \cong A_4$	12	$\left\langle\, a,b \,\middle|\, a^2, b^3, (ab)^3 \,\right\rangle$
D_n	$2n$	$\left\langle\, r,\sigma \,\middle|\, r^n, \sigma^2, (r\sigma)^2 \,\right\rangle$	$O \cong S_4$	24	$\left\langle\, a,b \,\middle|\, a^2, b^3, (ab)^4 \,\right\rangle$
DC_n	$4n$	$\left\langle\, r,\sigma \,\middle|\, r^{2n}, r^n=\sigma^2, \sigma r \sigma^{-1} = r^{-1} \,\right\rangle$	$E \cong A_5$	60	$\left\langle\, a,b \,\middle|\, a^2, b^3, (ab)^5 \,\right\rangle$
Q	8	$\left\langle\, a,b \,\middle|\, aba=b\,, bab=a \,\right\rangle$	$\mathsf{SL}(2,\mathbb{Z})$	∞	$\left\langle\, a,b \,\middle|\, aba=bab, (aba)^4 \,\right\rangle$
Q_{16}	16	$\left\langle\, a,b,c \,\middle|\, a^4=b^2=c^2=abc \,\right\rangle$	$\mathsf{PSL}(2,\mathbb{Z})$	∞	$\left\langle\, a,b \,\middle|\, a^2, b^3 \,\right\rangle$
$\pi_1(S)$	∞	$\left\langle\, \{x_n,y_n\} \,\middle|\, \langle x_1,y_1\rangle \cdots \langle x_g,y_g\rangle \,\right\rangle$	$F_{\mathcal{G}}$	∞	$\left\langle\, \mathcal{G} \,\middle|\, \emptyset \,\right\rangle$

Table 1.6: Examples of discrete group presentations. DC_n is the *dicyclic group*, which is order $4n$. T, O, and E are the tetrahedral, octahedral (cubic), and icosahedral groups, respectively, which describe the rotational symmetries of those regular polyhedra. Q_{16} is the *generalized quaternion group*. $\pi_1(S)$ is the fundamental group of a surface of genus g, which is generated by $2g$ loops and $\langle \bullet, \bullet \rangle$ is the commutator.

Note that if G has presentation $\left\langle\, \mathcal{G} \,\middle|\, \mathfrak{R} \,\right\rangle$ and H has presentation $\left\langle\, \mathcal{H} \,\middle|\, \mathfrak{S} \,\right\rangle$, then the direct product $G \times H$ has presentation $\left\langle\, \mathcal{G}, \mathcal{H} \,\middle|\, \mathfrak{R}, \mathfrak{S}, [\mathcal{G}, \mathcal{H}] \,\right\rangle$. where $[\mathcal{G}, \mathcal{H}]$ signifies that all generators from the set $\mathcal{G}$ commute with all generators from the set $\mathcal{H}$. The *free product* $G \star H$ has presentation $\left\langle\, \mathcal{G}, \mathcal{H} \,\middle|\, \mathfrak{R}, \mathfrak{S} \,\right\rangle$. Thus, since the presentation of the dihedral group D_4 is $\left\langle\, r,\sigma \,\middle|\, r^4, \sigma^2, (r\sigma)^2 \,\right\rangle$, the presentation of $D_{4h} = D_4 \times \mathbb{Z}_2$ is

$$\left\langle\, r,\sigma,c \,\middle|\, r^4, \sigma^2, (r\sigma)^2, c^2, rc=cr, \sigma c = c\sigma \,\right\rangle \quad . \tag{1.49}$$

In the presentation for Q, $a = \mathtt{i}$ and $b = \mathtt{j}$. How can we show $a^4 = 1$? From $a = bab$ and $b = aba$, we have $a^2 = a(bab) = (aba)b = b^2$. Then $a^3 = a^2 a = b^2 a = b(bab)b^{-1} = bab^{-1}$. It follows that $a^4 = a(bab^{-1}) = (aba)b^{-1} = bb^{-1} = 1$, and of course $b^4 = (b^2)^2 = (a^2)^2 = a^4 = 1$ as well. Similarly, from the above presentation for Q_{16}, one can show that $a^4 = b^2 = c^2 = abc$ are all of order two, and an equivalent presentation is $\left\langle\, a,b \,\middle|\, a^4 = b^2 = abab \,\right\rangle$. Note that some groups have no finite presentation, but necessarily they must be of infinite order.

1.5 Lie Groups

1.5.1 Definition of a Lie group

Algebra and topology – two great tastes that taste great together! A *Lie group* is a *manifold*[34] G which is endowed with a group structure such that multiplication $G \times G \mapsto G : (g, g') \to gg'$ and inverse $G \mapsto G : g \to g^{-1}$ are smooth.

[34]There are two broad classifications of manifolds: *intake manifolds*, which distribute fuel and air to engine cylinders, and *exhaust manifolds*, which direct exhaust to the rear of the vehicle. Also a manifold is a topological space that is everywhere locally homeomorphic to $\mathbb{R}^n$ for some fixed integer n.

This definition is perhaps a bit too slick. Let's say we have a smooth manifold $\mathcal{M}$ and a map $g : \mathcal{M} \mapsto G$, where G is our Lie group. That is to say, the group operations consists of $\{g(x) \mid x \in \mathcal{M}\}$ where $g(x)\, g(y) = g(z)$ for some $z(x, y)$. Here x, y, and z are points on $\mathcal{M}$. There are two important axioms:

(i) *smoothness of group composition* : The function $z(x, y)$ is differentiable.

(ii) *smoothness of inverse* : The function $y = \psi(x)$, where $\big[g(x)\big]^{-1} = g(y)$, is differentiable.

As an example, consider the group $\mathsf{SL}(2, \mathbb{R})$, which is the set of real 2×2 matrices with determinant 1, also known as "the special linear group of rank two over the reals". Each element $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathsf{SL}(2, \mathbb{R})$ can be parameterized by the three real numbers $\{a, b, c\}$, since $ad - bc = 1$ requires $d = (1 + bc)/a$. (A different parameterization much be chosen in the vicinity of $a = 0$.) $\mathsf{SL}(2, \mathbb{R})$ is an example of a *matrix group*. Other examples include $\mathsf{GL}(n, \mathbb{R})$ (real invertible $n \times n$ matrices), $\mathsf{O}(3)$ (rank three real orthogonal matrices), $\mathsf{Sp}(4, \mathbb{R})$ (rank four real symplectic matrices), $\mathsf{SU}(3) \times \mathsf{SU}(2) \times \mathsf{U}(1)$ (some contrived group the particle physicists seem to think is important - *as if!*), *etc.* See §1.3.8 above on $\mathsf{SU}(2)$.

Lie groups that are not matrix groups

It is quite convenient that every Lie group we will study is a matrix group, hence algebraically the only operations we will need are matrix multiplication and matrix inversion. The *metaplectic group* $\mathsf{Mp}(2n, \mathbb{R})$, which is a double cover of the symplectic group $\mathsf{Sp}(2n, \mathbb{R})$, is an example of a Lie group which is not a matrix group, but, truth be told, I have no idea what the hell I'm talking about here.

Hall[35] provides a concrete example of a Lie group which is not a matrix group:

$$G = \mathbb{R} \times \mathbb{R} \times S^2 = \Big\{ g \equiv (x, y, w) \,\Big|\, x \in \mathbb{R},\, y \in \mathbb{R},\, w \in S^1 \subset \mathbb{C} \Big\} \tag{1.50}$$

under the group operation $G \times G \mapsto G$ defined by

$$(x_1, y_1, w_1) \cdot (x_2, y_2, w_2) = (x_1 + x_2\,,\, y_1 + y_2\,,\, e^{ix_1 y_2}\, w_1 w_2) \quad . \tag{1.51}$$

Note that $w_{1,2}$ are expressed as unimodular complex numbers. The inverse operation is

$$g^{-1} = (-x\,,\, -y\,,\, e^{ixy} w) \quad . \tag{1.52}$$

One can check that G under the above multiplication law satisfies the axioms for a Lie Group. Yet it can be proven (see Hall, §4.8) that there is no continuous injective homomorphism of G into any $\mathsf{GL}(n, \mathbb{C})$, so G is not a matrix Lie group.

1.5.2 The big happy family of matrix Lie groups

First, a mathy definition:

[35] B. C. Hall, *Lie Groups, Lie Algebras, and their Representations*, 2nd edition, p. 25. (Henceforth "Hall".)

DEFINITION : A *matrix Lie group* is any subgroup G of $\mathsf{GL}(n,\mathbb{C})$ (*i.e.* complex invertible $n \times n$ matrices) such that if A_n is any sequence of matrices in G and A_n converges to some matrix A, then either $A \in G$ or A is noninvertible[36]. Thus, G is a closed subgroup of $\mathsf{GL}(n,\mathbb{C})$.

Perhaps the best way to appreciate the content of this definition is to provide some examples of subgroups of $\mathsf{GL}(n,\mathbb{C})$ which fail to be Lie groups[37]. Consider, for example the group G of all real $n \times n$ invertible matrices with all rational entries. Since the limit of a sequence of rational numbers may be irrational, this group is not a Lie group. Another example: let G be the set of 2×2 matrices of the form $M(\theta) = \mathsf{diag}\{e^{i\theta}, e^{i\theta\sqrt{2}}\}$ with $\theta \in \mathbb{R}$. Clearly the matrix $-1 \notin G$, since $e^{i\theta} = -1$ requires $\theta = (2n+1)\pi$, and since $(2n+1)\sqrt{2}\pi$ is not an odd multiple of π for any n. However, one can easily find a sequence of rationals of the form $(2k+1)/(2n+1)$ with converges to $\sqrt{2}$, so the corresponding sequence of matrices converges to an invertible matrix, -1, which is not in G.

Now let's meet the family:

- *General and special linear groups* : The Lie group $\mathsf{GL}(n,\mathbb{R})$ denotes the group of invertible $n \times n$ matrices A with real entries. It is a manifold of dimension n^2, corresponding to the number of real freedoms associated with a general $n \times n$ matrix[38]. Similarly, $\mathsf{GL}(n,\mathbb{C})$ is the group of invertible $n \times n$ matrices A with complex entries, of real dimension $2n^2$. One can also define the *quaternionic general linear group* $\mathsf{GL}(n,\mathbb{H})$ to be all invertible $n \times n$ matrices A with quaternionic entries. Its dimension is then $4n^2$.

  In each case, we can apply the further restriction that the determinant is $\det A = 1$. This imposes one real constraint on $\mathsf{GL}(n,\mathbb{R})$, resulting in the MLG $\mathsf{SL}(n,\mathbb{R})$, whose real dimension is $\dim \mathsf{SL}(n,\mathbb{R}) = n^2 - 1$. Applied to $\mathsf{GL}(n,\mathbb{C})$, the determinant condition amounts to one complex constraint, hence the real dimension is $\dim \mathsf{SL}(n,\mathbb{C}) = 2(n^2-1)$. For quaternionic matrices, $\det A = 1$ imposes four real constraints, so $\dim \mathsf{SL}(n,\mathbb{H}) = 4(n^2-1)$.

- *Orthogonal and special orthogonal groups* : The orthogonal group $\mathsf{O}(n)$ consists of all matrices $R \in \mathsf{GL}(n,\mathbb{R})$ such that $R^{\mathsf{T}}R = E$, where R^{T} denotes the matrix transpose of R, *i.e.* $R^{\dagger}_{ij} = R_{ji}$. Orthogonal transformations of vectors preserve the inner product $\langle \boldsymbol{x}|\boldsymbol{y}\rangle = \sum_i x_i\, y_i$, *i.e.* $\langle R\boldsymbol{x}|R\boldsymbol{y}\rangle = \langle \boldsymbol{x}|R^{\mathsf{T}}R|\boldsymbol{y}\rangle = \langle \boldsymbol{x}|\boldsymbol{y}\rangle$. Note that this entails $\det R = \pm 1$. Orthogonal matrices with $\det R = +1$ are known as *proper rotations*, while those with $\det R = -1$ are *improper rotations*. This distinction splits the $\mathsf{O}(n)$ into two disconnected components. One cannot continuously move throughout the group manifold of $\mathsf{O}(n)$ between a proper and an improper rotation. The special orthogonal group $\mathsf{SO}(n)$ consists of proper rotations only. Thus $\mathsf{SO}(n) \subset \mathsf{O}(n) \subset \mathsf{GL}(n,\mathbb{R})$.

  We can count the real dimension of $\mathsf{O}(n)$ by the following argument. The condition $R^{\mathsf{T}}R = E$ entails n constraints along the diagonal and $\frac{1}{2}n(n-1)$ constraints above the diagonal[39]. Thus, we have $\frac{1}{2}n(n+1)$ constraints on n^2 real numbers, and we conclude $\dim \mathsf{O}(n) = \dim \mathsf{SO}(n) = \frac{1}{2}n(n-1)$.

[36] Convergence of the matrix sequence $A_n \to A$ means that each matrix element of A_n converges to the corresponding element of A.

[37] Hall, ch. 1.

[38] The invertibility condition does not change the dimension.

[39] Since $R^{\mathsf{T}}R$ is symmetric by construction, there are no new conditions arising from those elements below the diagonal.

- *Generalized orthogonal groups* : The general orthogonal group $\mathsf{O}(n,k)$ is defined to be the subgroup of matrices $L \in \mathsf{GL}(n+k,\mathbb{R})$ such that $L^{\mathsf{T}} I_{n,k} L = I_{n,k}$, where

$$I_{n,k} = \begin{pmatrix} 1_{n\times n} & 0_{n\times k} \\ 0_{k\times n} & -1_{k\times k} \end{pmatrix} \quad . \tag{1.53}$$

This is a generalization of the orthogonality condition, and one which preserves the metric

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = \sum_{i=1}^{n} x_i \, y_i - \sum_{j=n+1}^{n+k} x_j \, y_j \quad . \tag{1.54}$$

One can check that again one has $\det L = \pm 1$ and that $\dim \mathsf{O}(n,k) = \frac{1}{2}(n+k)(n+k-1)$. Perhaps the most famous example is the Lorentz group $\mathrm{O}(3,1)$. Whereas $\mathsf{O}(n)$ and $\mathsf{SO}(n)$ are *compact* Lie groups, $\mathsf{O}(n,k)$ is *noncompact* when $nk \neq 0$.

- *Unitary and special unitary groups* : The unitary group $\mathsf{U}(n)$ consists of all matrices $U \in \mathsf{GL}(n,\mathbb{C})$ such that $U^\dagger U = E$, where $U^\dagger$ denotes the Hermitian conjugate of U, *i.e.* $U^\dagger_{ij} = U^*_{ji}$. Unitary transformations of vectors preserve the complex inner product $\langle \boldsymbol{x} | \boldsymbol{y} \rangle = \sum_i x_i^* \, y_i$, which says that $\langle U\boldsymbol{x} | U\boldsymbol{y} \rangle = \langle \boldsymbol{x} | U^\dagger U | \boldsymbol{y} \rangle = \langle \boldsymbol{x} | \boldsymbol{y} \rangle$. Note that this entails $|\det U| = 1$, *i.e.* $\det U = e^{i\alpha}$ for some $\alpha \in [0, 2\pi)$. The special unitary group $\mathsf{SU}(n)$ consists of those $U \in \mathsf{U}(n)$ with $\det U = 1$. Thus we have $\mathsf{SU}(n) \subset \mathsf{U}(n) \subset \mathsf{GL}(n,\mathbb{C})$.

Let's count the real dimension of $\mathsf{U}(n)$. The matrix $U^\dagger U$ is Hermitian by construction, so once again we total up the constraints associated with its diagonal and off-diagonal elements. Along the diagonal, we have n real constraints. Above the diagonal, we have $\frac{1}{2}n(n-1)$ complex constraints, which is equivalent to $n(n-1)$ real constraints. Thus, we have n^2 real constraints on n^2 complex elements of U, and we conclude that the real dimension of $\mathsf{U}(n)$ is $\dim \mathsf{U}(n) = n^2$. For $\mathsf{SU}(n)$, setting the determinant $\det U = 1$ adds one more real constraint (on the phase of $\det U$), and thus $\dim \mathsf{SU}(n) = n^2 - 1$.

As with the orthogonal groups, we may generalize the unitary groups to

$$\mathsf{U}(n,k) = \left\{ U \in \mathsf{GL}(n,\mathbb{C}) \,|\, U^\dagger I_{n,k} \, U = I_{n,k} \right\} \tag{1.55}$$

where $I_{n,k}$ is as defined in Eqn. 1.53.

- *Symplectic groups*[40] : Here we encounter a bit of an embarrassing mess, because the notation and definition for the different MLGs known as symplectic groups is inconsistent throughout the literature. The first symplectic MLG we shall speak of is $\mathsf{Sp}(2n,\mathbb{R})$, defined to be real matrices $M \in \mathsf{GL}(2n,\mathbb{R})$ which satisfy $M^{\mathsf{T}} J M = J$, where

$$J = \begin{pmatrix} 0_{n\times n} & 1_{n\times n} \\ -1_{n\times n} & 0_{n\times n} \end{pmatrix} \quad . \tag{1.56}$$

[40] Wikipedia tells us that the term "symplectic" was coined by Hermann Weyl in an effort to obviate a previous terminological confusion. It is a *calque* of the word "complex". A calque is a word-for-word or root-for-root translation of an expression imported from another language. The word "superconductor" is a calque from the Dutch *supergeleider*. "Thought experiment" of course calques the German *Gedankenexperiment*. "Rest in peace" calques the Latin *requiescat in pace*. Hilariously, French Canadian "chien chaud" calques English *hot dog*. Prior to Weyl, what we call today the symplectic group $\mathsf{Sp}(2n,\mathbb{R})$ was called the "line complex group". The English word "complex" comes from the Latin *com-plexus*, meaning "together braided". In Greek, this becomes $\sigma\upsilon\mu\pi\lambda\varepsilon\kappa\tau\iota\kappa\omega\varsigma$, or *sym-plektikos*.

Note that $J^2 = -E$. This is again a generalization of the orthogonality condition[41]. In counting the dimension of $\mathsf{Sp}(2n,\mathbb{R})$, note that $M^{\mathsf{T}}JM$ is a real, antisymmetric matrix of rank $2n$. There are then n^2 conditions on the upper right $n \times n$ block, and $\frac{1}{2}n(n-1)$ conditions on the above-diagonal elements in each of the upper left and lower right blocks, for a grand total of $n(2n-1)$ constraints on $4n^2$ elements, hence $\dim \mathsf{Sp}(2n,\mathbb{R}) = n(2n+1)$. At first sight, it might seem that $\det M = \pm 1$, but a nifty identity involving Pfaffians provides an further restriction. The *Pfaffian* of any antisymmetric matrix $B = -B^{\mathsf{T}}$ is defined as

$$\mathsf{Pf}\, B \equiv \frac{1}{2^n\, n!} \sum_{\sigma \in S_{2n}} \mathsf{sgn}(\sigma)\, B_{\sigma(1)\,\sigma(2)}\, B_{\sigma(3)\,\sigma(4)} \cdots B_{\sigma(2n-1)\,\sigma(2n)} \quad . \tag{1.57}$$

One can show that $\det B = (\mathsf{Pf}\, B)^2$. For our purposes, the following identity, which holds for any invertible matrix A, is very useful:

$$\mathsf{Pf}(A^{\mathsf{T}}JA) = (\det A)\,(\mathsf{Pf}\, J) \quad . \tag{1.58}$$

Setting $A = M \in \mathsf{Sp}(2n,\mathbb{R})$, we find $\det M = +1$. This says that symplectic matrices are both volume preserving as well as orientation preserving. Clearly any $M \in \mathsf{Sp}(2n,\mathbb{R})$ preserves the bilinear form $\langle \boldsymbol{x}|J|\boldsymbol{y}\rangle = \sum_{i=1}^{n}(x_i\, y_{i+n} - x_{i+n}\, y_i)$, where $\langle \boldsymbol{x}|\boldsymbol{y}\rangle$ is the usual Euclidean dot product:

$$\langle\, M\boldsymbol{x}\,|\,J\,|\,M\boldsymbol{y}\,\rangle = \langle\, \boldsymbol{x}\,|\,M^{\mathsf{T}}JM\,|\,\boldsymbol{y}\,\rangle = \langle\, \boldsymbol{x}\,|\,J\,|\,\boldsymbol{y}\,\rangle \quad . \tag{1.59}$$

The group $\mathsf{Sp}(2n,\mathbb{R})$ is noncompact. Note that we could reorder the row and column indices by interleaving each group and instead define J to consist of repeating 2×2 blocks $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ along its diagonal, *i.e.* $J_{ij} = +1$ if $(i,j) = (2l-1, 2l)$, and -1 if $(i,j) = (2l, 2l-1)$, and 0 otherwise.

The group $\mathsf{Sp}(2n,\mathbb{C})$ consists of all matrices $Z \in \mathsf{GL}(2n,\mathbb{C})$ satisfying $Z^{\mathsf{T}}JZ = J$. Note that it is still the matrix transpose and not the Hermitian conjugate which appears in the first term. $\mathsf{Sp}(2n,\mathbb{C})$, like $\mathsf{Sp}(2n,\mathbb{R})$, is noncompact. Counting constraints, we have n^2 complex degrees of freedom in the upper right $n \times n$ block of the complex antisymmetric matrix $Z^{\mathsf{T}}JZ$, and $\frac{1}{2}n(n-1)$ complex freedoms above the diagonal in each of the upper left and lower right blocks, for a total of $\mathsf{n}(2n-1)$ complex constraints on $4n^2$ complex entries in Z. Thus, the number of real degrees of freedom in $\mathsf{Sp}(2n,\mathbb{C})$ is $\dim \mathsf{Sp}(2n,\mathbb{C}) = 2n(2n+1)$, which is twice the dimension of $\mathsf{Sp}(2n,\mathbb{R})$.

There is also the group $\mathsf{Sp}(n) = \mathsf{Sp}(2n,\mathbb{C}) \cap \mathsf{U}(2n)$, sometimes denoted $\mathsf{USp}(2n)$[42], because it is isomorphic to the group of unitary symplectic matrices of rank $2n$. One also has $\mathsf{Sp}(n) \cong \mathsf{U}(n,\mathbb{H})$, the quaternionic unitary group of rank n. $\mathsf{Sp}(n)$ is compact and of real dimension $n(2n+1)$.

Finally, consider the group $\mathsf{G}(2n)$ defined by

$$\mathsf{G}(2n) = \left\{ M \in \mathsf{GL}(n,\mathbb{C}) \,|\, M^{\dagger}JM = J \right\} \quad , \tag{1.60}$$

[41] The notion of symplectic structure is strongly associated with Hamiltonian mechanics, where phase space is even-dimensional, consisting of n coordinates q_σ and n conjugate momenta p_σ. Defining the rank $2n$ vector $\boldsymbol{\xi}^{\mathsf{T}} = (\boldsymbol{q}^{\mathsf{T}}, \boldsymbol{p}^{\mathsf{T}})$, the equations of motion are $\dot{\xi}_j = J_{ij}\, \partial H/\partial \xi_j$. A canonical transformation to a new set of generalized coordinates and momenta $\boldsymbol{\Xi}$ must preserve this form of the equations of motion, which means that it must preserve the Poisson bracket $\{A,B\}_\xi = \sum_{i,j} J_{ij}(\partial A/\partial\xi_i)(\partial B/\partial\xi_j)$. Requiring $\{A,B\}_\xi = \{A,B\}_\Xi$ then entails $M^{\mathsf{T}}JM = J$, where $M_{ai} = \partial\Xi_a/\partial\xi_i$ is the Jacobian of the transformation.

[42] Note that if G and H are both Lie groups, then their intersection $G \cap H$ is also a Lie group.

which is the group of *conjugate symplectic matrices* of rank $2n$. If we define the unitary matrix

$$V \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1_{n\times n} & 1_{n\times n} \\ i1_{n\times n} & -i1_{n\times n} \end{pmatrix} \quad , \tag{1.61}$$

then we have that $V^\dagger J V = iI_{n,n}$. Thus, defining $\widetilde{M} = V^\dagger M V$, we have

$$\widetilde{M}^\dagger I_{n,n}\,\widetilde{M} = V^\dagger M^\dagger \big(V I_{n,n} V^\dagger\big) M V = V^\dagger M^\dagger \big(-iJ\big) M V = -iV^\dagger J V = I_{n,n} \quad , \tag{1.62}$$

which says that $\widetilde{M} \in \mathsf{U}(n,n)$. Thus we have that $\mathsf{G}(2n) \cong \mathsf{U}(n,n)$.

Again, do not be surprised if in the literature you find different notation. Sometimes $\mathsf{Sp}(2n,\mathbb{R})$ is abbreviated as $\mathsf{Sp}(2n)$, and sometimes even as $\mathsf{Sp}(n)$.

- *Euclidean and Poincaré groups* : The Euclidean group $\mathsf{E}(n)$ in n dimensions is the group of all bijective, distance-preserving automorphisms[43] of $\mathbb{R}^n$. It can be shown that any element $T \in \mathsf{E}(n)$ can be expressed as a rotation (proper or improper) followed by a translation. Thus each such T may be represented as a rank $n+1$ real matrix,

$$T \equiv (\boldsymbol{d}, R) = \begin{pmatrix} R & \boldsymbol{d} \\ \mathbf{0} & 1 \end{pmatrix} \quad , \tag{1.63}$$

where $R \in \mathsf{O}(n)$, $\boldsymbol{d} \in \mathbb{R}^n$ is an n-component column vector, and $\mathbf{0} = (0\,,\,\ldots\,,\,0)$ is an n-component row vector. Clearly $\dim \mathsf{E}(n) = \dim \mathsf{O}(n) + \dim \mathbb{R}^n = \frac{1}{2}n(n+1)$. Acting on the vector $\boldsymbol{v} \in \mathbb{R}^{n+1}$ whose transpose is $\boldsymbol{v}^{\mathsf{T}} = (x_1, \ldots, x_n, 1)$, one has

$$T\boldsymbol{v} = \begin{pmatrix} R & \boldsymbol{d} \\ \mathbf{0} & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{x} \\ 1 \end{pmatrix} = \begin{pmatrix} R\boldsymbol{x} + \boldsymbol{d} \\ 1 \end{pmatrix} \quad , \tag{1.64}$$

Note that

$$T^{-1} = \begin{pmatrix} R^{-1} & -R^{-1}\boldsymbol{d} \\ \mathbf{0} & 1 \end{pmatrix} = (-R^{-1}\boldsymbol{d}, R^{-1}) \quad . \tag{1.65}$$

The group multiplication rule is

$$(\boldsymbol{d}_2, R_2)(\boldsymbol{d}_1, R_1) = \begin{pmatrix} R_2 & \boldsymbol{d}_2 \\ \mathbf{0} & 1 \end{pmatrix} \begin{pmatrix} R_1 & \boldsymbol{d}_1 \\ \mathbf{0} & 1 \end{pmatrix} = \begin{pmatrix} R_2 R_1 & R_2\boldsymbol{d}_1 + \boldsymbol{d}_2 \\ \mathbf{0} & 1 \end{pmatrix} = (\boldsymbol{d}_2 + R_2\,\boldsymbol{d}_1, R_2\,R_1) \quad . \tag{1.66}$$

Note that $\mathsf{E}(n)$ is not simply a direct product of the orthogonal group $\mathsf{O}(n)$ and the group of translations $\mathbb{R}^n$ (under addition), because $(\boldsymbol{d}_2\,, R_2)(\boldsymbol{d}_1\,, R_1) \neq (\boldsymbol{d}_1 + \boldsymbol{d}_2, R_2\,R_1)$. Rather, we write $\mathsf{E}(n) = \mathbb{R}^n \rtimes \mathsf{O}(n)$, which says that the Euclidean group is a *semidirect product* of $\mathbb{R}^n$ and $\mathsf{O}(n)$ (see §1.5.3 below). Note that $\mathbb{R}^n \lhd \mathsf{E}(n)$, *i.e.* $\mathbb{R}^n$ is a normal subgroup, but $\mathsf{O}(n)$ is *not* a normal subgroup of $\mathsf{E}(n)$.

To define the Poincaré group $\mathsf{P}(n,1)$, simply increase the dimension to add a 'time' coordinate. A general element of $\mathsf{P}(n,1)$ is written

$$(\boldsymbol{d}, L) = \begin{pmatrix} L & \boldsymbol{d} \\ \mathbf{0} & 1 \end{pmatrix} \quad , \tag{1.67}$$

[43] An *endomorphism* is a map from a set to itself. An invertible endomorphism is called an automorphism.

where $L \in \mathsf{O}(n,1)$ and $\boldsymbol{d} \in \mathbb{R}^{n+1}$. The multiplication law is the same as that for $\mathsf{E}(n)$, and the Poincaré group also has a semidirect product structure: $\mathsf{P}(n,1) = \mathbb{R}^{n+1} \rtimes \mathsf{O}(n,1)$. Accordingly, $\dim \mathsf{P}(n,1) = \frac{1}{2}(n+1)(n+2)$.

- *Less common cases* : One can define the *complex orthogonal group* $\mathsf{O}(n,\mathbb{C})$ as the set of matrices $W \in \mathsf{GL}(n,\mathbb{C})$ such that $W^{\mathsf{T}}W = E$. This rarely arises in physical settings. Clearly $\det W = \pm 1$, and $\dim \mathsf{O}(n,\mathbb{C}) = n(n-1)$. One can then restrict $\mathsf{SO}(n,\mathbb{C})$ to those $W \in \mathsf{O}(n,\mathbb{C})$ with determinant one, with no further reduction in dimension. Personally I am not so sure that $\mathsf{O}(n,\mathbb{C})$ should be counted as part of our big happy family of matrix Lie groups. He's more like your weird hairy uncle who lives in your grandparents' basement apartment. We might include him, but only for tax purposes[44].

  The subset of all matrices $A \in \mathsf{GL}(n,\mathbb{R})$ with $A_{ij} = 0$ whenever $i > j$ is an abelian Lie group consisting of all real $n \times n$ upper triangular matrices. It is a good exercise to show how the inverse of any given element may be constructed. The *unitriangular group* $\mathsf{UT}(n,\mathbb{R})$ is defined to be the subgroup of $\mathsf{GL}(n,\mathbb{R})$ consisting of all matrices A for which $A_{ij} = 0$ whenever $i > j$ and $A_{ii} = 1$. That is, all the elements below the diagonal are 0, all the elements along the diagonal are 1, and all the elements above the diagonal are arbitrary real numbers.

1.5.3 More on semidirect products

Given a group G with a subgroup H and a normal subgroup $N \lhd G$, then $G = N \rtimes H$ if and only if $G = NH$ where $N \cap H = \{E\}$. This last condition is equivalent to requiring that for any $g \in G$, there exist unique $h \in H$ and $n \in N$ such that $g = nh$.[45] This may be taken as a definition of the semidirect product. Although this subsection is located within the material on Lie groups, the notion of semidirect product applies equally well to discrete groups. One can even form the semidirect product of a continuous group with a discrete group.

More generally, though, let G and K be groups, and let $\varphi : K \times G \to K$ with $(k,g) \to \varphi_g(k)$. The semidirect product $K \rtimes G$ with respect to φ is defined to be the set of elements (k,g) with $k \in K$ and $g \in G$ subject to the multiplication law

$$(k_2, g_2)\,(k_1, g_1) = \big(k_2\,\varphi_{g_2}(k_1)\,,\; g_2\,g_1\big) \quad . \tag{1.68}$$

One then has that $K \rtimes G$ satisfies the group axioms provided

$$\varphi_g(kk') = \varphi_g(k)\,\varphi_g(k') \qquad \text{and} \qquad \varphi_g\big(\varphi_{g'}(k)\big) = \varphi_{gg'}(k) \quad , \tag{1.69}$$

which are required for associativity of multiplication in $K \rtimes G$. Please note that there are *three* group multiplication laws in play here: (i) multiplication in G (*i.e.* gg'), (ii) multiplication in K (*i.e.* kk'), and (iii) multiplication in $K \rtimes G$ (*i.e.* Eqn. 1.69). Note also that $\varphi_g(k)\,\varphi_{g'}(k')$ is the K-product of two elements of K, *i.e.* $\varphi_g(k)$ and $\varphi_{g'}(k')$. In our example of $\mathsf{E}(n) = \mathbb{R}^n \rtimes \mathsf{O}(n)$, group multiplication in $K = \mathbb{R}^n$ is vector addition, group multiplication in $G = \mathsf{O}(n)$ is matrix multiplication, and the map φ is matrix-vector multiplication.

[44] $\mathsf{O}(n,\mathbb{C})$ is very different from $\mathsf{SU}(n)$. For starters, $\mathsf{O}(n,\mathbb{C})$ is not compact.

[45] Or that $g = hn$, for that matter – but generally with different h and n, than in the decomposition $g = nh$, of course!

Consider the semidirect product $G \equiv \mathbb{Z}_n \rtimes \mathbb{Z}_2$ where $\mathbb{Z}_n \cong \{E, r, \ldots, r^{n-1}\}$ with $r^n = E$ and $\mathbb{Z}_2 \cong \{E, \sigma\}$ with $\sigma^2 = E$. Now let $\varphi_\sigma(r^\ell) = \sigma r^\ell \sigma$ act by conjugation[46]. To completely define φ, we must specify the image of $\varphi_\sigma(r^\ell) = \sigma r^\ell \sigma$ in $\mathbb{Z}_n$ for each ℓ, and we choose $\sigma r^\ell \sigma = r^{n-\ell} = r^{-\ell}$. Now I claim that $G \cong D_n$, where the group isomorphism $\psi\, G \to D_n$ maps $(r^\ell, E) \in G$ to $r^\ell \in D_n$, and $(r^\ell, \sigma) \in G$ to $r^\ell \sigma \in D_n$. Thus, the semidirect product of two abelian groups may be nonabelian, depending on the features of the mapping φ.

1.5.4 Topology of the happy family

You already know that compact means "closed and bounded" in the context of subsets of $\mathbb{R}^n$, for example. The same criteria may be applied to matrix groups. A matrix Lie group G is compact if the following two conditions hold:

- If $A_n \in G$ is a sequence in G which converges to some matrix A, then $A \in G$.
- There exists a positive real number C such that, for any $A \in G$, $|A_{ij}| < C$ for all i, j.

The first condition says G is closed, and the second condition says it is bounded.

Two other terms that pop up in describing continuous spaces are *connected* and *simply connected*. A connected manifold is one where any two points may be joined by a continuous curve[47]. Any disconnected Lie group G may be uniquely decomposed into a union of its *components*. The component which contains the identity (there can be only one) is then a subgroup of G. The group $\mathsf{O}(n)$ is not connected, because there is no continuous path in the space of orthogonal matrices which connects a proper rotation and an improper rotation. Nor is $\mathsf{GL}(1, \mathbb{R})$, *i.e.* the group of nonzero real numbers under multiplication, because the two components $\mathbb{R}_+$ and $\mathbb{R}_-$ cannot be connected by a continuous path which goes not go through zero. Thus, $\mathsf{GL}(1, \mathbb{R})$ has two *components*, as does $\mathsf{O}(n)$. For the same reason, $\mathsf{GL}(n, \mathbb{R})$ is also disconnected and breaks up into components with positive and negative determinant. If $A(t)$ with $t \in [0, 1]$ is a smooth path in the space of $n \times n$ real matrices with $\det A(0) > 0$ and $\det A(1) < 0$, then by the intermediate value theorem there must be a $t^* \in [0, 1]$ for which $\det A(t^*) = 0$, which means $A(t^*) \notin \mathsf{GL}(n, \mathbb{R})$. Note that $\mathsf{GL}(n, \mathbb{C})$ is connected for all n, because the determinant is complex, and we can always choose a path connecting any two complex matrixes $A(0)$ and $A(1)$ which "goes around" the the set of matrices with $\det A = 0$.

A simply connected manifold is one where every closed curve can be continuously contracted to a point. The 2-sphere S^2 and the 2-torus T^2 are both connected, but S^2 is simply connected whereas T^2 is not, since a closed path which has net winding around either (or both) of the toroidal cycles cannot be continuously contracted to a point. The group of unimodular complex numbers under multiplication, $\mathsf{U}(1)$, is isomorphic to a circle S^1, with the identification of $z = e^{i\theta}$. Thus, it is the same group as the real numbers modulo 1 under addition. Clearly the MLG $\mathsf{U}(1)$ is connected, but it is not simply connected, since the path $z(t) = e^{2\pi i n t}$ for $t \in [0, 1]$ winds n times around the circle and is non-contractable.

[46] Note that $\sigma^{-1} = \sigma$.

[47] Topologists call this property *path connectedness* as opposed to connectedness *per se*, which is a somewhat weaker condition. But it turns out that a matrix Lie group is connected if and only if it is path connected.

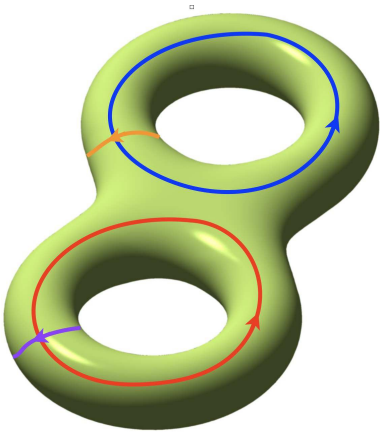


Figure 1.4: The double torus, with fundamental group generators a_1 (blue), b_1 (orange), a_2 (red), and b_2 (purple).

Continuous deformation of closed loops on any manifold $\mathcal{M}$ allows us to define equivalence classes of loops. Two loops are in the same equivalence class if they can be smoothly deformed into one another. These loop equivalence classes themselves form a group, where the group operation is defined by attaching loops to each other. The inverse of a given loop is that same loop executed in reverse. This group of loop equivalence classes is called the *fundamental group* (or *first homotopy group*) of the manifold, and is denoted $\pi_1(\mathcal{M})$. If $\mathcal{M}$ is simply connected, $\pi_1(\mathcal{M})$ is trivial. Else $\pi_1(\mathcal{M})$ may be either abelian or nonabelian. Clearly $\pi_1(S^1) \cong \mathbb{Z}$, as closed loops on the circle may be classified by their winding number, and paths of different winding number cannot be continuously deformed into one another. One has $\pi_1(T^2) \cong \mathbb{Z} \times \mathbb{Z}$, but the fundamental group of the *double torus*, which is to say a torus with an extra handle[48] (see Fig. 1.4), is an infinite nonabelian group with the presentation

$$\left\langle\, a_1, b_1, a_2, b_2 \,\middle|\, a_1\, b_1\, a_1^{-1}\, b_1^{-1}\, a_2\, b_2\, a_2^{-1}\, b_2^{-1} \,\right\rangle \quad . \tag{1.70}$$

One sometimes sees the notation $\pi_0(\mathcal{M})$, apparently denoting the "zeroth homotopy group" of $\mathcal{M}$. This is a misnomer, since $\pi_0(\mathcal{M})$ is not a group, but rather a set, corresponding to the connected components of $\mathcal{M}$. The order of this set is the number of connected components, and it is convenient to simply define $\pi_0(\mathcal{M})$ to be this number. Thus $\pi_0\big(\mathsf{O}(n)\big) = 2$, corresponding to the proper and improper rotations. Tab. 1.7 summarizes the topological properties of our happy family of matrix Lie groups[49].

Finally, consider the familiar case of $\mathsf{SO}(3)$, which consists of rotations in three dimensional Euclidean space by an angle ξ about an axis $\hat{\boldsymbol{n}} \in S^2$. Thus, each pair $(\xi, \hat{\boldsymbol{n}})$ labels an element $g(\xi, \hat{\boldsymbol{n}}) \in \mathsf{SO}(3)$. If we let $\xi \in [0, 2\pi)$, then we have $g(2\pi - \xi, -\hat{\boldsymbol{n}}) = g(\xi, \hat{\boldsymbol{n}})$, which means that points in the group manifold with $(\xi', \hat{\boldsymbol{n}}') = (2\pi - \xi, -\hat{\boldsymbol{n}})$ are *identified*. Now we might as well do away with all values of ξ greater than π, since they are all redundant labels, and take $\xi \in [0, \pi]$. The group manifold of $\mathsf{SO}(3)$ is then a solid sphere in $\mathbb{R}^3$ of radius π, with the following important distinction: antipodal points on the boundary are identified: $g(\pi, \hat{\boldsymbol{n}}) = g(\pi, -\hat{\boldsymbol{n}})$. This means that $\mathsf{SO}(3)$ is not simply connected, as shown in Fig.. 1.5.

[48] The double torus is a Riemann surface of genus $g = 2$. It resembles some sort of exotic breakfast pastry.

[49] A topologist, it is said, is someone who is unable to distinguish between a donut and a coffee cup.

G	compact?	$\pi_0(G)$	$\pi_1(G)$	G	compact?	$\pi_0(G)$	$\pi_1(G)$
$\mathsf{GL}(n,\mathbb{R})$	no	2	–	$\mathsf{GL}(n,\mathbb{C})$	no	1	$\mathbb{Z}$
$\mathsf{Sp}(2n,\mathbb{R})$	no	1	$\mathbb{Z}$	$\mathsf{Sp}(2n,\mathbb{C})$	no	2	–
$\mathsf{SL}(n,\mathbb{R})$ $(n\geq 3)$	no	1	$\mathbb{Z}_2$	$\mathsf{SL}(n,\mathbb{C})$	no	1	$\{1\}$
$\mathsf{SL}(2,\mathbb{R})$	no	1	$\mathbb{Z}$	$\mathsf{SO}(2)$	yes	1	$\mathbb{Z}$
$\mathsf{O}(n)$	yes	2	–	$\mathsf{SO}(n)$ $(n\geq 3)$	yes	1	$\mathbb{Z}_2$
$\mathsf{U}(n)$	yes	1	$\mathbb{Z}$	$\mathsf{SU}(n)$	yes	1	$\{1\}$
$\mathsf{Sp}(n)$	yes	1	$\{1\}$	$\mathsf{UT}(n,\mathbb{R})$	yes	1	$\{1\}$
$\mathsf{SO}(n,1)$	no	2	–	$\mathsf{O}(n,1)$	no	4	–
$\mathsf{E}(n)$	no	2	–	$\mathsf{P}(n,1)$	no	4	–

Table 1.7: Topological properties of matrix Lie groups.

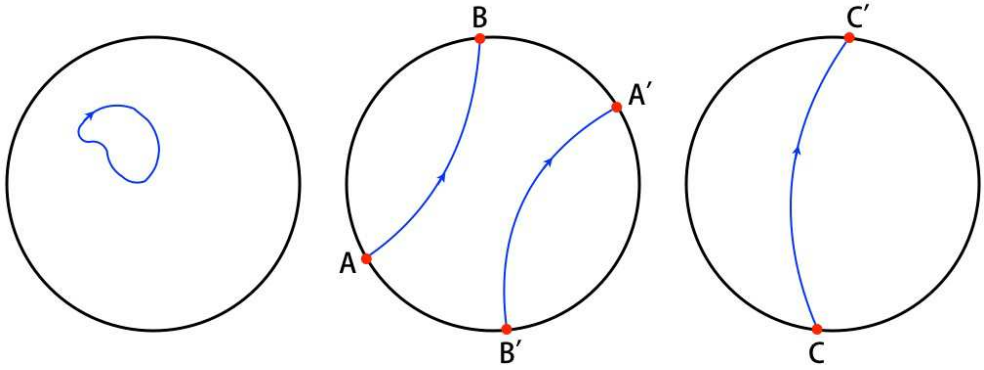


Figure 1.5: The fundamental group of $\mathsf{SO}(3)$ is $\mathbb{Z}_2$. Left: a contractible loop. Center: another contractible loop. Points A and A′ are identified, as are B and B′. If B is moved toward A along the boundary, then B′ moves toward A′. Right: a noncontractible loop. Points C and C′ are identified, and the blue path connecting them is a non-contractable loop. In all cases, the black sphere corresponds to group elements with $\xi = \pi$ and different values of $\hat{\boldsymbol{n}}$.

1.5.5 Matrix exponentials and the Lie algebra

Another mathy definition:

> DEFINITION : The *Lie algebra* $\mathfrak{g}$ of a matrix Lie group G is the set of all matrices X such that $\exp(tX) \in G$ for all $t \in \mathbb{R}$. Alternatively, $\mathfrak{g}$ is the *tangent space* to G at its identity E, *i.e.* the set of derivatives of all smooth curves in G passing through E.

I'm assuming you all know that the matrix exponential $\exp(X)$ is defined through its Taylor series, which is convergent for any real or complex matrix X. You should also know that for any matrix function $f(A)$ with a convergent power series expansion, one has

$$C^{-1} f\big(A\big)\, C = f\big(C^{-1} A\, C\big) \quad , \quad \big[f(A)\big]^{\mathsf{T}} = f\big(A^{\mathsf{T}}\big) \quad , \quad \big[f(A)\big]^{*} = f^{*}\big(A^{*}\big) \quad , \tag{1.71}$$

where $f^*(X)$ is defined by the same power series as $f(X)$, after complex conjugation of all the coefficients. In particular, the above are all true for $f(X) = \exp(X)$. Another handy True Fact is that for any nonsingular matrix A, $\ln \det A = \mathsf{Tr} \ln A$.

Warning! Physicists generally define the Lie algebra $\mathfrak{g}$ of G from the map $X \to \exp(-itX)$ rather than $X \to \exp(tX)$. We will hold by the math convention for now.

We now state three Important Facts about matrix Lie algebras:

(i) If $X, Y \in \mathfrak{g}$ then $\alpha X + \beta Y \in \mathfrak{g}$ where α and β are scalars in some field $\mathbb{F}$.

(ii) If $X, Y \in \mathfrak{g}$ then $[X, Y] = XY - YX \in \mathfrak{g}$.

(iii) The Jacobi identity holds for all $X, Y, Z \in \mathfrak{g}$:

$$\big[X, [Y, Z]\big] + \big[Y, [Z, X]\big] + \big[Z, [X, Y]\big] = 0 \quad . \tag{1.72}$$

We won't prove any of these[50]. The first says that $\mathfrak{g}$ is a vector space over the field $\mathbb{F}$. The second introduces the *Lie bracket* $[\bullet, \bullet]$, known to us physicists as the commutator, and says that $\mathfrak{g}$ is closed under the bracket. The third follows from the definition of the Lie bracket[51].

To provide some motivation to the second Important Fact, consider the product $e^X\, e^Y$ using Dynkin's expression of the Baker-Campbell-Hausdorff (BCH) formula[52],

$$\ln\left(e^X\, e^Y\right) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \sum_{\substack{r_1, s_1 \\ r_1 + s_1 > 0}} \cdots \sum_{\substack{r_n, s_n \\ r_n + s_n > 0}} \frac{\big[X^{r_1} Y^{s_1} X^{r_2} Y^{s_2} \cdots X^{r_n} Y^{s_n}\big]}{\sum_{i=1}^{n} (r_i + s_i) \cdot \prod_{j=1}^{n} r_j!\, s_j!} \quad , \tag{1.73}$$

where

$$\big[X^{r_1} Y^{s_1} X^{r_2} Y^{s_2} \cdots X^{r_n} Y^{s_n}\big] = \underbrace{[X, [X, \cdots [X}_{r_1}, \underbrace{[Y, [Y, \cdots [Y}_{s_1}, \cdots \underbrace{[X, [X, \cdots [X}_{r_n}, \underbrace{[Y, [Y, \cdots [Y}_{s_n}]] \cdots]] \quad . \tag{1.74}$$

Thus,

$$\exp(X)\, \exp(Y) = \exp\Big(X + Y + \tfrac{1}{2}\big[X, Y\big] + \tfrac{1}{12}\big[X, \big[X, Y\big]\big] + \tfrac{1}{12}\big[Y, \big[Y, X\big]\big] + \ldots\Big) \quad . \tag{1.75}$$

Notice that every term inside the round bracket on the RHS, other than $X + Y$, is formed from nested commutators. Thus if $[X, Y] \in \mathfrak{g}$ for all $X, Y \in \mathfrak{g}$, then the product $e^X\, e^Y = e^Z$ with $Z \in \mathfrak{g}$.

[50] See Hall §3.3 for the proofs.

[51] The formal definition of a finite-dimensional real/complex Lie algebra is a finite-dimensional real/complex vector space $\mathfrak{g}$ together with a map $[\bullet, \bullet]$ from $\mathfrak{g} \times \mathfrak{g}$ into $\mathfrak{g}$ called the *Lie bracket*, such that (i) $[\bullet, \bullet]$ is bilinear, (ii) $[X, Y] = -[Y, X]$ for all $X, Y \in \mathfrak{g}$, and (iii) $\big[X, [Y, Z]\big] + \big[Y, [Z, X]\big] + \big[Z, [X, Y]\big]$ for all $X, Y, Z \in \mathfrak{g}$. For Lie algebras of matrix Lie groups, the Lie bracket is the commutator.

[52] See https://en.wikipedia.org/wiki/Baker-Campbell-Hausdorff_formula.

Why should we care about Lie algebras?

Why are we interested in Lie algebras to begin with? Aren't their corresponding Lie groups enough? One reason is that Lie algebras describe the *infinitesimal form* of continuous symmetries[53]. A Lie algebra $\mathfrak{g}$ is the *linearization* of a Lie group G. In this sense, Lie algebras are *much simpler* than Lie groups because they describe only the latter's tangent space in the vicinity of its identity. Mathematically, Lie groups are homogeneous structures in which any given point *locally* "looks like" any other point: if g is in the neighborhood of g_0, then $h \equiv g g_0^{-1} h_0$ is in the neighborhood of h_0[54]. Thus, from an understanding of $\mathfrak{g}$, we can deduce *almost* all the properties of G itself[55]. The inverse of linearization, which takes us from $\mathfrak{g}$ to G, is the exponential map. Since algebras are vector spaces, we may apply in the study of Lie algebras many of the powerful tools of linear algebra, such as basis vectors and inner products. For two infinitesimal group operations $g = e^{\epsilon X}$ and $h = e^{\epsilon Y}$, their product is $gh = e^{\epsilon(X+Y)+\mathcal{O}(\epsilon^2)}$. Thus, group composition of two elements in the vicinity of the identity corresponds to simple vector addition in the Lie algebra! However, when we evaluate the group commutator $\langle g, h\rangle = g^{-1}h^{-1}gh$, we find that the $\mathcal{O}(\epsilon)$ term vanishes, and

$$e^{-\epsilon X} e^{-\epsilon Y} e^{\epsilon X} e^{\epsilon Y} = \exp\left(\epsilon^2 [X, Y] + \mathcal{O}(\epsilon^3)\right) \quad . \tag{1.76}$$

Thus consideration of the infinitesimal group commutator $\langle \bullet, \bullet \rangle$ requires the introduction of additional structure in the linear vector space of $\mathfrak{g}$, *i.e.* the notion of the Lie bracket.

Some concrete examples of Lie algebras

$\mathsf{GL}(n, \mathbb{R})$: The Lie algebra $\mathsf{gl}(n, \mathbb{R})$ is the set of all real $n \times n$ matrices. Similarly, $\mathsf{gl}(n, \mathbb{C})$ is the set of all complex $n \times n$ matrices.

$\mathsf{SL}(n, \mathbb{R})$: Adding the determinant condition puts a restriction on $\mathsf{sl}(n, \mathbb{R})$, namely that $\det \exp(tX) = 1$. Taking the logarithm, we obtain the condition $\mathsf{Tr}\, X = 0$. Hence $\mathsf{sl}(n, \mathbb{R})$ is the set of all real traceless $n \times n$ matrices. And of course $\mathsf{sl}(n, \mathbb{C})$ is the set of all complex traceless $n \times n$ matrices.

$\mathsf{O}(n)$: Now we demand $\exp(tX^{\mathsf{T}})\, \exp(tX) = E$, hence $\exp(tX^{\mathsf{T}}) = \exp(-tX)$. Taking the logarithm, we obtain $X^{\mathsf{T}} = -X$. Thus, $\mathsf{o}(n)$ is the set of all real antisymmetric $n \times n$ matrices. This is easy!

$\mathsf{U}(n)$: *Mutatis mutandis*, $\mathsf{u}(n)$ consists of the set of complex antihermitian $n \times n$ matrices, *i.e.* matrices A for which $A_{ji} = -A^*_{ij}$.

$\mathsf{Sp}(2n, \mathbb{R})$: We require $\exp(tX^{\mathsf{T}})\, J \exp(tX) = J$. Multiplying on the right by $-\exp(-tX)\, J$, we obtain $\exp(tX^{\mathsf{T}}) = -J \exp(-tX) J = \exp(tJXJ)$, since $J^{-1} = -J$. Thus, we arrive at the condition $X^{\mathsf{T}} = JXJ$ for any real $n \times n$ matrix $X \in \mathsf{sp}(2n, \mathbb{R})$. It is straightforward to show that this means X is of the form

$$X = \begin{pmatrix} A & B \\ C & -A^{\mathsf{T}} \end{pmatrix} \quad , \tag{1.77}$$

[53] In physics, much useful information is deduced from the consideration of infinitesimal continuous symmetries. For example, the existence of conserved currents via Noether's theorem.

[54] For this reason, the properties of the neighborhood of any point in G are reduced to a study of the properties of the neighborhood of E, which is to say the Lie algebra $\mathfrak{g}$ of G.

[55] One obvious thing we can't infer from $\mathfrak{g}$ is whether G has any disconnected parts. The Lie algebras corresponding to $\mathsf{O}(n)$ and $\mathsf{SO}(n)$ are both $\mathsf{o}(n)$.

where A is an arbitrary $n \times n$ matrix, and $B = B^{\mathsf{T}}$ and $C = C^{\mathsf{T}}$ are arbitrary symmetric $n \times n$ matrices. The same conditions hold for any complex $n \times n$ matrix $X \in \mathsf{sp}(2n, \mathbb{C})$. Finally, we may conclude $\mathsf{sp}(n) = \mathsf{sp}(2n, \mathbb{C}) \cap \mathsf{u}(2n)$.

1.5.6 Structure constants

We noted above that the Lie algebra $\mathfrak{g}$ of a matrix Lie group G is the set of all smooth curves in G passing through the identity E. Consider, for example, the group $\mathsf{SL}(2, \mathbb{R})$, which is of real dimension three. In the vicinity of the identity, we can write

$$g(x^1, x^2, x^3) = \begin{pmatrix} 1 + x^1 & x^2 \\ x^3 & \frac{1+x^2x^3}{1+x^1} \end{pmatrix} \quad . \tag{1.78}$$

One can check by inspection that $\det g(x^1, x^2, x^3) = 1$ and that $g(0, 0, 0) = E$. Now expand in the three local coordinates $\{x^1, x^2, x^3\}$:

$$\begin{aligned} g(x^1, x^2, x^3) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} x^1 + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} x^2 + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} x^3 + \mathcal{O}(x^2) \\ &\equiv E + \sum_{a=1}^{3} x^a \, X_a + \mathcal{O}(x^2) \quad , \end{aligned} \tag{1.79}$$

where

$$X_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad X_2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad , \quad X_3 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{1.80}$$

are a set of *generators* for the Lie algebra $\mathsf{sl}(2, \mathbb{R})$ which may be taken as *basis vectors* in the vector space of that algebra. Note in general that if $\{X_a\}$ are taken as a set of basis vectors for some Lie algebra $\mathfrak{g}$ that we may write $\exp(x^a X_a) \exp(y^a X_a) = \exp(z^a X_a)$, where $z = z(x, y)$, which follows from Dynkin's version of BCH.

Can we reconstruct the Lie group G from its Lie algebra $\mathfrak{g}$? Not always. By employing exponentiation, we can form the group consisting of all matrices of the form $\exp(x^a X_a)$ (note summation convention here). For $\mathsf{sl}(n, \mathbb{R})$, there are a total of $n^2 - 1$ generators, and via exponentiation we can indeed reconstruct all of $\mathsf{SL}(n, \mathbb{R})$. But suppose we try to do this with $\mathsf{o}(n)$ and $\mathsf{O}(n)$. In that case the generators are a $\frac{1}{2}n(n-1)$ element basis of real traceless antisymmetric matrices, hence $\det \exp(x^a X_a) = 1$, and we are missing the improper rotations. So via exponentiation, we can in general only reconstruct from $\mathfrak{g}$ alone the component of G which contains the identity E.

Since each Lie algebra $\mathfrak{g}$ is closed under the action of the Lie bracket (commutation), the generators X_a must satisfy

$$\big[X_a, X_b\big] = {C_{ab}}^c \, X_c \quad , \tag{1.81}$$

for some sets of numbers ${C_{ab}}^c$, which are called the *structure constants* of the Lie algebra. Note that ${C_{ab}}^c = -{C_{ba}}^c$ owing to the antisymmetry of the Lie bracket. Taking, for example, the three generators of $\mathsf{sl}(2, \mathbb{R})$ from Eqn. 1.80, one finds $\big[X_1, X_2\big] = 2X_2$, $\big[X_1, X_3\big] = -2X_3$, and $\big[X_2, X_3\big] = X_1$. Thus ${C_{12}}^2 = -{C_{21}}^2 = 2$, ${C_{13}}^3 = -{C_{31}}^3 = -2$, and ${C_{23}}^1 = -{C_{32}}^1 = 1$, with all other $C_c^{ab} = 0$. Again, in the

physics literature one generally finds this written as $\big[T^a, T^b\big] = i f_{ab}{}^c\, T^c$ for the generators $\{T^a\}$, where $X_a = -iT^a$ and $f_{ab}{}^c = C_{ab}{}^c$.

Since $\mathfrak{g}$ is a vector space, any complete and linearly independent set of generators will do. For example, we could have chosen

$$X_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad X_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad X_3 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad , \tag{1.82}$$

in which case one finds the nonzero structure constants $C_{12}{}^3 = 2$, $C_{13}{}^2 = -2$, and $C_{32}{}^1 = -2$. In addition, we could have multiplied each of the generators by an arbitrary nonzero scale factor, with corresponding consequences for the $C_{ab}{}^c$. One way to mitigate this ambiguity is to choose a normalization condition for the generators, such as

$$\mathsf{Tr}\big(X_a X_b\big) = \lambda_a\, \delta^{ab} \quad \text{(no sum)} \quad . \tag{1.83}$$

If the Lie algebra is *semisimple*, one can further restrict $|\lambda_a| = 1$ for all a, but we cannot change the sign of any of the λ_a.

One last tidbit: As a consequence of the Jacobi identity, the structure constants obey the relation

$$C_{bc}{}^d\, C_{da}{}^e + C_{ab}{}^d\, C_{dc}{}^e + C_{ca}{}^d\, C_{db}{}^e = 0 \quad . \tag{1.84}$$

Thus, if we define the matrices $X_{ab}{}^c \equiv -C_{ab}{}^c$, Eqn. 1.84 may be written as

$$-\,X_{bc}{}^d\, X_{ad}{}^e - C_{ab}{}^d\, X_{dc}{}^e + X_{ac}{}^d\, X_{bd}{}^e = 0 \quad , \tag{1.85}$$

which says $\big[X_a, X_b\big]_{ce} = C_{ab}{}^d\, \big(X_d\big)_{ce}$, *i.e.* $\big[X_a, X_b\big] = C_{ab}{}^c\, X_c$. In other words, the structure constants themselves generate a representation of the algebra, called the *adjoint representation*. For example, if we choose the structure constants computed from Eqn. 1.82, we obtain the 3×3 representation

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2 \\ 0 & 2 & 0 \end{pmatrix} \quad , \quad X_2 = \begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 0 \end{pmatrix} \quad , \quad X_3 = \begin{pmatrix} 0 & -2 & 0 \\ -2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{1.86}$$

One can then check $\big[X_a, X_b\big] = C_{ab}{}^c\, X_c$.

1.6 Appendix : Ideal Bose Gas Condensation

We begin with the grand canonical Hamiltonian $K = H - \mu N$ for the ideal Bose gas,

$$K = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu)\, b^\dagger_{\boldsymbol{k}} b_{\boldsymbol{k}} - \sqrt{N} \sum_{\boldsymbol{k}} \left(\nu_{\boldsymbol{k}}\, b^\dagger_{\boldsymbol{k}} + \bar\nu_{\boldsymbol{k}}\, b_{\boldsymbol{k}} \right) \quad . \tag{1.87}$$

Here $b^\dagger_{\boldsymbol{k}}$ is the creation operator for a boson in a state of wavevector $\boldsymbol{k}$, hence $\big[b_{\boldsymbol{k}}\,,\, b^\dagger_{\boldsymbol{k}'}\big] = \delta_{\boldsymbol{k}\boldsymbol{k}'}$. The dispersion relation is given by the function $\varepsilon_{\boldsymbol{k}}$, which is the energy of a particle with wavevector $\boldsymbol{k}$. We must have $\varepsilon_{\boldsymbol{k}} - \mu \geq 0$ for all $\boldsymbol{k}$, lest the spectrum of K be unbounded from below. The fields $\{\nu_{\boldsymbol{k}}, \bar\nu_{\boldsymbol{k}}\}$ break a global $\mathsf{O}(2)$ symmetry.

Students who have not taken a course in solid state physics can skip the following paragraph, and be aware that $N = V/v_0$ is the total volume of the system in units of a fundamental "unit cell" volume v_0. The thermodynamic limit is then $N \to \infty$. Note that N is not the boson particle number, which we'll call N_b.

Solid state physics boilerplate : We presume a setting in which the real space Hamiltonian is defined by some boson hopping model on a Bravais lattice. The wavevectors $\boldsymbol{k}$ are then restricted to the first Brillouin zone, $\hat{\Omega}$, and assuming periodic boundary conditions are quantized according to the condition $\exp\bigl(iN_l\,\boldsymbol{k}\cdot\boldsymbol{a}_l\bigr) = 1$ for all $l \in \{1,\ldots,d\}$, where $\boldsymbol{a}_l$ is the $l^{\rm th}$ fundamental direct lattice vector and N_l is the size of the system in the $\boldsymbol{a}_l$ direction; d is the dimension of space. The total number of unit cells is $N \equiv \prod_l N_l$. Thus, quantization entails $\boldsymbol{k} = \sum_l (2\pi n_l/N_l)\,\boldsymbol{b}_l$, where $\boldsymbol{b}_l$ is the $l^{\rm th}$ elementary reciprocal lattice vector ($\boldsymbol{a}_l\cdot\boldsymbol{b}_{l'} = 2\pi\delta_{ll'}$) and n_l ranges over N_l distinct integers such that the allowed $\boldsymbol{k}$ points form a discrete approximation to $\hat{\Omega}$.

To solve, we first shift the boson creation and annihilation operators, writing

$$K = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu)\,\beta^\dagger_{\boldsymbol{k}}\beta_{\boldsymbol{k}} - N\sum_{\boldsymbol{k}} \frac{|\nu_{\boldsymbol{k}}|^2}{\varepsilon_{\boldsymbol{k}}-\mu} \quad , \tag{1.88}$$

where

$$\beta_{\boldsymbol{k}} = b_{\boldsymbol{k}} - \frac{\sqrt{N}\,\nu_{\boldsymbol{k}}}{\varepsilon_{\boldsymbol{k}}-\mu} \qquad , \qquad \beta^\dagger_{\boldsymbol{k}} = b^\dagger_{\boldsymbol{k}} - \frac{\sqrt{N}\,\bar{\nu}_{\boldsymbol{k}}}{\varepsilon_{\boldsymbol{k}}-\mu} \quad . \tag{1.89}$$

Note that $\bigl[\beta_{\boldsymbol{k}}\,,\,\beta^\dagger_{\boldsymbol{k}'}\bigr] = \delta_{\boldsymbol{k}\boldsymbol{k}'}$ so the above transformation is canonical. The Landau free energy $\Omega = -k_{\rm B}T\ln\Xi$, where $\Xi = {\rm Tr}\, e^{-K/k_{\rm B}T}$, is given by

$$\Omega = Nk_{\rm B}T\int_{-\infty}^{\infty} d\varepsilon\; g(\varepsilon)\;\ln\bigl(1 - e^{(\mu-\varepsilon)/k_{\rm b}T}\bigr) - N\sum_{\boldsymbol{k}}\frac{|\nu_{\boldsymbol{k}}|^2}{\varepsilon_{\boldsymbol{k}}-\mu} \quad , \tag{1.90}$$

where $g(\varepsilon)$ is the density of energy states per unit cell,

$$g(\varepsilon) = \frac{1}{N}\sum_{\boldsymbol{k}}\delta\bigl(\varepsilon-\varepsilon_{\boldsymbol{k}}\bigr) \xrightarrow[N\to\infty]{} v_0\int_{\hat{\Omega}}\frac{d^dk}{(2\pi)^d}\,\delta\bigl(\varepsilon-\varepsilon_{\boldsymbol{k}}\bigr) \quad . \tag{1.91}$$

Note that

$$\psi_{\boldsymbol{k}} \equiv \frac{1}{\sqrt{N}}\,\bigl\langle b_{\boldsymbol{k}}\bigr\rangle = -\frac{1}{N}\,\frac{\partial\Omega}{\partial\bar{\nu}_{\boldsymbol{k}}} = \frac{\nu_{\boldsymbol{k}}}{\varepsilon_{\boldsymbol{k}}-\mu} \quad . \tag{1.92}$$

In the condensed phase, $\psi_{\boldsymbol{k}}$ is nonzero.

The Landau free energy (grand potential) is a function $\Omega(T,N,\mu,\nu,\bar{\nu})$. We now make a Legendre transformation,

$$Y(T,N,\mu,\psi,\bar{\psi}) = \Omega(T,N,\mu,\nu,\bar{\nu}) + N\sum_{\boldsymbol{k}}\bigl(\nu_{\boldsymbol{k}}\bar{\psi}_{\boldsymbol{k}} + \bar{\nu}_{\boldsymbol{k}}\psi_{\boldsymbol{k}}\bigr) \quad . \tag{1.93}$$

Note that

$$\frac{\partial Y}{\partial\bar{\nu}_{\boldsymbol{k}}} = \frac{\partial\Omega}{\partial\bar{\nu}_{\boldsymbol{k}}} + N\psi_{\boldsymbol{k}} = 0 \quad , \tag{1.94}$$

by the definition of $\psi_{\boldsymbol{k}}$. Similarly, $\partial Y/\partial\nu_{\boldsymbol{k}} = 0$. We now have

$$Y(T,N,\mu,\psi,\bar\psi) = Nk_{\rm B}T\int\limits_{-\infty}^{\infty}\!\!d\varepsilon\;g(\varepsilon)\;\ln\left(1-e^{(\mu-\varepsilon)/k_{\rm b}T}\right) + N\sum_{\boldsymbol{k}}(\varepsilon_{\boldsymbol{k}}-\mu)\,|\psi_{\boldsymbol{k}}|^2 \quad . \tag{1.95}$$

Therefore, the boson particle number per unit cell is given by the *dimensionless density*,

$$n = \frac{N_b}{N} = -\frac{1}{N}\frac{\partial Y}{\partial\mu} = \sum_{\boldsymbol{k}}|\psi_{\boldsymbol{k}}|^2 + \int\limits_{-\infty}^{\infty}\!\!d\varepsilon\;\frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_{\rm B}T}-1} \quad , \tag{1.96}$$

and the relation between the condensate amplitude $\psi_{\boldsymbol{k}}$ and the field $\nu_{\boldsymbol{k}}$ is given by

$$\nu_{\boldsymbol{k}} = \frac{1}{N}\frac{\partial Y}{\partial\bar\psi_{\boldsymbol{k}}} = (\varepsilon_{\boldsymbol{k}}-\mu)\,\psi_{\boldsymbol{k}} \quad . \tag{1.97}$$

Recall that $\nu_{\boldsymbol{k}}$ acts as an external field. Let the dispersion $\varepsilon_{\boldsymbol{k}}$ be minimized at $\boldsymbol{k} = \boldsymbol{K}$. Without loss of generality, we may assume this minimum value is $\varepsilon_{\boldsymbol{K}} = 0$. We see that if $\nu_{\boldsymbol{k}} = 0$ then one of two must be true:

(i) $\psi_{\boldsymbol{k}} = 0$ for all $\boldsymbol{k}$

(ii) $\mu = \varepsilon_{\boldsymbol{K}}$, in which case $\psi_{\boldsymbol{K}}$ can be nonzero.

Thus, for $\nu = \bar\nu = 0$ and $\mu > 0$, we have the usual equation of state,

$$n(T,\mu) = \int\limits_{-\infty}^{\infty}\!\!d\varepsilon\;\frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_{\rm B}T}-1} \quad , \tag{1.98}$$

which relates the intensive variables n, T, and μ. When $\mu = 0$, the equation of state becomes

$$n(T,\mu=0) = \overbrace{\sum_{\boldsymbol{K}}|\psi_{\boldsymbol{K}}|^2}^{n_0} + \overbrace{\int\limits_{-\infty}^{\infty}\!\!d\varepsilon\;\frac{g(\varepsilon)}{e^{\varepsilon/k_{\rm B}T}-1}}^{n_>(T)} \quad , \tag{1.99}$$

where now the sum is over only those $\boldsymbol{K}$ for which $\varepsilon_{\boldsymbol{K}} = 0$. Typically this set has only one member, $\boldsymbol{K} = 0$, but it is quite possible, due to symmetry reasons, that there are more such $\boldsymbol{K}$ values. This last equation of state is one which relates the intensive variables n, T, and n_0, where

$$n_0 = \sum_{\boldsymbol{K}}|\psi_{\boldsymbol{K}}|^2 \tag{1.100}$$

is the dimensionless condensate density. If the integral $n_>(T)$ in Eqn. 1.99 is finite, then for $n > n_0(T)$ we must have $n_0 > 0$. Note that, for any T, $n_>(T)$ diverges logarithmically whenever $g(0)$ is finite. This means that Eqn. 1.98 can always be inverted to yield a finite $\mu(n,T)$, no matter how large the value of n,

in which case there is no condensation and $n_0 = 0$. If $g(\varepsilon) \propto \varepsilon^\alpha$ with $\alpha > 0$, the integral converges and $n_>(T)$ is finite and monotonically increasing for all T. Thus, for fixed dimensionless number n, there will be a *critical temperature* $T_{\rm c}$ for which $n = n_>(T_{\rm c})$. For $T < T_{\rm c}$, Eqn. 1.98 has no solution for any μ and we must appeal to eqn. 1.99. The condensate density, given by $n_0(n,T) = n - n_>(T)$, is then finite for $T < T_{\rm c}$, and vanishes for $T \geq T_{\rm c}$.

In the condensed phase, the phase of the order parameter ψ inherits its phase from the external field ν, which is taken to zero, in the same way the magnetization in the symmetry-broken phase of an Ising ferromagnet inherits its direction from an applied field h which is taken to zero. The important feature is that in both cases the applied field is taken to zero *after* the approach to the thermodynamic limit.

Chapter 2

Theory of Group Representation

2.1 Basic Definitions

This chapter is not about the legalities of class action lawsuits. Rather, when we speak of a *group representation*, we mean a map from the space of elements of some abstract group G to a space of operators $\hat{D}(G)$ which act linearly on some vector space $\mathcal{V}$. The fancy way to say this is that a representation is a map from G to $\mathsf{End}(\mathcal{V})$, the space of *endomorphisms* of $\mathcal{V}$.[1]

2.1.1 Group elements cry out for representation

Check it:

> DEFINITION : Let G be a group and let $\mathcal{V}$ be a vector space. A *linear representation*[2] of G is a homomorphism $\hat{D} : G \mapsto \mathsf{End}(\mathcal{V})$. The *dimension* of the representation is $\dim(\mathcal{V})$. The representation is *faithful* if $\hat{D}(G)$ is an isomorphism. Otherwise it is said to be *degenerate*.

In plain English: each group element $g \in G$ maps to an operator[3] $\hat{D}(g)$ which acts on the vector space $\mathcal{V}$. For us, $\mathcal{V}$ will be a finite-dimensional subspace of the full Hilbert space $\mathcal{H}$, for some quantum mechanical Hamiltonian, which transforms into itself under symmetry group operations. If $\mathcal{V}$ is n-dimensional, we can choose a basis $\{|\,\mathrm{e}_i\,\rangle\}$ with $i \in \{1, \ldots, n\}$. The action of $\hat{D}(g)$ on each basis state is given by

$$\hat{D}(g)\,|\,\mathrm{e}_k\,\rangle = |\,\mathrm{e}_i\,\rangle\,D^{(n)}_{ik}(g) \quad , \tag{2.1}$$

where $D^{(n)}(g) \in \mathsf{GL}(n,\mathbb{C})$ is an $n \times n$ matrix. That $\hat{D}$ is a homomorphism means $\hat{D}(g)\,\hat{D}(g') = \hat{D}(gg')$, which entails $D^{(n)}(g)\,D^{(n)}(g') = D^{(n)}(gg')$. We shall interchangeably refer to both $\hat{D}(G)$ as well as

[1] An endomorphism is a map from a set to itself. An automorphism is an invertible endomorphism.

[2] We use the term "linear representation" to distinguish it from what is called a "projective representation", which we introduce in §2.1.5. Most of the time we shall abbreviate the former as simply "representation".

[3] Here and henceforth we shall endeavor to properly attire all our operators with stylish hats.

$D^{(n)}(G)$ as representations, though formally one is in terms of operators acting on $\mathcal{V}$ and the other in terms of matrices, which presumes some choice of basis for $\mathcal{V}$. If the representation is unitary, we may write it as $\hat{U}(G)$.

2.1.2 Equivalent and reducible representations

Let $D^{(n)}(G)$ and $\widetilde{D}^{(n)}(G)$ be two n-dimensional matrix representations of G, and suppose $\exists\, S \in \mathsf{GL}(n,\mathbb{C})$ such that $\widetilde{D}^{(n)}(g) = S^{-1} D^{(n)}(g)\, S$ for all $g \in G$. Then D and $\widetilde{D}$ are said to be *equivalent* representations.

How can we test for equivalence? One diagnostic we can apply is based on the identity $\mathsf{Tr}\,(S^{-1} A\, S) = \mathsf{Tr}\, A$. We call

$$\chi(g) \equiv \mathsf{Tr}\, D(g) \tag{2.2}$$

the *character* of g in the representation $D(G)$. Note that all group elements in a given equivalence class have the same character, because $\chi(h^{-1}gh) = \chi(g)$. So one thing we can say at this point is that if the characters of the same class differ in D and $\widetilde{D}$, then the representations are not equivalent.

Now let's talk about reducibility. Two definitions:

> DEFINITION : Let $\hat{D}(G)$ be a representation of G acting on the vector space $\mathcal{V}$. A subspace $\mathcal{V}_1 \subset \mathcal{V}$ is *invariant* if $\hat{D}(g)\,|\psi\rangle \in \mathcal{V}_1 \;\forall\; |\psi\rangle \in \mathcal{V}_1$. An invariant subspace is called *minimal* (or *proper*) if it contains no nontrivial invariant subspaces[4].
>
> DEFINITION : A representation $\hat{D}(G)$ acting on $\mathcal{V}$ is *irreducible* if there is no nontrivial invariant subspace $\mathcal{V}_1 \subset \mathcal{V}$ under the action of $\hat{D}(G)$. Otherwise the representation is *reducible*. If the orthogonal complement[5] $\mathcal{V}_1^\perp$ is also invariant, the representation is said to be *fully reducible*.

What does reducibility entail for a matrix representation $D^{(n)}(G)$? Let the reducible subspace $\mathcal{V}_1$ be spanned by vectors $\{|\mathrm{e}_1\rangle, \ldots, |\mathrm{e}_{n_1}\rangle\}$, with its complement $\mathcal{V}_1^\perp$ spanned by $\{|\mathrm{e}_{n_1+1}\rangle, \ldots, |\mathrm{e}_{n_1+n_2}\rangle\}$, where $n_1 + n_2 \equiv n = \mathsf{dim}(\mathcal{V})$. According to Eqn. 2.1, we must have

$$D^{(n)}(g) = \left[\begin{array}{c|c} D^{(n_1)}(g) & C^{(n_1,n_2)}(g) \\ \hline 0 & D^{(n_2)}(g) \end{array}\right] \tag{2.3}$$

where $D^{(n_1)}(G)$ and $D^{(n_2)}(G)$ are each smaller matrix representations of G, and, adopting an obvious and simplifying notation,

$$C(gh) = D_1(g)\, C(h) + C(g)\, D_2(h) \quad , \tag{2.4}$$

with $C(E) = 0$. Note that transitivity is then satisfied, *i.e.*

$$\begin{aligned} C(ghk) &= D_1(gh)\, C(k) + C(gh)\, D_2(k) \\ &= D_1(g)\, C(hk) + C(g)\, D_2(hk) \\ &= D_1(gh)\, C(k) + D_1(g)\, C(h)\, D_2(k) + C(g)\, D_2(hk) \quad . \end{aligned} \tag{2.5}$$

[4] *I.e.* no invariant subspaces other than $\mathcal{V}_1$ itself and the null vector $\{0\}$.

[5] An unexpected and out-of-context accolade. For example, *"Get the hell out of this lane before we run into that truck!!"* followed by "Dude, those are really nice cufflinks."

If $\mathcal{V}_1^\perp$ is invariant, then $C^{(n_1,n_2)}(g) = 0$ for all g and $D^{(n)}(G)$ is block diagonal, meaning that $D^{(n)}(G)$ is fully reducible.

We may now prove the following theorem:

- ◇ *Any unitary representation $\hat{D}(G)$ that is reducible is fully reducible.*

The proof is trivial. In Eqn. 2.3, the upper right $n_1 \times n_2$ rectangular block of $D^\dagger D = \mathbb{1}$ is $D_1^\dagger C = 0$. But D_1 is invertible, hence $C = 0$. Full reducibility means that we can express any unitary representation as a *direct sum* over irreducible representations, *viz.*

$$\begin{aligned} D(g) =& \overbrace{D^{\Gamma_1}(g) \oplus \cdots \oplus D^{\Gamma_1}(g)}^{n_{\Gamma_1} \text{ times}} \oplus \overbrace{D^{\Gamma_2}(g) \oplus \cdots \oplus D^{\Gamma_2}(g)}^{n_{\Gamma_2} \text{ times}} \oplus \cdots \\ =& \bigoplus_\Gamma n_\Gamma \, D^\Gamma(g) \quad , \end{aligned} \tag{2.6}$$

where each irreducible representation Γ_j appears $n(\Gamma_j) \equiv n_{\Gamma_j}$ times. If we call $D(g) \equiv D^\Psi(g)$ the matrix of g in the Ψ representation, then the reduction of Ψ is

$$\Psi = n_{\Gamma_1} \, \Gamma_1 \oplus n_{\Gamma_2} \, \Gamma_2 \oplus \cdots \ . \tag{2.7}$$

2.1.3 Conjugate and adjoint representations

If the matrices $D(G)$ form a representation Γ of the group G, then their complex conjugates $D(G)^*$ also form a representation of G, which we call Γ^*, called the *conjugate representation* of Γ. This is because, defining $D^*(g) = [D(g)]^*$,

$$D^*(g) \, D^*(h) = \big[D(g) \, D(h)\big]^* = D^*(gh) \quad . \tag{2.8}$$

If $D(G)$ is a real representation, then $\Gamma^* \cong \Gamma$.

Similarly, the matrices $[D(G)^{\mathsf{T}}]^{-1}$, *i.e.* the inverse transposes of $D(G)$, also form a representation, called the *adjoint representation* of Γ. This is because, with $D^{\mathsf{T}}(g) \equiv [D(g)]^{\mathsf{T}}$ and $\overline{D}(g) \equiv [D^{\mathsf{T}}(g)]^{-1}$,

$$\overline{D}(g)\overline{D}(h) = [D^{\mathsf{T}}(g)]^{-1}[D^{\mathsf{T}}(h)]^{-1} = [D^{\mathsf{T}}(h) \, D^{\mathsf{T}}(g)]^{-1} = \big[[D(g) \, D(h)]^{\mathsf{T}}\big]^{-1} = [D^{\mathsf{T}}(gh)]^{-1} = \overline{D}(gh) \quad . \tag{2.9}$$

Note that for unitary representations, the complex and adjoint representations are one and the same.

It is left as an exercise to the student to prove that $D(G)$, $D^*(G)$, and $\overline{D}(G)$ are either all reducible or all irreducible.

2.1.4 Unitary representations of finite groups

So it turns out that every representation $D^{(n)}(G)$ of a finite group is equivalent to a unitary representation. To show this, we need to find an invertible matrix S such that $S^{-1} D^{(n)}(g) \, S \in \mathsf{U}(n)$ for all $g \in G$. It

almost seems too much to ask, but as we're about to see, it is quite easy to construct such an S. We'll suppress the superscript on $D^{(n)}(g)$ and remember throughout that we are talking about an n-dimensional representation.

Start by forming the matrix

$$H = \sum_{g\in G} D^\dagger(g)\, D(g) \quad . \tag{2.10}$$

Clearly $H = H^\dagger$ is Hermitian, which means it can be diagonalized by a unitary matrix $V \in \mathsf{U}(n)$. We write

$$V^\dagger H V = \Lambda = \mathsf{diag}(\lambda_1, \ldots, \lambda_n) \quad , \tag{2.11}$$

with $\lambda_j > 0$ for all j (you should prove this). Now define $\widetilde{D}(g) = V^\dagger D(g)\, V$, in which case

$$\Lambda = V^\dagger H V = \sum_{g\in G} \widetilde{D}^\dagger(g)\, \widetilde{D}(g) \qquad , \qquad \lambda_k = \sum_{g\in G} \sum_{l=1}^{n} \left|\widetilde{D}_{lk}(g)\right|^2 \quad . \tag{2.12}$$

We may now form the matrices $\Lambda^{\pm 1/2}$, and define

$$B(g) = \Lambda^{1/2}\, \widetilde{D}(g)\, \Lambda^{-1/2} \quad . \tag{2.13}$$

We now show that $B(g)$ is unitary for all g:

$$\begin{aligned} B^\dagger(g) B(g) = \Lambda^{-1/2}\, \widetilde{D}^\dagger(g)\, \Lambda\, \widetilde{D}(g)\, \Lambda^{-1/2} &= \Lambda^{-1/2} \sum_{h\in G} \widetilde{D}^\dagger(g)\, \widetilde{D}^\dagger(h)\, \widetilde{D}(h)\, \widetilde{D}(g)\, \Lambda^{-1/2} \\ &= \Lambda^{-1/2} \overbrace{\sum_{h\in G} \widetilde{D}^\dagger(hg)\, \widetilde{D}(hg)}^{\Lambda}\, \Lambda^{-1/2} = \mathbb{1} \quad , \end{aligned} \tag{2.14}$$

where we have invoked the rearrangement theorem to write the sum over all hg for fixed g as a sum over group elements. So we have shown $B(g) = S^{-1} D(g)\, S$ is unitary for all g, with $S = V\Lambda^{-1/2}$. Note that not all symmetries can be realized unitarily. For example, time-reversal, which we shall discuss in due time, is an anti-unitary symmetry.

The above proof relies on the convergence of the sum for H in Eqn. 2.10. For discrete groups of finite order, or for compact continuous (Lie) groups, this convergence is guaranteed. But for groups of infinite order or noncompact Lie groups, convergence is not guaranteed. The Lorentz group, for example, has nonunitary representations.

2.1.5 Projective representations

I highly recommend you skip this section.

What? You're still here? OK, but strap in as we introduce the concept of a *projective representation*[6]. In a projective representation, the multiplication rule is preserved up to a phase, *i.e.*

$$\hat{D}(g)\, \hat{D}(h) = \omega(g,h)\, \hat{D}(gh) \quad , \tag{2.15}$$

[6]I am grateful to my colleague John McGreevy for explaining all sorts of crazy math shit to me.

where $\omega(g,h) \in \mathbb{C}$ for all $g, h \in G$ is called a *cocycle*. Hence $\hat{D}(G)$ is no longer a homomorphism. We still require associativity, meaning

$$\begin{aligned}\hat{D}(g)\,\hat{D}(h)\,\hat{D}(k) &= \big[\hat{D}(g)\,\hat{D}(h)\big]\hat{D}(k) = \omega(g,h)\,\hat{D}(gh)\,\hat{D}(k) = \omega(g,h)\,\omega(gh,k)\,\hat{D}(ghk) \\ &= \hat{D}(g)\big[\hat{D}(h)\,\hat{D}(k)\big] = \omega(h,k)\,\hat{D}(g)\,\hat{D}(hk) = \omega(g,hk)\,\omega(h,k)\,\hat{D}(ghk) \quad ,\end{aligned} \tag{2.16}$$

which therefore requires

$$\frac{\omega(g,h)}{\omega(h,k)} = \frac{\omega(g,hk)}{\omega(gh,k)} \quad . \tag{2.17}$$

Perhaps the simplest discrete example is that of the abelian group $\mathbb{Z}_2 \times \mathbb{Z}_2$, which consists of the elements $\big\{E, \sigma, \tau, \sigma\tau\big\}$, with $\sigma^2 = \tau^2 = E$ and $\sigma\tau = \tau\sigma$. Consider now the projective representation where

$$D(\sigma) = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad D(\tau) = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad D(\sigma\tau) = iY \equiv \Lambda = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad , \tag{2.18}$$

where X, Y, Z are the familiar Pauli matrices, and $D(E)$ is of course the 2×2 identity matrix. Then $\omega(\sigma,\tau) = \omega(\sigma,\sigma\tau) = \omega(\sigma\tau,\tau) = 1$ but $\omega(\tau,\sigma) = \omega(\sigma\tau,\sigma) = \omega(\tau,\sigma\tau) = -1$. Below we shall find that representation of abelian groups are always one-dimensional. Not so for projective representations! Here we have an example of an abelian group with a two-dimensional irreducible projective representation. Incidentally, we can *lift* the projective representation to a conventional linear representation, of a different group $\widetilde{G}$, acting on the same two-dimensional vector space. $\widetilde{G}$ is called a *central extension* of G.[7] In our case, $\widetilde{G} \subset \mathsf{SU}(2)$ consists of the eight elements $\big\{\pm E, \pm Z, \pm X \ \pm\Lambda\big\}$, with the multiplication table given by

$$(\pm E)^2 = (\pm Z)^2 = (\pm X)^2 = E \quad , \quad (\pm\Lambda)^2 = -E \tag{2.19}$$

and

$$ZX = -XZ = \Lambda \quad , \quad Z\Lambda = -\Lambda Z = X \quad , \quad \Lambda X = -X\Lambda = Z \quad . \tag{2.20}$$

Clearly $\widetilde{G}$ is nonabelian, and as we remarked in chapter 1, there are only two distinct nonabelian groups of order eight. So $\widetilde{G}$ must either be the dihedral group D_4 or the quaternion group Q. You should figure out which one it is for yourself before proceeding to the next paragraph.

To be more clear, an *extension* $\widetilde{G}$ of a group G by an abelian group A is given by an *exact sequence* of homomorphisms,

$$1 \longrightarrow A \xrightarrow{\ \psi\ } \widetilde{G} \xrightarrow{\ \pi\ } G \longrightarrow 1 \quad . \tag{2.21}$$

Exactness means that the kernel of every map in the sequence is the image of the map which precedes it, and that ψ is injective while π is surjective. Furthermore $\mathsf{im}(\psi) \lhd \widetilde{G}$, *i.e.* the image of ψ in $\widetilde{G}$ is a normal subgroup. The extension is said to be *central* if $\mathsf{im}(\psi) \subseteq Z(\widetilde{G})$, *i.e.* if the image $\psi(A)$ lies within the center of $\widetilde{G}$. The first map in the sequence, $1 \longrightarrow A$, is a trivial injection of the one element group $\mathbb{Z}_1 = \{1\}$ to the identity in A (it is so trivial we don't bother distinguishing it with a name). Similarly the last map $G \longrightarrow 1$ is the trivial surjection onto $\mathbb{Z}_1$.

In our previous example, the group $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ is lifted to $\widetilde{G} = D_4$ by means of the abelian group $A = \mathbb{Z}_2$. Thus, let $\mathbb{Z}_2 = \{1, m\}$, $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, \tau, \sigma, \sigma\tau\}$, and $D_4 = \{E, -E, \Lambda, -\Lambda, X, -X, Z, -Z\}$. We

[7] For example, the central extension for UCSD is 858-534-2230.

write the exact sequence vertically from top to bottom, and next to it the action of the maps ψ and π on the group elements, as well as the trivial initial injection and final surjection from/to the group $\mathbb{Z}_1$:

$$
\begin{array}{ccc}
1 & & 1 \\
\downarrow & & \downarrow \\
\mathbb{Z}_2 & & E \\
\downarrow{\scriptstyle \psi} & & \downarrow{\scriptstyle \psi} \\
D_4 & : & E \\
\downarrow{\scriptstyle \pi} & & \downarrow{\scriptstyle \pi} \\
\mathbb{Z}_2 \times \mathbb{Z}_2 & & E \\
\downarrow & & \downarrow \\
1 & & 1
\end{array}
\qquad
\begin{array}{c}
m \\
\downarrow{\scriptstyle \psi} \\
-E \\
\downarrow{\scriptstyle \pi} \\
E \\
\downarrow \\
1
\end{array}
\qquad
\begin{array}{c}
\Lambda \\
\downarrow{\scriptstyle \pi} \\
\sigma\tau \\
\downarrow \\
1
\end{array}
\qquad
\begin{array}{c}
-\Lambda \\
\downarrow{\scriptstyle \pi} \\
\sigma\tau \\
\downarrow \\
1
\end{array}
\qquad
\begin{array}{c}
X \\
\downarrow{\scriptstyle \pi} \\
\tau \\
\downarrow \\
1
\end{array}
\qquad
\begin{array}{c}
-X \\
\downarrow{\scriptstyle \pi} \\
\tau \\
\downarrow \\
1
\end{array}
\qquad
\begin{array}{c}
Z \\
\downarrow{\scriptstyle \pi} \\
\sigma \\
\downarrow \\
1
\end{array}
\qquad
\begin{array}{c}
-Z \\
\downarrow{\scriptstyle \pi} \\
\sigma \\
\downarrow \\
1
\end{array}
$$

A central extension is not necessarily unique. For example, $\mathbb{Z}_2 \times \mathbb{Z}_2$ can also be lifted via $\mathbb{Z}_2$ to the quaternion group Q.

Student exercise : Check that all this stuff works out. *I.e.* that ψ and π are group homomorphisms, that $\mathsf{im}(\psi) = \mathsf{ker}(\pi)$, that $\mathsf{im}(\psi) \lhd \widetilde{G}$, *etc.*

One can also have projective representations of continuous groups. Consider, for example, the case of $\mathsf{U}(1) \cong \mathsf{O}(2)$. The group elements are labeled by points $z \in S^1$ which live on the circle, *i.e.* unimodular $\big(|z| = 1\big)$ complex numbers. *I.e.* $z = e^{i\theta}$ with $\theta \in [\,0, 2\pi)$, which is called the *fundamental domain* of θ. Let us represent $\mathsf{U}(1)$ projectively, via $\hat{U}(\theta) = \exp(iq\theta)$ where $q \in \mathbb{Z} + \frac{1}{2}$, *i.e.* q is a half odd integer. Now let's multiply. At first it might seem quite trivial: $\hat{U}(\theta)\,\hat{U}(\theta') = \hat{U}(\theta + \theta')$. *What could possibly go wrong?* Well, the problem is that $\theta + \theta'$ doesn't always live in the fundamental domain. The group operation on the original $\mathsf{U}(1)$ should be thought of as addition of the angles modulo 2π, in which case

$$\hat{U}(\theta)\,\hat{U}(\theta') = \omega(\theta,\theta')\,\hat{U}(\theta + \theta' \;\mathsf{mod}\; 2\pi) \qquad , \qquad \omega(\theta,\theta') = \begin{cases} +1 & \text{if } 0 \le \theta + \theta' < 2\pi \\ -1 & \text{if } 2\pi \le \theta + \theta' < 4\pi \end{cases} \quad . \tag{2.22}$$

We saw above how each element of $\mathbb{Z}_2 \times \mathbb{Z}_2$ could be associated with two elements in its central extension D_4 via the lift $(E, \sigma, \tau, \sigma\tau) \to (\pm E, \pm Z, \pm X, \pm \Lambda)$. One could loosely say that D_4 is a "double cover" of $\mathbb{Z}_2 \times \mathbb{Z}_2$. The collocation *covering group* refers to the central extension of a Lie group. For example, the group $\mathsf{SU}(2)$ is a double cover of $\mathsf{SO}(3)$, because each matrix $R \in \mathsf{SO}(3)$ can be assigned to two matrices $\pm U$ in $\mathsf{SU}(2)$. Accordingly, $\mathsf{SO}(3)$ can be projectively represented by $\mathsf{SU}(2)$. To see the double cover explicitly, let $U(\xi, \hat{\boldsymbol{n}}) = \exp\big(-\frac{i}{2}\,\xi\,\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\big) \in \mathsf{SU}(2)$. It is left as an exercise to the student to show that

$$U\,\sigma^a\,U^\dagger = R_{ab}\,\sigma^b \quad , \tag{2.23}$$

with

$$R_{ab} = n^a\,n^b + \big(\delta^{ab} - n^a\,n^b\big)\cos\xi - \epsilon_{abc}\,n^c\,\sin\xi \quad . \tag{2.24}$$

For example, if $\hat{\boldsymbol{n}} = \hat{\boldsymbol{z}}$ we have

$$R = \begin{pmatrix} \cos\xi & -\sin\xi & 0 \\ \sin\xi & \cos\xi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{2.25}$$

Clearly $R \in \mathsf{SO}(3)$, and each $R(\xi, \hat{\boldsymbol{n}})$ labels a unique such group element, aside from the identification $R(\pi, \hat{\boldsymbol{n}}) = R(\pi, -\hat{\boldsymbol{n}})$. Yet both $\pm U$ map to R, hence the double cover. Another way to say this is $\mathsf{SU}(2)/\mathbb{Z}_2 \cong \mathsf{SO}(3)$.

A more familiar example to condensed matter physicists is that of the *magnetic translation group*, which is the group of space translations in the presence of a uniform magnetic field. Let's first consider ordinary translations in $d = 3$ dimensions. The translation operator is $\hat{t}(\boldsymbol{d}) = \exp(i\boldsymbol{p} \cdot \boldsymbol{d}/\hbar) = \exp(\boldsymbol{d} \cdot \boldsymbol{\nabla})$. Note that $\hat{t}(\boldsymbol{d})\,\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} + \boldsymbol{d})$. Since the different components of $\boldsymbol{p}$ commute, we have $\hat{t}(\boldsymbol{d})\,\hat{t}(\boldsymbol{d}') = \hat{t}(\boldsymbol{d} + \boldsymbol{d}')$, hence $\hat{t}\big(\mathbb{R}^3, +\big)$ is a representation of the group $\mathbb{R}^3$, where the group operation is vector addition.

In the presence of a uniform magnetic field $\boldsymbol{B}$, the kinetic energy becomes $\hat{T} = \boldsymbol{\pi}^2/2m$, where the *cyclotron momentum* $\boldsymbol{\pi}$ is given by $\boldsymbol{\pi} = \boldsymbol{p} + \frac{e}{c}\boldsymbol{A}$ and $\boldsymbol{\nabla} \times \boldsymbol{A} = \boldsymbol{B}$. Its different components in general do not commute. Rather, $\big[\pi^\alpha, \pi^\beta\big] = -i(\hbar e/c)\,\varepsilon_{\alpha\beta\gamma} B^\gamma$. One then defines the *guiding center momentum* operator $\boldsymbol{\kappa} \equiv \boldsymbol{\pi} - \frac{e}{c}\boldsymbol{B} \times \boldsymbol{r}$, and finds $\big[\kappa^\alpha, \kappa^\beta\big] = +i(\hbar e/c)\,\varepsilon_{\alpha\beta\gamma} B^\gamma$ as well as $\big[\kappa^\alpha, \pi^\beta\big] = 0$. The *magnetic translation operator* is then defined as $\hat{t}_{\boldsymbol{B}}(\boldsymbol{d}) \equiv \exp(i\boldsymbol{\kappa} \cdot \boldsymbol{d}/\hbar)$. This commutes with the kinetic energy, but one finds

$$\hat{t}_{\boldsymbol{B}}(\boldsymbol{d})\,\hat{t}_{\boldsymbol{B}}(\boldsymbol{d}') = \exp\big(-i\pi \boldsymbol{B} \cdot \boldsymbol{d} \times \boldsymbol{d}'/\phi_0\big)\,\hat{t}_{\boldsymbol{B}}(\boldsymbol{d} + \boldsymbol{d}') \quad , \tag{2.26}$$

where $\phi_0 = hc/e$ is the Dirac flux quantum. In this case, then, we have a projective representation of the abelian group of translations in $\mathbb{R}^3$. Note that $\big[\hat{t}_{\boldsymbol{B}}(\boldsymbol{d})\,,\,\hat{t}_{\boldsymbol{B}}(\boldsymbol{d}')\big] = 0$ if and only if $\boldsymbol{B} \cdot \boldsymbol{d} \times \boldsymbol{d}' = q\phi_0$, where $q \in \mathbb{Z}$, which says that the parallelogram with sides $\boldsymbol{d}$ and $\boldsymbol{d}'$ encloses an area containing an integer number of Dirac quanta.

2.2 The Great Orthogonality Theorem

We now return to the warm, comforting safe-space of discrete groups with finite dimension, and their proper representations, and embark on a path toward a marvelous result known as the "Great Orthogonality Theorem". To reach this sublime state of enlightenment, we first need two lemmas[8] due to I. Schur[9].

2.2.1 Schur's first lemma

> LEMMA : Let $\hat{D}(G)$ be an irreducible representation of G on a vector space $\mathcal{V}$, and $\hat{C}$ an arbitrary linear operator on $\mathcal{V}$. If $\big[\hat{D}(g), \hat{C}\big] = 0$ for all $g \in G$, then $\hat{C} = \lambda \hat{\mathbb{1}}$ is a multiple of the identity.

We've already seen how any irreducible representation of a finite group is equivalent to a unitary representation, hence without loss of generality we may assume $\hat{D}(G)$ is unitary. We will also assume $\hat{C}$ is Hermitian. This imposes no restriction, because from an arbitrary $\hat{C}$ we may form $\hat{C}_+ = \frac{1}{2}(\hat{C} + \hat{C}^\dagger)$ and $\hat{C}_- = \frac{1}{2i}(\hat{C} - \hat{C}^\dagger)$, both of which are Hermitian, and prove the theorem for $\hat{C}_\pm$ separately.

[8] "[A lemma] is a stepping stone on the path to proving a theorem" - some math blog.
[9] Awful pun: We can trust in these lemmas because their author was Schur.

With $\hat{C} = \hat{C}^\dagger$, we may find a unitary operator $\hat{W}$ such that $\hat{W}^\dagger \hat{C}\, \hat{W} = \hat{\Lambda}$, where $\hat{\Lambda}$ is diagonal in our basis. In other words, we may use $\hat{W}$ to transform to a new basis $|\tilde{e}_{a\mu}\rangle$ where $\hat{C}\,|\tilde{e}_{a\mu}\rangle = \lambda_a |\tilde{e}_{a\mu}\rangle$. Here a labels the distinct eigenvalues of $\hat{C}$, and μ is an auxiliary index parameterizing the subspace $\mathcal{V}_a \subset \mathcal{V}$ with eigenvalue λ_a. Since $\hat{D}(g)$ commutes with $\hat{C}$ for all $g \in G$, each $\mathcal{V}_a$ is an invariant subspace. But by assumption $\hat{D}(G)$ is an irreducible representation, in which case the only invariant subspace is $\mathcal{V}$ itself. In that case, $\hat{C}$ can only have one eigenvalue, hence $\hat{C} = \lambda \hat{\mathbb{1}}$ for some $\lambda \in \mathbb{R}$. QED

COROLLARY : If G is abelian, its irreducible representations are all of dimension one.

To prove the corollary, note that if G is abelian, then for any $h \in G$, we have $\big[\hat{D}(g), \hat{D}(h)\big] = 0$ for all $g \in G$. By the lemma, $\hat{D}(h) = \lambda_h \hat{\mathbb{1}}$ for all $h \in G$. As an example, consider the cyclic group C_n, consisting of elements $\big\{E, R, R^2, \ldots, R^{n-1}\big\}$. The operator $\hat{R}$ must then correspond to a unimodular complex number $e^{i\theta}$, and $\hat{R}^n = 1$ requires $\theta = 2\pi j/n$ with $j \in \{0, 1, \ldots, n-1\}$ labeling the representation. Thus, C_n has n one-dimensional representations, each of which is of course irreducible.

2.2.2 Schur's second lemma

LEMMA : Let $\hat{D}_1(G)$ and $\hat{D}_2(G)$ be two irreducible representations of a finite group G, acting on vector spaces $\mathcal{V}_1$ and $\mathcal{V}_2$, respectively. Let $\hat{L} : \mathcal{V}_2 \mapsto \mathcal{V}_1$ be a linear operator such that $\hat{L}\hat{D}_2(g) = \hat{D}_1(g)\hat{L}$ for all $g \in G$. Then either (i) $\hat{L} = 0$ or (ii) $\mathcal{V}_1 \cong \mathcal{V}_2$ and $\hat{D}_1(G)$ is equivalent to $\hat{D}_2(G)$.

Note that this means that the matrices $D_1^{(n_1)}(g)$ and $D_2^{(n_2)}(g)$ satisfy $L D_1^{(n_1)}(g) = D_2^{(n_2)}(g) L$, where L is a $n_2 \times n_1$ rectangular matrix corresponding to $\hat{L}$.

To prove this lemma, we start by considering the space $\mathsf{im}(\hat{L}) = \Big\{ \hat{L}\,|\psi_2\rangle \;\Big|\; |\psi_2\rangle \in \mathcal{V}_2 \Big\}$, which is the image of the operator $\hat{L}$. This is an invariant subspace for $\hat{D}_1(G)$ because

$$\hat{D}_1(g)\,\hat{L}\,|\,\psi_2\,\rangle = \hat{L}\,\hat{D}_2(g)\,|\,\psi_2\,\rangle = \hat{L}\,|\,\tilde{\psi}_2\,\rangle \in \mathsf{im}(\hat{L})\;\forall\; g \in G \quad . \tag{2.27}$$

But if $\hat{D}_1(G)$ is an irreducible representation, either $\mathsf{im}(\hat{L}) = 0$ or $\mathsf{im}(\hat{L}) = \mathcal{V}_1$.

Next, consider the kernel $\mathsf{ker}(\hat{L}) = \Big\{ |\psi_2\rangle \in \mathcal{V}_2 \;\Big|\; \hat{L}\,|\psi_2\rangle = 0 \Big\}$. This is invariant under $\hat{D}_2(G)$ because

$$\hat{L}\,\hat{D}_2(g)\,|\,\psi_2\,\rangle = \hat{D}_1(g)\,\hat{L}\,|\,\psi_2\,\rangle = 0 \quad . \tag{2.28}$$

So either $\mathsf{ker}(\hat{L}) = 0$ or $\mathsf{ker}(\hat{L}) = \mathcal{V}_2$.

So we conclude that either

$$\text{(i) } \mathsf{im}(\hat{L}) = 0 \text{ and } \mathsf{ker}(\hat{L}) = \mathcal{V}_2 \qquad \text{or} \qquad \text{(ii) } \mathsf{im}(\hat{L}) = \mathcal{V}_1 \text{ and } \mathsf{ker}(\hat{L}) = 0 \quad .$$

Case (i) says $\hat{L} = 0$, *i.e.* every vector $\mathcal{V}_2$ maps to zero. Case (ii) says $\mathcal{V}_1 \cong \mathcal{V}_2$ and $\hat{L}$ is an isomorphism. Hence $\hat{L}$ is invertible and we may write $\hat{D}_2(g) = \hat{L}^{-1}\,\hat{D}_1(g)\,\hat{L}$ for all $g \in G$, which is to say the two representations are equivalent[10].

[10] Mathematicians call a lemma like this where there are two possible cases a *dilemma*.

2.2.3 Great Orthogonality Theorem

Someone wise once said, "when life gives you lemmas, make a proof".

THEOREM : Let G be a finite group, Γ an irreducible representation of G, and $D^{\Gamma}(g)$ the matrix of g in the representation Γ. Then

$$\boxed{\sum_{g\in G} D^{\Gamma}_{ki}(g^{-1})\, D^{\Gamma'}_{i'k'}(g) = \frac{N_G}{d_\Gamma}\,\delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'}} \tag{2.29}$$

where $N_G = |G|$ is the order of G and $d_\Gamma = \dim(\Gamma)$ is the dimension of the representation Γ.

It is important to stress that equivalent representations are not distinguished; they are considered to be the same representation. Also, note that if the representations are all unitary, we may write

$$\sum_{g\in G} D^{\Gamma^*}_{ik}(g)\, D^{\Gamma'}_{i'k'}(g) = \frac{N_G}{d_\Gamma}\,\delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'} \quad , \tag{2.30}$$

where $D^{\Gamma^*}(g) = \big[D^{\Gamma}(g)\big]^*$, *i.e.* the matrix of g in the conjugate representation Γ^* is the complex conjugate of the matrix of g in the representation Γ. Note that the matrices $D^{\Gamma^*}(g)$ and $D^{\Gamma}_{ik}(g)$ are not necessarily of the same dimension. *I.e.* i and k in Eqns. 2.29, 2.30 run from 1 to d_Γ while i' and k' run from 1 to $d_{\Gamma'}$. We say that two general (not necessarily irreducible) representations Ψ and Ψ' are *orthogonal* if

$$\sum_{g\in G} D^{\Psi^*}_{ik}(g)\, D^{\Psi'}_{i'k'}(g) = 0 \quad . \tag{2.31}$$

We will see that this means that Ψ and Ψ', when fully reduced into IRREPs, contain no IRREPs in common.

As an example of the G.O.T. in action, consider the cyclic group C_n, with elements $\{E, R, R^2, \ldots, R^{n-1}\}$. We know that there are n irreducible representations (IRREPs), all of which are one-dimensional. Each IRREP Γ is labeled by an integer j_Γ, with $D^{\Gamma}(R^k) = \exp(2\pi i j_\Gamma k/n)$. Then

$$\sum_{k=0}^{n-1} D^{\Gamma^*}(R^k)\, D^{\Gamma'}(R^k) = \sum_{k=0}^{n-1} e^{2\pi i(j_{\Gamma'} - j_\Gamma)k/n} = n\,\delta_{\Gamma\Gamma'} \quad . \tag{2.32}$$

To prove the theorem, let M be a $d_\Gamma \times d_{\Gamma'}$ matrix, and

$$L = \sum_{g\in G} D^{\Gamma}(g^{-1})\, M\, D^{\Gamma'}(g) \quad , \tag{2.33}$$

which is also of dimensions $d_\Gamma \times d_{\Gamma'}$. By the rearrangement theorem, $D^{\Gamma}(h^{-1})\, L\, D^{\Gamma'}(h) = L$ for all $h \in G$, *i.e.* $L\, D^{\Gamma'}(h) = D^{\Gamma}(h)\, L$. We now appeal to Schur's lemmas, and conclude that either (i) $\Gamma \neq \Gamma'$ and $L = 0$, or (ii) $\Gamma = \Gamma'$ and $L = \lambda E$. Now choose the matrix $M^{(kk')}_{jj'} = \delta_{jk}\,\delta_{j'k'}$, where $k \in \{1, \ldots, d_\Gamma\}$ and $k' \in \{1, \ldots, d_{\Gamma'}\}$ are arbitrary. Here (kk') is a label for a family of $d_\Gamma\, d_{\Gamma'}$ matrices. We then have

$$L^{(kk')}_{ii'} = \sum_{g\in G} D^{\Gamma}_{ik}(g^{-1})\, D^{\Gamma'}_{k'i'}(g) \quad . \tag{2.34}$$

We've already noted that if $\Gamma \neq \Gamma'$, then $L^{(kk')} = 0$. If $\Gamma = \Gamma'$, we must have $L^{(kk')}_{ii'} = \lambda_{kk'}\,\delta_{ii'}$, with

$$\lambda_{kk'} = \frac{1}{d_\Gamma}\mathsf{Tr}\,L^{(kk')} = \frac{1}{d_\Gamma}\sum_{g\in G} D^\Gamma_{ik}(g^{-1})\,D^\Gamma_{k'i}(g) = \frac{1}{d_\Gamma}\sum_{g\in G}\left[D^\Gamma(g)\,D^\Gamma(g^{-1})\right]_{k'k} = \frac{N_G}{d_\Gamma}\,\delta_{kk'} \quad , \tag{2.35}$$

and we are done!

Without loss of generality, we may restrict our attention to unitary representations. Let us define the vector

$$\psi^{(\Gamma ik)}_g \equiv \sqrt{\frac{d_\Gamma}{N_G}}\,D^\Gamma_{ik}(g) \quad , \tag{2.36}$$

where (Γik) is a label, with $i,k \in \{1,\ldots,d_\Gamma\}$, and where the group element g indexes the components of ψ. The GOT can then be restated as an orthonormality condition on these vectors, *i.e.*

$$\left\langle\, \boldsymbol{\psi}^{(\Gamma ik)} \,\middle|\, \boldsymbol{\psi}^{(\Gamma' i'k')} \,\right\rangle = \delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'} \quad , \tag{2.37}$$

which is kind of cool. Since each $\boldsymbol{\psi}^{(\Gamma ik)}$ lives in a vector space of N_G dimensions, we know that the total number of these vectors cannot exceed N_G, *i.e.*

$$\sum_\Gamma d_\Gamma^2 \leq N_G \quad . \tag{2.38}$$

Indeed, after we discuss the *regular representation*, we shall prove that the set $\{\boldsymbol{\psi}^{(\Gamma ik)}\}$ is complete as well as orthonormal. Completeness then entails the equality $\sum_\Gamma d_\Gamma^2 = N_G$, as well as

$$\sum_\Gamma \sum_{i,k=1}^{d_\Gamma} \psi^{(\Gamma ik)}_g \left(\psi^{(\Gamma ik)}_{g'}\right)^* = \frac{1}{N_G}\sum_\Gamma d_\Gamma \sum_{i,k=1}^{d_\Gamma} D^\Gamma_{ik}(g)\,D^{\Gamma *}_{ik}(g') = \delta_{gg'} \quad , \tag{2.39}$$

which is also quite wonderful[11].

2.3 Group Characters

Recall the definition of the *character* of the group element g in the representation Γ, $\chi^\Gamma(g) = \mathsf{Tr}\,D^\Gamma(g)$, where $D^\Gamma(G)$ are the matrices of the representation Γ, which may be taken to be unitary. We remarked earlier that $\chi^\Gamma(h^{-1}gh) = \chi^\Gamma(g)$, due to cyclic invariance of the trace, means that two elements g and g' in the same conjugacy class have the same character[12]. Therefore, it is convenient to focus on the conjugacy classes themselves, labeling them $\mathcal{C}$. The expression $\chi^\Gamma(\mathcal{C})$ then will refer to the character of each element in the conjugacy class $\mathcal{C}$. The identity element always forms its own class, and we accordingly have the following important result:

- ⋄ *The dimension of any representation Γ is the character of the identity:* $d_\Gamma \equiv \mathsf{dim}(\Gamma) = \chi^\Gamma(E)$.

Note also that if a class $\mathcal{C}$ contains the inverse of each of its elements, then $\chi^\Gamma(\mathcal{C})$ is real in every unitary representation, since then $\chi^\Gamma(g) = \chi^\Gamma(g^{-1}) = \left[\chi^\Gamma(g)\right]^*$.

[11] We might well call this the "Great Completeness Theorem".

[12] The fact that character is so intimately associated with class may seem politically incorrect and even distressful to some. If this makes you feel unsafe, try to remember that we are talking about group theory.

$\mathcal{C} \rightarrow$ $\Gamma \downarrow$	$\mathcal{C}_1$ $\{E\}$	$3\mathcal{C}_2$ $\{\sigma, \sigma', \sigma''\}$	$2\mathcal{C}_3$ $\{R, W\}$
A_1	1	1	1
A_2	1	-1	1
E	2	0	-1
Υ	3	1	0

Table 2.1: Character table for $C_{3v} \cong D_3$. The representations A_1, A_2 , and E are irreducible.

2.3.1 Example : D_3

Recall the dihedral group $D_3 \cong C_{3v} \cong S_3$, with elements $(E, R, W, \sigma, \sigma', \sigma'')$. In chapter one, we identified its three conjugacy classes, $\mathcal{C}_1 = \{E\}$, $\mathcal{C}_2 = \{\sigma, \sigma', \sigma''\}$, and $\mathcal{C}_3 = \{R, W\}$, and we met up with *four* of its representations. The first two are one-dimensional, and we call them A_1 and A_2 . The 1×1 matrices of the A_1 representation are given by

$$D^{A_1}(E) = 1 \quad , \quad D^{A_1}(R) = 1 \quad , \quad D^{A_1}(W) = 1 \quad , \quad D^{A_1}(\sigma) = 1 \quad , \quad D^{A_1}(\sigma') = 1 \quad , \quad D^{A_1}(\sigma'') = 1 \quad . \tag{2.40}$$

In the A_2 representation, the 1×1 matrices are

$$D^{A_2}(E) = 1 \quad , \quad D^{A_2}(R) = 1 \quad , \quad D^{A_2}(W) = 1 \quad , \quad D^{A_2}(\sigma) = -1 \quad , \quad D^{A_2}(\sigma') = -1 \quad , \quad D^{A_2}(\sigma'') = -1 \, . \tag{2.41}$$

The third representation, called E, is two-dimensional, with

$$D^E(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^E(R) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \qquad D^E(W) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}$$

$$D^E(\sigma) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^E(\sigma') = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \qquad D^E(\sigma'') = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \quad . \tag{2.42}$$

Finally, recall the defining representation of S_3 , which we call Υ :

$$D^\Upsilon(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad D^\Upsilon(R) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad D^\Upsilon(W) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

$$D^\Upsilon(\sigma) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad D^\Upsilon(\sigma') = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad D^\Upsilon(\sigma'') = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{2.43}$$

Let's construct the character table for D_3. Taking the traces, we obtain the results in Tab. 2.1. Note the notation $3\mathcal{C}_2$ and $2\mathcal{C}_3$, which refer to the 3-element class $\mathcal{C}_2$ and the 2-element class $\mathcal{C}_3$, respectively. The

representation Υ is reducible, and it turns out that $\Upsilon = A_1 \oplus E$. Indeed, one sees that

$$\chi^{\Upsilon}(g) = \chi^{A_1}(g) + \chi^{E}(g) \quad . \tag{2.44}$$

We shall see how reducible representations may be decomposed further below.

Remark about reality of characters

If a class $\mathcal{C}$ contains the inverse of each of its elements, then $\chi^{\Gamma}(\mathcal{C})$ is real in every unitary representation, since then $\chi^{\Gamma}(g) = \chi^{\Gamma}(g^{-1}) = \big[\chi^{\Gamma}(g)\big]^*$. This is the case for all classes of $C_{3v} \cong D_3$, for example. It is *not* the case in general, and certainly not for most abelian groups in particular, because in an abelian group, all classes contain a single element, but the only elements which are their own inverses are those elements of order $n = 1$ or $n = 2$. For example, if we eliminate the reflection symmetries, C_{3v} is broken down to $C_3 \cong Z_3$. Without the mirrors, we lose the conjugacy of R and W, since $\sigma R \sigma^{-1} = \sigma R \sigma = W$, which also holds when σ is replaced by either of the other mirrors σ' and σ''. Thus, the class $2\mathcal{C}_3$ in C_{3v} breaks up into two distinct classes $\mathcal{C}_3\ (R)$ and $\mathcal{C}_3^{-1}\ (W)$ within C_3. In two of the IRREPs, the $C_3^{\pm 1}$ classes have complex characters, as shown in Tab. 2.2.

2.3.2 Orthogonality theorem for characters

Taking the trace of each of the matrices in Eqn. 2.29, we obtain[13]

$$\sum_{g \in G} \chi^{\Gamma}(g^{-1})\, \chi^{\Gamma'}(g) = N_G\, \delta_{\Gamma\Gamma'} \quad . \tag{2.45}$$

Henceforth we shall assume all representations are unitary, in which case $\chi^{\Gamma}(g^{-1}) = \big[\chi^{\Gamma}(g)\big]^* = \chi^{\Gamma^*}(g)$. We may replace the above sum over group elements by a sum over conjugacy classes $\mathcal{C}$, resulting in

$$\sum_{\mathcal{C}} N_{\mathcal{C}}\, \chi^{\Gamma^*}(\mathcal{C})\, \chi^{\Gamma'}(\mathcal{C}) = N_G\, \delta_{\Gamma\Gamma'} \quad , \tag{2.46}$$

where $N_{\mathcal{C}}$ is the number of elements in class $\mathcal{C}$. If we set $\Gamma = \Gamma'$, we have

$$\sum_{\mathcal{C}} N_{\mathcal{C}}\, \big|\chi^{\Gamma}(\mathcal{C})\big|^2 = N_G \quad . \tag{2.47}$$

Note that for D_3, which has six elements, the representations A_1 and A_2 in Tab. 2.1 appropriately yield $1 \cdot 1^2 + 3 \cdot 1^2 + 2 \cdot 1^2 = 6$. Similarly, for E we have $1 \cdot 2^2 + 3 \cdot 0^2 + 2 \cdot (-1)^2 = 6$. But for Υ the LHS of Eqn. 2.47 gives $1 \cdot 3^2 + 3 \cdot 1^2 + 2 \cdot 0^2 = 12$, hence we can immediately tell that Υ must be reducible. For irreducible representations, we have the following:

THEOREM : Two IRREPs Γ and Γ' are equivalent if and only if $\chi^{\Gamma}(g) = \chi^{\Gamma'}(g)$ for all $g \in G$.

This proof is left as an exercise to the reader. Note that an IRREP Γ is equivalent to its complex conjugate Γ^* if and only if Γ is real.

[13] In Eqn. 2.29, recall that $i, k \in \{1, \ldots, d_\Gamma\}$ and $i', k' \in \{1, \ldots, d_{\Gamma'}\}$.

2.3.3 Dirac characters

Recall from chapter 1 the notion of a group algebra $\mathcal{G}$, which consists of linear combinations of the form $\boldsymbol{x} = \sum_{g\in G} x_g\, g$. Consider now the quantity

$$\Omega_a = \sum_{g\in\mathcal{C}_a} g \quad , \tag{2.48}$$

where the sum is over all group elements in the conjugacy class $\mathcal{C}_a$, where a ranges from 1 to the total number of classes. Ω_a is known as a *Dirac character*. Unlike the group characters we have discussed thus far, which are complex numbers, Dirac characters are elements of the group algebra. What makes them special is that each Ω_a commutes with every element of G, because taking $g^{-1}\Omega_a\, g$ simply reorders the terms in the above sum. We shall now prove that any element of $\mathcal{G}$ which commutes with the entire group G must be a linear combination of the Dirac characters. To see this, write a general element $\boldsymbol{x} \in \mathcal{G}$ as $\boldsymbol{x} = \sum_{g\in G} x_g\, g$, where each $x_g \in \mathbb{C}$. Then for any $r \in G$,

$$r^{-1}\,\boldsymbol{x}\,r = \sum_{h\in G} x_h\, r^{-1}hr = \sum_{g\in G} x_{rgr^{-1}}\, g \quad , \tag{2.49}$$

and therefore if $r^{-1}\,\boldsymbol{x}\,r = \boldsymbol{x}$, then equating the coefficients of g we have $x_g = x_{rgr^{-1}}$ for all $r \in G$, which says that x_g is a *class function*, *i.e.* it takes the same value for every element of a given conjugacy class.

Since each Ω_a commutes with all group elements, so does the product $\Omega_a\,\Omega_b$, and the above result then entails a relation of the form

$$\Omega_a\,\Omega_b = \sum_c F_{abc}\,\Omega_c \quad , \tag{2.50}$$

where the F_{abc} are called the *class coefficients*. Recall that the identity element E forms its own class, which we can always call Ω_1, so that $F_{1bc} = F_{b1c} = \delta_{bc}$.

For the group C_{3v}, with classes $\mathcal{C}_1 = \{E\}$, $\mathcal{C}_2 = \{R, W\}$, and $\mathcal{C}_3 = \{\sigma, \sigma', \sigma''\}$,

$$\begin{aligned}
\Omega_2\,\Omega_2 &= (R+W)(R+W) = 2E + R + W = 2\Omega_1 + \Omega_2 \\
\Omega_2\,\Omega_3 &= (R+W)(\sigma+\sigma'+\sigma'') = \sigma'' + \sigma + \sigma' + \sigma' + \sigma'' + \sigma = 2\,\Omega_3 \\
\Omega_3\,\Omega_3 &= (\sigma+\sigma'+\sigma'')(\sigma+\sigma'+\sigma'') = 3E + 3R + 3W = 3\,\Omega_1 + 3\,\Omega_2 \quad .
\end{aligned} \tag{2.51}$$

Thus,

$$\begin{aligned}
&F_{111} = F_{122} = F_{212} = F_{133} = F_{313} = 1 \\
&F_{221} = 2 \quad , \quad F_{222} = 1 \quad , \quad F_{233} = F_{323} = 2 \quad , \quad F_{331} = 3 \quad , \quad F_{332} = 3 \quad ,
\end{aligned} \tag{2.52}$$

with all other $F_{abc} = 0$. Because the Dirac characters all commute, any equation solved by the Ω_a will be solved by their eigenvalues ω_a[14]. We always have $\omega_1 = 1$. We then must solve the three equations

$$\omega_2^2 = 2 + \omega_2 \qquad , \qquad \omega_2\,\omega_3 = 2\,\omega_3 \qquad , \qquad \omega_3^2 = 3 + 3\,\omega_2 \quad . \tag{2.53}$$

[14] *Eigenvalues?!* How are we suddenly talking about *eigenvalues*? Well, you see, as we noted toward the end of §1.3.1, the group algebra $\mathcal{G}$ is in fact a vector space $\mathcal{A}$ with basis vectors $g \in G$, endowed with a linear multiplication law $\mathcal{A} \times \mathcal{A} \to \mathcal{A}$. Thus, any element of the algebra is also a linear operator, and linear operators have eigenvalues. So there.

If $\omega_3 = 0$, the third of these gives $\omega_2 = -1$, which is consistent with the first, and therefore $\boldsymbol{\omega} = (1, -1, 0)$. If $\omega_3 \neq 0$, the second equation gives $\omega_2 = 2$, again consistent with the first, and thus $\omega_3^2 = 9$, and so there are two possible solutions $\boldsymbol{\omega} = (1, 2, 3)$ and $\boldsymbol{\omega} = (1, 2, -3)$.

Relation to group characters

Suppose $D^\Gamma(G)$ is an irreducible matrix representation of G, and define the matrix

$$\Lambda_a = \sum_{g \in \mathcal{C}_a} D^\Gamma(g) \quad . \tag{2.54}$$

Then for all $h \in G$, we have $D^\Gamma(h^{-1})\,\Lambda_a\,D^\Gamma(h) = \Lambda_a$, and by Schur's first lemma it must be that each $\Lambda_a = \lambda_a \mathbb{1}$ is a multiple of the identity matrix. But then

$$\mathsf{Tr}\,\Lambda_a = d_\Gamma\,\lambda_a = \sum_{g \in \mathcal{C}_a} \chi^\Gamma(g) = N_{\mathcal{C}_a}\,\chi^\Gamma(\mathcal{C}_a) \quad , \tag{2.55}$$

and therefore

$$\Lambda_a = \frac{N_{\mathcal{C}_a}}{d_\Gamma}\,\chi^\Gamma(\mathcal{C}_a)\,\mathbb{1} \quad . \tag{2.56}$$

But clearly the Λ_a satisfy the same algebra as the Ω_a, *i.e.*

$$\Lambda_a\,\Lambda_b = \sum_c F_{abc}\,\Lambda_c \quad , \tag{2.57}$$

which yields the following relation for group characters:

$$\chi^\Gamma(\mathcal{C}_a)\,\chi^\Gamma(\mathcal{C}_b) = d_\Gamma \sum_l f_{abc}\,\chi^\Gamma(\mathcal{C}_c) \quad , \tag{2.58}$$

where $f_{abc} \equiv \left(N_{\mathcal{C}_c}/N_{\mathcal{C}_a}N_{\mathcal{C}_b}\right) F_{abc}$.

2.4 Decomposition of Representations

2.4.1 Reducible representations

We claim that the reduction of a reducible representation Ψ into IRREPs is unique. To see this, suppose

$$\Psi = \bigoplus_\Gamma n_\Gamma(\Psi)\,\Gamma \qquad \Rightarrow \qquad \chi^\Psi(\mathcal{C}) = \sum_\Gamma n_\Gamma(\Psi)\,\chi^\Gamma(\mathcal{C}) \quad . \tag{2.59}$$

We now derive an explicit formula for the decomposition $\{n_\Gamma(\Psi)\}$. Using the character orthogonality equation, we have

$$\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma^*}(\mathcal{C})\,\chi^\Psi(\mathcal{C}) = \sum_{\Gamma'} n_{\Gamma'}(\Psi)\,\overbrace{\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma^*}(\mathcal{C})\,\chi^{\Gamma'}(\mathcal{C})}^{N_G\,\delta_{\Gamma\Gamma'}} = N_G\,n_\Gamma(\Psi) \quad . \tag{2.60}$$

Thus, the number of times the IRREP Γ appears in the decomposition of Ψ is

$$n_\Gamma(\Psi) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}}\, \chi^{\Gamma^*}(\mathcal{C})\, \chi^{\Psi}(\mathcal{C}) \quad . \tag{2.61}$$

Note that if $\Psi = \Gamma'$ is itself an IRREP, the above formula correctly gives $n_\Gamma(\Gamma') = \delta_{\Gamma\Gamma'}$.

Note further that we can define the vectors

$$V^\Gamma_{\mathcal{C}} = \sqrt{\frac{N_{\mathcal{C}}}{N_G}}\, \chi^\Gamma(\mathcal{C}) \quad , \tag{2.62}$$

which are labeled by IRREPs Γ, and whose indices run over the equivalence classes $\mathcal{C}$. Character orthogonality then entails

$$\langle\, \boldsymbol{V}^\Gamma \,|\, \boldsymbol{V}^{\Gamma'} \,\rangle = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}}\, \chi^{\Gamma^*}(\mathcal{C})\, \chi^{\Gamma'}(\mathcal{C}) = \delta_{\Gamma\Gamma'} \quad . \tag{2.63}$$

Note that the vector space $\{\boldsymbol{V}^\Gamma\}$ is spanned by the vectors corresponding to all IRREPs, and that these vectors must be complete if every representation can be decomposed into IRREPs. Thus, we conclude the following:

- ◇ *The number of* IRREP*s is the number of classes:* $\sum_\Gamma 1 = \sum_{\mathcal{C}} 1$.

Completeness then entails $\sum_\Gamma |\, \boldsymbol{V}^\Gamma \,\rangle\langle\, \boldsymbol{V}^\Gamma \,| = \mathbb{1}$, *i.e.*

$$\sum_\Gamma \chi^{\Gamma^*}(\mathcal{C})\, \chi^\Gamma(\mathcal{C}') = \frac{N_G}{N_{\mathcal{C}}}\, \delta_{\mathcal{C}\mathcal{C}'} \quad , \tag{2.64}$$

from which it follows that

$$\chi^\Psi(\mathcal{C}) = \sum_\Gamma n_\Gamma(\Psi)\, \chi^\Gamma(C) \quad , \tag{2.65}$$

i.e. the characters of a reducible representation are given by the sums of the characters of their constituents. This is quite obvious when one considers that any reducible representation may be brought to block diagonal form, where the individual blocks are the constituent IRREPs.

2.4.2 Projection onto a particular representation

Suppose, on your birthday, you are given a unitary matrix representation $\Delta(G)$ of a popular finite discrete group. You have reason to believe $\Delta(G)$ is reducible[15], and you are a very impatient person, so you don't want to spend your time sifting through $\Delta(G)$ for your favorite IRREPs – especially not on your birthday. You would like to access them directly! How to do it?

The first thing to do is to go borrow a set of matrices $D^\Gamma_{\mu\nu}$ for all the IRREPs of G. Then construct the following expressions:

$$\Pi^\Gamma_{\mu\nu} = \frac{d_\Gamma}{N_G} \sum_{g\in G} D^{\Gamma^*}_{\mu\nu}(g)\, \Delta(g) \quad , \tag{2.66}$$

[15] It may have come in a very large box, for example.

which for each set of labels (Γ, μ, ν) is a matrix of the same rank as $\Delta(G)$. The $\Pi^\Gamma_{\mu\nu}$ are *projection matrices* onto the $\mu^{\rm th}$ row of the IRREP Γ. The following three marvelous things are true:

(i) The product of projectors is

$$\Pi^\Gamma_{\mu\nu}\,\Pi^{\Gamma'}_{\mu'\nu'} = \delta_{\Gamma\Gamma'}\,\delta_{\nu\mu'}\,\Pi^\Gamma_{\mu\nu'} \quad . \tag{2.67}$$

(ii) Hermitian conjugate: $\left(\Pi^\Gamma_{\mu\nu}\right)^\dagger = \Pi^\Gamma_{\nu\mu}$, *i.e.*

$$\left(\Pi^\Gamma_{\mu\nu}\right)^*_{ji} = \left(\Pi^\Gamma_{\nu\mu}\right)_{ij} \quad . \tag{2.68}$$

(iii) Resolution of identity (where there is an implied sum on μ):

$$\sum_\Gamma \Pi^\Gamma_{\mu\mu} = \mathbb{1} \quad , \tag{2.69}$$

You will have fun proving these results for yourself! Note that $P^\Gamma_\mu \equiv \Pi^\Gamma_{\mu\mu}$ with no sum on μ satisfies

$$P^\Gamma_\mu\,P^{\Gamma'}_{\mu'} = \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,P^\Gamma_\mu \quad , \tag{2.70}$$

i.e. each P^Γ_μ is a rank one projector onto the μ row of the Γ IRREP. Summing over all rows of all IREPs yields $\sum_{\Gamma,\mu} P^\Gamma_\mu = \mathbb{1}$. However, note that it is the projectors of *fixed column index* which transform according to a particular IRREP, because[16]

$$\Delta(g)\,\Pi^\Gamma_{\mu\nu} = \sum_\rho \Pi^\Gamma_{\rho\nu}\,D^\Gamma_{\rho\mu}(g) \quad . \tag{2.71}$$

Finally let's take the trace on μ and ν in Eqn. 2.66 and form $\Pi^\Gamma = \sum_\mu \Pi^\Gamma_{\mu\mu} = \sum_\mu P^\Gamma_\mu$, *i.e.*

$$\Pi^\Gamma \equiv \frac{d_\Gamma}{N_G}\sum_{g\in G}\chi^{\Gamma^*}(g)\,\Delta(g) \quad . \tag{2.72}$$

This also acts as a projection matrix onto Γ, since $\Pi^\Gamma\,\Pi^{\Gamma'} = \delta_{\Gamma\Gamma'}\,\Pi^\Gamma$.

Consider now an arbitrary vector $\boldsymbol{\psi}$, and form the vector $\boldsymbol{\psi}^{(\Gamma\mu)} = \Pi^\Gamma_{\mu\nu}\,\boldsymbol{\psi}$. The index ν is fixed and suppressed in $\boldsymbol{\psi}^{(\Gamma\mu)}$. That is, we form the vector whose $i^{\rm th}$ component is

$$\psi^{(\Gamma\mu)}_i = \frac{d_\Gamma}{N_G}\sum_{g\in G} D^{\Gamma^*}_{\mu\nu}(g)\,\Delta_{ij}(g)\,\psi_j \quad . \tag{2.73}$$

Then, appealing to Eqn. 2.71,

$$\Delta_{ij}(g)\,\psi^{(\Gamma\mu)}_j = \psi^{(\Gamma\rho)}_i\,D^\Gamma_{\rho\mu}(g) \quad , \tag{2.74}$$

with implied sums on j and ρ. We've just projected an arbitrary vector $\boldsymbol{\psi}$ onto one which transforms according to the $\mu^{\rm th}$ row of the IRREP Γ, *i.e.* $\boldsymbol{\psi}^{(\Gamma\mu)}$.

[16] Prove it!

2.4.3 The regular representation

The regular representation of any finite discrete group is defined as follows. Define the group multiplication table so that the entry for row g_a and column g_b is $g_a^{-1} g_b$ rather than the usual $g_a\, g_b$. By this convention, all diagonal entries will be the identity element, E. The matrices of the regular representation are all of rank N_G, which is of course the rank of the multiplication table, and $D^{\rm reg}_{g,g'}(h)$ is defined to be one everywhere h occurs in the above reorganized table, and zero otherwise. In other words,

$$D^{\rm reg}_{g,g'}(h) = \delta_{g',\,gh} = \begin{cases} 1 & \text{if } g' = gh \\ 0 & \text{if } g' \neq gh \end{cases} \quad . \tag{2.75}$$

Note that

$$\sum_{g'\in G} D^{\rm reg}_{g,g'}(h)\, D^{\rm reg}_{g',g''}(k) = \sum_{g'\in G} \delta_{g',\,gh}\, \delta_{g'',\,g'k} = \delta_{g'',\,ghk} = D^{\rm reg}(hk) \quad , \tag{2.76}$$

and so $D^{\rm reg}(G)$ is a valid representation. We may now prove the following:

THEOREM : $\Gamma_{\rm reg} = \bigoplus_\Gamma d_\Gamma\, \Gamma$.

In other words, each IRREP appears in $\Gamma_{\rm reg}$ as many times as its dimension. To show this, first note that

$$\chi^{\Gamma_{\rm reg}}(h) = \sum_{g\in G} \delta_{g,gh} = N_G\, \delta_{h,E} \tag{2.77}$$

since $g = gh$ entails $h = E$. Next, we invoke Eqn. 2.61 with $\Psi = \Gamma_{\rm reg}$. From the above result, only the identity class contributes to the sum over equivalence classes $\mathcal{C}$, in which case

$$n_\Gamma(\Gamma_{\rm reg}) = \chi^\Gamma(E) = d_\Gamma \quad . \tag{2.78}$$

As a bonus, we can now establish the equality in Eqn. 2.38, since

$$N_G = \chi^{\Gamma_{\rm reg}}(E) = \sum_\Gamma n_\Gamma(\Gamma_{\rm reg})\, \chi^\Gamma(E) = \sum_\Gamma d_\Gamma^2 \quad . \tag{2.79}$$

Therefore the order of any finite group is the sum of the squares of the dimensions of its irreducible representations. QED

2.4.4 Induced and subduced representations

The regular representation is a special case of something called an *induced representation*. Suppose $H \subset G$ is a subgroup. As we saw in chapter 1, this entails that N_G/N_H is an integer, and there is a unique *coset construction* where we can write

$$G = \sum_{j=1}^{N_G/N_H} r_j\, H \quad . \tag{2.80}$$

Uniqueness means that the set $\{r_j\}$ is fixed by H. Now suppose we have a representation $D_{ab}(H)$. We now define

$$\widetilde{D}_{ia\,,\,jb}(g) = \sum_{h\in H} D_{ab}(h)\,\delta_{r_i h\,,\,gr_j} \quad , \tag{2.81}$$

where

$$\delta_{r_i h\,,\,gr_j} = \begin{cases} 1 & \text{if } r_i h = g r_j \\ 0 & \text{otherwise} \end{cases} \quad . \tag{2.82}$$

Then one finds

$$\begin{aligned} \widetilde{D}_{ia\,,\,jb}(g)\,\widetilde{D}_{jb\,,\,kc}(g') &= \sum_{h,h'\in H} D_{ab}(h)\,D_{bc}(h')\,\delta_{r_i h\,,\,gr_j}\,\delta_{r_j h'\,,\,g' r_k} \\ &= \sum_{\tilde h\in H} D_{ac}(\tilde h)\,\delta_{r_i \tilde h\,,\,gg' r_k} = \widetilde{D}_{ia\,,\,kc}(gg') \quad , \end{aligned} \tag{2.83}$$

and so $\widetilde{D}(G)$ is a representation of the larger group G. Note that if $D_{ab}(h) = 1$, then $\widetilde{D}_{ij}(g) = \sum_{h\in H}\delta_{r_i h\,,\,gr_j}$ and that if $H = \{E\}$ then $\widetilde{D}(G)$ is just the regular representation. The character of g in the induced representation is then

$$\widetilde{\chi}(g) = \mathsf{Tr}\,\widetilde{D}(g) = \sum_{h\in H}\chi(h)\,\sum_i \delta_{g\,,\,r_i h r_i^{-1}} \quad . \tag{2.84}$$

Let G be a group and $H \subset G$ a proper subgroup of G. Then any representation $D^{\Psi}(G)$ is also a representation of H, called the *subduced representation* $\Psi^{\downarrow}(H)$, with

$$D^{\Psi^{\downarrow}}(h) = D^{\Psi}(h) \quad . \tag{2.85}$$

Even if $D^{\Psi}(G)$ is reducible, the subduced representation $D^{\Psi^{\downarrow}}(H)$ need not necessarily be irreducible. For example, the subduced representation on to the identity is the unit matrix of rank d_Ψ, which is clearly reducible since it is a direct sum of d_Ψ one-dimensional trivial representations. If $D^{\Psi}(G)$ is reducible, then so is $D^{\Psi^{\downarrow}}(H)$. Thus, if $D^{\Psi^{\downarrow}}(H)$ is irreducible, then necessarily $D^{\Psi}(G)$ be reducible. Furthermore, if Ψ and Ψ' are two IRREPs of G, if there exists a subgroup $H \subset G$ such that $\Psi^{\downarrow}$ and $\Psi'^{\downarrow}$ are orthogonal, meaning they contain no common IRREPs of H, then Ψ and Ψ' are orthogonal. This is easily proven using the coset decomposition, writing $G = \sum_a r_a H$, so that

$$D^{\Psi}_{ik}(g) = D^{\Psi}_{ik}(rh) = \sum_m D^{\Psi}_{im}(r)\,D^{\Psi}_{mk}(h) \tag{2.86}$$

for some $h \in H$ and $r \notin H$. Multiplying the complex conjugate of this expression by the corresponding expression for $D^{\Psi'}_{i'k'}(g)$, and then summing over $g \in G$, we have

$$\sum_{g\in G} D^{\Psi^*}_{ik}(g)\,D^{\Psi'}_{i'k'}(g) = \sum_{m,m'}\sum_r D^{\Psi^*}_{im}(r)\,D^{\Psi'}_{i'm'}(r)\sum_{h\in H} D^{\Psi^*}_{mk}(h)\,D^{\Psi'}_{m'k'}(h) \quad , \tag{2.87}$$

which vanishes if $\Psi^{\downarrow}$ and $\Psi'^{\downarrow}$ are orthogonal representations on H.

2.4.5 Summary of key results

Here we summarize the key results. For unitary representations of a finite group G:

- Great Orthogonality Theorem : $\sum_{g\in G} D^{\Gamma^*}_{ik}(g)\, D^{\Gamma'}_{i'k'}(g) = (N_G/d_\Gamma)\,\delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'}$.
- Great Completeness Theorem : $\sum_{\Gamma,i,k} d_\Gamma\, D^{\Gamma^*}_{ik}(g)\, D^{\Gamma}_{ik}(g') = N_G\,\delta_{gg'}$.
- *Group characters* : $\chi^\Gamma(\mathcal{C}) \equiv \mathsf{Tr}\, D^\Gamma(g)$, where g is any element in the conjugacy class $\mathcal{C}$.
- *Character tables* : Rows indexed by IRREPs Γ, columns indexed by classes $\mathcal{C}$. Identity IRREP row entries are all 1's. Identity class column entries are $d_\Gamma = \mathsf{Tr}\, D^\Gamma(E)$.
- *Row orthogonality* : $\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma^*}(\mathcal{C})\,\chi^{\Gamma'}(\mathcal{C}) = N_G\,\delta_{\Gamma\Gamma'}$.
- *Column orthogonality* : $\sum_\Gamma \chi^{\Gamma^*}(\mathcal{C})\,\chi^{\Gamma}(\mathcal{C}') = (N_G/N_{\mathcal{C}})\,\delta_{\mathcal{C}\mathcal{C}'}$.
- *Decomposition* : The IRREP Γ appears $n_\Gamma(\Psi) = N_G^{-1}\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma^*}(\mathcal{C})\,\chi^{\Psi}(\mathcal{C})$ times in Ψ.
- *Projection matrices* : If $\Delta(G)$ is a reducible representation, $\Pi^\Gamma_{\mu\nu} = (d_\Gamma/N_G)\sum_{g\in G} D^{\Gamma^*}_{\mu\nu}(g)\,\Delta(g)$ projects onto the $\mu^{\rm th}$ row of the Γ IRREP.

Here $N_G = |G|$ is the number of elements in G, $d_\Gamma = \mathsf{dim}(\Gamma)$ is the dimension of the representation Γ, and $N_{\mathcal{C}}$ is the number of group elements in the conjugacy class $\mathcal{C}$.

2.4.6 Example character tables

Thus far we have not encountered any complex values of $\chi^\Gamma(g)$, but such cases are quite common. Consider, for example, the cyclic group C_3 consisting of $\{E, R, W\}$. C_n is abelian for all n, hence each element is its own class. We've seen how the 1×1 matrix $D^\Gamma(R^k)$ is given by $\omega^{k\,j_\Gamma}$ with $\omega = \exp(2\pi i/n)$, where $j_\Gamma \in \{0,\ldots,n-1\}$ labels the IRREP, and $k \in \{0,\ldots,n-1\}$. Tab. 2.2 shows the character table for C_3. Note that $\Gamma_3 = \Gamma_2^*$ is the complex conjugate of the Γ_2 representation.

C_3	E	R	W
Γ_1	1	1	1
Γ_2	1	ω	ω^2
Γ_3	1	ω^2	ω

Table 2.2: Character table for C_3.

We saw in chapter one that the eight element quaternion group, $Q = \{\pm E, \pm \mathtt{i}, \pm \mathtt{j}, \pm \mathtt{k}\}$ has five conjugacy classes. Aside from the trivial one-dimensional identity representation Γ_1, it has three other inequivalent one-dimensional IRREPs, called *sign representations*. The first of these we call Γ_2, the 1×1 matrices for which are $D^{\Gamma_2}(\pm E, \pm\mathtt{i}) = +1$ while $D^{\Gamma_2}(\pm\mathtt{j}, \pm\mathtt{k}) = -1$. One can check this is a valid group

Q	$\{E\}$	$\{-E\}$	$\{\mathtt{i},-\mathtt{i}\}$	$\{\mathtt{j},-\mathtt{j}\}$	$\{\mathtt{k},-\mathtt{k}\}$
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	1	-1	1	-1
Γ_4	1	1	-1	-1	1
Ψ	2	-2	0	0	0

Table 2.3: Character table for the quaternion group Q.

homomorphism. Permuting $\pm\mathtt{i}$, $\pm\mathtt{j}$, and $\pm\mathtt{k}$ gives the other two one-dimensional IRREPs. One can then easily infer that there is one remaining IRREP of dimension 2. The character table for the quaternion group Q is shown in Tab. 2.3.

While the character table for a group G contains a wealth of important information, it does not always distinguish G up to isomorphism. That is, it is possible for two different groups to have the same character table. Such is the case with Q and D_4, for example. The dihedral group D_4 also has five classes, which we can call E (the identity), C_2 (rotation by π), C_4 (rotations by $\pm\frac{1}{2}\pi$), C_2' (reflections in $y=0$ and in $x=0$), and C_2'' (reflections in $y=x$ and in $y=-x$). Tab. 3.2 shows its character table[17], which you should compare with Tab. 2.3.

D_4	E	C_2	$2C_4$	$2C_2'$	$2C_2''$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

Table 2.4: Character table for the dihedral group D_4.

Recall that the eight matrices $\{\pm E, \pm Z, \pm X, \pm \mathit{\Lambda}\}$ from §2.1.5 form a real two-dimensional representation of either D_4 or Q (you were supposed to figure out which). Applying the GOT with $N_G = 8$ and $d_\Gamma = 2$, we have

$$2\,E_{ik}\,E_{i'k'} + 2\,Z_{ik}\,Z_{i'k'} + 2\,X_{ik}\,X_{i'k'} + 2\,\mathit{\Lambda}_{ik}\,\mathit{\Lambda}_{i'k'} = 4\,\delta_{ii'}\,\delta_{kk'} \quad . \tag{2.88}$$

Recall $\mathit{\Lambda} = iY = -\mathit{\Lambda}^{\mathsf{T}}$, hence we may write the above relation as

$$X_{ik}\,X_{k'i'} + Y_{ik}\,Y_{k'i'} + Z_{ik}\,Z_{k'i'} = 2\,\delta_{ii'}\,\delta_{kk'} - \delta_{ik}\,\delta_{i'k'} \quad , \tag{2.89}$$

which is recognized as the familiar Pauli matrix identity $\sigma^a_{\alpha\beta}\,\sigma^a_{\mu\nu} = 2\,\delta_{\alpha\nu}\,\delta_{\beta\mu} - \delta_{\alpha\beta}\,\delta_{\mu\nu}$.

[17] Note that there is a representation labeled E, which you should take care not to confuse with the identity element.

2.4.7 Character table for $\mathbb{Z}_2 \times G$

Consider any group G with classes $\mathcal{C}_j$ and representations Γ_a and take its direct product with $\mathbb{Z}_2$, whose elements are written $\{E, \varepsilon\}$ with $\varepsilon^2 = 1$. Then $\varepsilon g = g\varepsilon$ for all $g \in G$, *i.e.* the operation ε commutes with all elements of G, hence ε forms its own class. Clearly $\mathbb{Z}_2 \times G$ has $2N_G$ elements, $\{E, g_2, \ldots, g_{N_G}, \varepsilon, \varepsilon g_2, \ldots, \varepsilon g_{N_G}\}$. The representation matrices in any representation satisfy $D(\varepsilon g) = D(\varepsilon)\, D(g)$, with $D(\varepsilon) = \pm \mathbb{1}$. Thus, each IRREP Γ_a of G spawns two IRREPs in $\mathbb{Z}_2 \times G$, labeled $\Gamma_{a\pm}$, whose representation matrices are

$$D^{\Gamma_{a\pm}}(g) = D^{\Gamma_a}(g) \qquad , \qquad D^{\Gamma_{a\pm}}(\varepsilon g) = \pm\, D^{\Gamma_a}(g) \quad . \tag{2.90}$$

Note that $\mathsf{dim}(\Gamma_{a\pm}) = \mathsf{dim}(\Gamma_a)$. The character table for $\mathbb{Z}_2 \times G$ is given in Tab. 2.5 in terms of the characters of G.

$\mathbb{Z}_2 \times G$	$\mathcal{C}_j$	$\varepsilon\,\mathcal{C}_j$
Γ_{a+}	$\chi^{\Gamma_a}(\mathcal{C}_j)$	$\chi^{\Gamma_a}(\mathcal{C}_j)$
Γ_{a-}	$\chi^{\Gamma_a}(\mathcal{C}_j)$	$-\chi^{\Gamma_a}(\mathcal{C}_j)$

Table 2.5: Character table for $\mathbb{Z}_2 \times G$.

In solid state physics, there are many structures which possess an *inversion symmetry* under $\boldsymbol{r} \to -\boldsymbol{r}$. Clearly this commutes with all rotations. Thus, the cubic group $O \cong S_4$ has 24 elements, but upon adding inversion, it becomes O_h with 48 elements. The dihedral group D_n is the symmetry group of the n-gon. Adding inversion or a horizontal reflection plane doubles its size from $2n$ to $4n$ elements, yielding the group D_{nh}.

2.4.8 Direct product representations

Given two representations (not necessarily IRREPs) Ψ_a and Ψ_b of a group G, we can form a new representation of G, written $\Psi_a \times \Psi_b$, and called the direct product representation. Given basis vectors $|\,\mathrm{e}_i\,\rangle \in \mathcal{V}$ and $|\,\tilde{\mathrm{e}}_p\,\rangle \in \mathcal{V}'$, with $1 \le i \le d_{\Psi_a}$ and $1 \le p \le d_{\Psi_b}$, the action of $\hat{D}(g)$ on the vector space $\mathcal{V} \otimes \mathcal{V}'$ in the product representation is given by

$$\hat{D}(g)\,|\,\mathrm{e}_k\,\rangle \otimes |\,\tilde{\mathrm{e}}_q\,\rangle = |\,\mathrm{e}_i\,\rangle \otimes |\,\tilde{\mathrm{e}}_p\,\rangle\, D^{\Psi_a}_{ik}(g)\, D^{\Psi_b}_{pq}(g) \quad . \tag{2.91}$$

Thus, the matrix form of $\hat{D}(g)$ in the product representation is

$$D^{\Psi_a \times \Psi_b}_{ip,\,kq}(g) = D^{\Psi_a}_{ik}(g)\, D^{\Psi_b}_{pq}(g) \quad . \tag{2.92}$$

The characters are then given by taking the trace, *i.e.*contracting with $\delta_{ik}\,\delta_{pq}$, yielding

$$\chi^{\Psi_a \times \Psi_b}(g) = \chi^{\Psi_a}(g)\,\chi^{\Psi_b}(g) \quad . \tag{2.93}$$

So the character of $g \in G$ in the product representation is the product of the characters of g in the initial representations.

We may now use Eqn. 2.61 to decompose the product representation into IRREPs, *viz.*

$$n_\Gamma(\Psi_a \times \Psi_b) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}}\, \chi^{\Gamma^*}(\mathcal{C})\, \chi^{\Psi_a}(\mathcal{C})\, \chi^{\Psi_b}(\mathcal{C}) \quad . \tag{2.94}$$

We then have

$$\Psi_a \times \Psi_b = \bigoplus_\Gamma n_\Gamma(\Psi_a \times \Psi_b)\, \Gamma \quad . \tag{2.95}$$

Eqns. 2.94 and 2.95 are extremely useful! Note that

$$d_a\, d_b = \sum_\Gamma n_\Gamma(\Psi_a \times \Psi_b)\, d_\Gamma \quad , \tag{2.96}$$

where $d_{a,b} = \dim(\Psi_{a,b})$. This is because the original matrices on the LHS of Eqn. 2.92 are of rank $d_a\, d_b$. If they are decomposed into blocks of rank d_Γ with each such block appearing n_Γ^{ab} times, the matrices must be the same size.

For practice, consider the product representation $E \times E$ of the group D_4. Consulting the character table Tab. 3.2, we see that $\left[\chi^E(\mathcal{C})\right]^2 = 4$ for $\mathcal{C} = E$ and $\mathcal{C} = C_2$, and is otherwise zero. Performing the decomposition, we find $n_\Gamma(E \times E) = 1$ for $\Gamma \in \{A_1, A_2, B_1, B_2\}$ but $n_E(E \times E) = 0$. Thus,

$$E \times E = A_1 \oplus A_2 \oplus B_1 \oplus B_2 \quad . \tag{2.97}$$

One also finds $A_2 \times B_1 = B_2$, $B_1 \times B_2 = A_1$, $B_2 \times E = B_2$, *etc.* For the group C_3, we have $\Gamma_2 \times \Gamma_2 = \Gamma_3$. All these results are consistent with the following fun fact:

- ◇ *The product of two* IRREPs $\Gamma_a \times \Gamma_b$ *contains the identity representation if and only if* $\Psi_b = \Psi_a^*$.

Direct products of different groups

Recall that the direct product $F = G \times H$ of groups G and H consists of elements (g, h) obeying the multiplication rule $(g, h)(g', h') = (gg', hh')$. Consider now a direct product of representations $\Psi_a^G \times \Psi_b^H$. The matrix representation of the product group element (g, h) is then

$$D^{\Psi_a^G \times \Psi_b^H}_{ip,kq}(g, h) = D^{\Psi_a^G}_{ik}(g)\, D^{\Psi_b^H}_{pq}(h) \quad , \tag{2.98}$$

with $1 \le i, k \le d_{\Psi_a^G}$ and $1 \le p, q \le d_{\Psi_b^H}$. The operators $\hat{D}(G \times H)$ act on basis vectors $|\, \mathrm{e}_i \,\rangle \otimes |\, \tilde{\mathrm{e}}_p \,\rangle \in \mathcal{V} \otimes \tilde{\mathcal{V}}$, according to

$$\hat{D}(g, h)\, |\, \mathrm{e}_k \,\rangle \otimes |\, \tilde{\mathrm{e}}_q \,\rangle = |\, \mathrm{e}_i \,\rangle \otimes |\, \tilde{\mathrm{e}}_p \,\rangle\, D^{\Psi_a^G}_{ik}(g)\, D^{\Psi_b^H}_{pq}(h) \quad . \tag{2.99}$$

In other words, $D^{\Psi_a^G \times \Psi_b^H}(g, h) = D^{\Psi_a^G}(g) \otimes D^{\Psi_b^H}(h)$. Thus, the character of (g, h) in this representation is

$$\chi^{\Psi_a^G \times \Psi_b^H}(g, h) = \chi^{\Psi_a^G}(g)\, \chi^{\Psi_b^H}(h) \quad , \tag{2.100}$$

and once again the character of the direct product is the product of the characters. Note that our earlier discussion fits in here if we apply the group homomorphism $G \mapsto G \times G$ where $\phi(g) = (g, g)$.

2.5 Real Representations

Here we follow the very clear discussion in §5-5 of Hammermesh. Consider an irreducible matrix representation $D(G)$ of a finite group G. We may, without loss of generality, assume $D(G)$ is a unitary, hence $D^*(G) = \overline{D}(G)$, *i.e.* the complex and adjoint representations coincide. If $D(G) = D^*(G)$, *i.e.* if $D(G)$ is real, then $\chi(g) \in \mathbb{R}$ for all $g \in G$. Conversely, if all the characters are real, then $\chi^*(g) = \chi(g)\ \forall\ g \in G$, which means that $D(G) \cong D^*(G)$[18]. The only case where $D(G)$ and $D^*(G)$ are *not* equivalent is when there are complex characters, *i.e.* $\mathrm{Im}\,\chi(g) \neq 0$ for some $g \in G$.

There are then three possibilities for the IRREPs of any finite group G:

(1) $D(G)$ is real or can be brought to real form. All characters are real: $\chi(g) \in \mathbb{R}\ \forall\ g \in G$.

(2) $D(G) \cong D^*(G)$, but cannot be brought to real form. Again, $\chi(g) \in \mathbb{R}\ \forall\ g \in G$.

(3) $D(G) \ncong D^*(G)$. Not all characters are real: $\exists\, g \in G$ s.t. $\mathrm{Im}\,\chi(g) \neq 0$.

Suppose $\chi(G) \in \mathbb{R}$, *i.e.* all the characters are real. Then we are dealing with cases (1) and (2), in which case there exists $S \in \mathsf{GL}(n,\mathbb{C})$ such that $SD(g)\,S^{-1} = \overline{D}(g) = D^*(g)$ for all $g \in G$.[19] Furthermore, this relation can be manipulated to give $S = D^{\mathsf{T}}(g)\,SD(g)$, which entails[20]

$$S^{-1}S^{\mathsf{T}} = D^{-1}(g)\,S^{-1}S^{\mathsf{T}}D(g) \tag{2.101}$$

for all $g \in G$. By Schur's first lemma, we must have $S^{-1}S^{\mathsf{T}} = \varepsilon\mathbb{1}$, *i.e.* $S^{\mathsf{T}} = \varepsilon S$. But taking the transpose of this equation gives $S = \varepsilon S^{\mathsf{T}} = \varepsilon^2 S$, which means $\varepsilon = \pm 1$. If $\varepsilon = -1$, we must have that $D(G)$ is even-dimensional, because $\det S = \det S^{\mathsf{T}} = \det(-S) = (-1)^n \det S$, where $n = \dim(G)$.

$\varepsilon = +1$ corresponds to case (1). In this case, S is both unitary and symmetric, and by Takagi's factorization[21], there exists a unitary matrix U such that $S = UU^{\mathsf{T}}$. Then $S^{-1} = U^*U^{-1}$, in which case $U^{\mathsf{T}}U\,D(g)\,U^\dagger U^* = D^*(g)$, which gives $UD(g)\,U^\dagger = U^*D^*(g)\,U^{\mathsf{T}} = \left[UD(g)\,U^\dagger\right]^*$ for all $g \in G$. Thus, $D(G)$ is unitarily equivalent to a real representation.

Note that any matrix of the form

$$S = \sum_{g\in G} D^{\mathsf{T}}(g) X D(g) \tag{2.102}$$

with X *arbitrary* satisfies $D^{\mathsf{T}}(h)\,S\,D(h) = S$ for all $h \in G$, by rearrangement. This would guarantee that $D(G) \cong D^*(G)$, so if case (3) pertains, we must have that *the RHS in Eqn. 2.102 vanishes for any X*. Thus, we must have $\sum_{g\in G} D_{ik}(g)D_{jl}(g) = 0$ for all $i,j,k,l \in \{1,\ldots,n\}$. The other two possibilities are that

[18] If $\chi^{\Gamma}(g) = \chi^{\Gamma^*}(g)$ for all $g \in G$, then applying the decomposition formula eqn. 2.61 gives $n_\Gamma(\Gamma^*) = 1$, which says that Γ and Γ^* are the same IRREP.

[19] This also tells us $\chi(g^{-1}) = \chi(g)$, since $\overline{D}(g) = D^{\mathsf{T}}(g^{-1})$.

[20] Taking the transpose, one has $D^{\mathsf{T}}(g)\,S^{\mathsf{T}}D(g) = S^{\mathsf{T}}$. Taking the inverse, $D^{-1}(g)\,S^{-1}\overline{D}(g) = S^{-1}$. Multiply to get Eqn. 2.101.

[21] Takagi [1927] proved that any complex symmetric matrix $A = A^{\mathsf{T}} \in \mathbb{C}^{n\times n}$ may be written in the form $A = VBV^{\mathsf{T}}$, where $V \in \mathsf{U}(n)$ and B is real and diagonal with all nonnegative entries. Thus $A = WB\,W^{\mathsf{T}}$ with $W \equiv V^{-1}$, in which case $B^\dagger B = W^*A^\dagger W^\dagger WA\,W^{\mathsf{T}} = W^*A^\dagger A\,W^{\mathsf{T}}$. It follows that if A is also unitary, then $B^\dagger B = \mathbb{1}$, hence $B = \mathbb{1}$ and so $A = VV^{\mathsf{T}}$. We pause to sadly recall how Mr. Takagi was ruthlessly murdered by Hans Gruber in the Bruce Willis action film *Die Hard*.

$S^{\intercal} = \varepsilon S$ with $\varepsilon = \pm 1$, corresponding to cases (1) and (2), respectively[22]. We can combine all three cases in the following equation:

$$\sum_{g\in G} D_{ik}(g)\, D_{jl}(g) = \varepsilon \sum_{g\in G} D_{jk}(g)\, D_{il}(g) \quad , \tag{2.103}$$

where $\varepsilon = 0, \pm 1$. Contracting the indices k with j and i with l then yields

$$\sum_{g\in G} \chi(g^2) = \varepsilon \sum_{g\in G} \chi^2(g) \quad . \tag{2.104}$$

For cases (1) and (2), we may invoke the GOT, taking the traces of both matrices on the LHS of Eqn. 2.30, which says $\sum_{g\in G} \chi^2(g) = N_G$. We then arrive at the following result, which is valid for any IRREP Γ:

$$\varepsilon_\Gamma = \frac{1}{N_G} \sum_{g\in G} \chi^\Gamma(g^2) \quad , \tag{2.105}$$

where $\varepsilon_\Gamma = +1, -1$, and 0 for cases (1), (2), and (3), respectively, is known as the *Frobenius-Schur indicator*.

We may immediately apply this result to C_3, whose character table is provided in Tab. 2.2 above. Note $R^2 = W$ and $W^2 = R$, so for the Γ_2 and Γ_3 representations, we have $\chi(E^2) + \chi(R^2) + \chi(W^2) = 0$, which says that neither Γ_2 nor Γ_3 is equivalent to a real representation. As a second example, consider the two-dimensional Ψ representation of the quaternion group Q, whose character table appears in Tab. 2.3. We have $(\pm E)^2 = E$ but $(\pm \mathtt{i})^2 = (\pm \mathtt{j})^2 = (\pm \mathtt{k})^2 = -E$, and since $\chi(\pm E) = \pm 2$, we have $\sum_{g\in Q} \chi(g^2) = 2 \cdot 2 + 6 \cdot (-2) = -8 = -N_G$, corresponding to $\varepsilon_\Psi = -1$. Thus $\Psi \cong \Psi^*$, but cannot be brought to real form. Indeed, we know that the elements $\mathtt{i}$, $\mathtt{j}$, and $\mathtt{k}$ in this representation may be represented by the 2×2 matrices $-iX$, $-iY$, and $-iZ$, respectively, where $\{X, Y, Z\}$ are the Pauli matrices. Thus, $D^\Psi(\pm \mathtt{i})$ and $D^\Psi(\pm \mathtt{k})$ contain complex matrix elements. Note that all the characters are still real.

There is one last bonus from this analysis. Consider an element $g \in G$ and let us ask how many elements h are there for which $g = h^2$. In other words, how many "square roots" does g have within the group? (Equivalently, how many times does g appear along the diagonal of the group multiplication table?) Call this number $\zeta(g)$. Then from Eqn. 2.105, we have

$$\sum_{g\in G} \zeta(g)\, \chi^\Gamma(g) = \varepsilon_\Gamma\, N_G \quad . \tag{2.106}$$

Note that $\zeta(g)$ does not depend on the representation Γ. Now we can use character orthogonality and the fact that $\zeta(g^{-1}) = \zeta(g)$ to derive

$$\zeta(g) = \sum_\Gamma \varepsilon_\Gamma\, \chi^\Gamma(g) \quad , \tag{2.107}$$

where the sum is now over IRREPs. For example, the number of square roots of the identity E is

$$\zeta(E) = \sum_\Gamma \varepsilon_\Gamma\, d_\Gamma \quad . \tag{2.108}$$

[22]Since $\varepsilon = 1$ is proven to correspond to case (1) and case (3) requires $\varepsilon = 0$, it must be that $\varepsilon = -1$ corresponds to case (2).

2.6 Representations of the Symmetric Group

Recall that the symmetric group S_n consists of all permutations σ on the set of n distinct elements, which we conventionally take to be the set $\{1,\ldots,n\}$. Thus i gets mapped to $\sigma(i)$. Under group multiplication, $\mu\sigma$ is the permutation mapping i to $\mu\big(\sigma(i)\big)$.

In §1.3.2, we learned how any element of the symmetric group S_n could be expressed as a product of cycles $(i_1\,i_2\,\cdots\,i_k)$, which means $\sigma(i_1)=i_2$, $\sigma(i_2)=i_3$, *etc.*, until finally $\sigma(i_k)=i_1$. For example,

$$\sigma=\begin{pmatrix}1&2&3&4&5&6&7&8\\7&2&6&8&1&3&5&4\end{pmatrix}=(175)(2)(36)(48)\quad . \tag{2.109}$$

We require that in the cyclic decomposition of any $\sigma\in S_n$, each integer $i\in\{1,\ldots,n\}$ occur exactly once. Cyclic decompositions remain invariant under cyclic permutation within the individual cycles, and under changing the order of the cycles. Thus, $(175)(2)(36)(48)$ is the same permutation as $(48)(2)(36)(175)$ or $(63)(571)(84)(2)$.

2.6.1 Partitions, Young diagrams and Young tableaux

A *partition* of a positive integer $n\in\mathbb{N}$ is a (necessarily finite) non-decreasing sequence of positive integers $\lambda=\{\lambda_1,\ldots,\lambda_k\}$ such that $\sum_{j=1}^k\lambda_j=n$. There is no known closed formula for the total number of partitions $p(n)$, although Hardy and Ramanujan proved the asymptotic formula[23]

$$p(n)\sim\frac{\exp\Big(\pi\sqrt{2n/3}\Big)}{4\sqrt{3}\,n}\quad . \tag{2.110}$$

Any cyclic decomposition of a permutation $\sigma\in S_n$ may be associated with a partition of n, where the $\{\lambda_i\}$ are the lengths of the individual cycles. Thus, in our earlier example, $\sigma=(175)(2)(36)(48)$ and $\lambda=\{3,2,2,1\}$. We can express this partition using a *Young diagram*, which is a set of empty boxes arranged in rows such that there are λ_1 boxes in row 1, *etc.*, and where the first boxes from each row are aligned in a single leftmost column. Thus,

$$\{3,2,2,1\}=\begin{array}{|c|c|c|}\hline\multicolumn{1}{c}{}&\multicolumn{1}{c}{}&\multicolumn{1}{c}{}\\\cline{1-3}\multicolumn{1}{c}{}&\multicolumn{1}{c}{}&\multicolumn{1}{c}{}\\\cline{2-3}\multicolumn{1}{c}{}&\multicolumn{1}{c}{}&\multicolumn{1}{c}{}\\\cline{2-3}\multicolumn{1}{c}{}&\multicolumn{1}{c}{}\\\cline{2-2}\end{array}\quad . \tag{2.111}$$

For obvious reasons, we call λ the *shape* of the permutation. Note that for a shape $\lambda=\{\lambda_1,\ldots,\lambda_k\}$, there are λ_1 columns and k rows in the associated Young diagram. If we want to specify a *particular* permutation, we need to label the boxes, yielding a *Young tableau*. Thus,

$$\sigma=(175)(2)(36)(48)=\begin{array}{|c|c|c|}\hline1&7&5\\\cline{1-3}3&6\\\cline{1-2}4&8\\\cline{1-2}2\\\cline{1-1}\end{array}\quad . \tag{2.112}$$

[23] Ramanujan managed to prove several other remarkable results, such as $p(5k+4)\equiv 0 \bmod 5$, $p(7k+5)\equiv 0 \bmod 7$, and $p(11k+6)\equiv 0 \bmod 11$. Given these results, one might suspect that $p(13k+7)\equiv 0 \bmod 13$, but in fact there are no additional congruences of the form $p(ak+b)\equiv 0 \bmod k$ for any prime a other than 5, 7, or 11. Number theory is often weird.

Due to the nature of cyclic permutations, this tableau is equivalent to any of the following:

$$\begin{array}{|c|c|c|}\hline 1&7&5\\\hline 3&6\\\cline{1-2}4&8\\\cline{1-2}2\\\cline{1-1}\end{array}\quad,\quad\begin{array}{|c|c|c|}\hline 5&1&7\\\hline 8&4\\\cline{1-2}3&6\\\cline{1-2}2\\\cline{1-1}\end{array}\quad,\quad\begin{array}{|c|c|c|}\hline 7&5&1\\\hline 6&3\\\cline{1-2}8&4\\\cline{1-2}2\\\cline{1-1}\end{array}\quad,\quad etc. \tag{2.113}$$

One important feature of cyclic permutations is that their length is preserved under conjugation. Thus,

$$\mu\,(175)(36)(48)(2)\,\mu^{-1} = \big(\mu(1)\,\mu(7)\,\mu(5)\big)\,\big(\mu(3)\,\mu(6)\big)\,\big(\mu(4)\,\mu(8)\big)\,\big(\mu(2)\big) \quad . \tag{2.114}$$

Thus, each shape λ specifies an equivalence class $\mathcal{C}_\lambda$, which we will simply abbreviate as λ. Recall from §1.3.2 that the number of possible decompositions of any $\sigma \in S_n$ into ν_1 1-cycles, ν_2 2-cycles, *etc.* is

$$N(\nu_1,\nu_2,\ldots,\nu_n) = \frac{n!}{1^{\nu_1}\,\nu_1!\,2^{\nu_2}\,\nu_2!\,\cdots\,n^{\nu_n}\,\nu_n!} \quad . \tag{2.115}$$

Thus $|\lambda| = N(\nu_1,\nu_2,\ldots,\nu_n)$, where the shape $\lambda = \{\lambda_1,\ldots,\lambda_k\}$ uniquely determines the set $\{\nu_1,\ldots,\nu_n\}$, according to

$$\nu_l = \sum_{i=1}^{k} \delta_{\lambda_i,\,l} \quad . \tag{2.116}$$

I.e. ν_l is the number of cycles of length l. We showed in §1.3.2 that

$$\sum_{\nu_1=0}^{\infty}\cdots\sum_{\nu_n=1}^{\infty} N(\nu_1,\nu_2,\ldots,\nu_n)\,\delta_{\nu_1+2\nu_2+\cdots+n\nu_n\,,\,n} = n! = \big|S_n\big| \quad , \tag{2.117}$$

so we have indeed accounted for all the equivalence classes.

2.6.2 S_3 and S_4

For the case $n = 3$, there are three classes, corresponding to the Young diagrams $\begin{array}{|c|}\hline\\\hline\\\hline\end{array}$, $\begin{array}{|c|c|}\hline\\\hline\\\cline{1-1}\end{array}$, and $\begin{array}{|c|c|c|}\hline\\\hline\end{array}$, of orders 1, 3, and 2, respectively. What about the IRREPs? We immediately know two one-dimensional IRREPs, namely the trivial IRREP $\Gamma_{\rm triv}$ and the sign IRREP $\Gamma_{\rm sgn}$. In the case of $D_3 \simeq S_3$, we called these IRREPs A_1 and A_2, respectively (see Tab. 2.1). The remaining representation of D_3, which we called E, is called the *standard representation* $\Gamma_{\rm std}$ of the S_3. Indeed, there is a standard representation for each S_n, and here is how to identify it. Start with the defining representation, which as you should recall from §1.3.2 is the n-dimensional representation in which $D_{ij}(\sigma) = \delta_{i\,,\,\sigma(j)}$. Acting on the vector space $\mathbb{R}^n$, this is clearly reducible because the one-dimensional subspace spanned by the vector $\boldsymbol{\psi}$ where $\psi_i = 1$ for all i is an invariant subspace. Since $D(\sigma)\,\boldsymbol{\psi} = \boldsymbol{\psi}$ for all $\sigma \in S_n$, we have that $\Gamma_{\rm def} = \Gamma_{\rm std} \oplus \Gamma_{\rm triv}$, *i.e.* the defining representation is a direct sum of the trivial representation and an $(n-1)$-dimensional representation $\Gamma_{\rm std}$ which turns out to be irreducible. Furthermore, since the characters of representations in direct sums are additive (see eqn. 2.65), we have $\chi^{\Gamma_{\rm std}}(\lambda) = \chi^{\Gamma_{\rm def}}(\lambda) - \chi^{\Gamma_{\rm triv}}(\lambda) = \chi^{\Gamma_{\rm def}}(\lambda) - 1$. Now in $\Gamma_{\rm def}$, the character of any element σ is simply the number of entries in the sequence $\{1\,2\,\cdots\,n\}$ which remain fixed by the action of σ. This is the number ν_1 of one-cycles in the corresponding partition λ. Thus

S_3			
N_λ	1	3	2
Γ_{triv}	1	1	1
Γ_{sgn}	1	-1	1
Γ_{std}	2	0	-1

Table 2.6: Character table for the symmetric group S_3.

$\chi^{\Gamma_{\text{def}}}\left(\text{}\right) = 3$, $\chi^{\Gamma_{\text{def}}}\left(\text{}\right) = 1$, and $\chi^{\Gamma_{\text{def}}}\left(\text{}\right) = 0$. We thus arrive at the character table in Tab. 2.6, which is of course identical to that of Tab. 2.1 for D_3. Note that

$$\sum_\lambda N_\lambda = \sum_\Gamma d_\Gamma^2 = 6 = \big|S_3\big| \quad . \tag{2.118}$$

Now let's consider the case of S_4. There are now five classes: , , , , and . Regarding the sign representation, we know that $\chi^{\Gamma_{\text{sgn}}}(\lambda)$ is given by $(-1)^{\#\text{ of cycles of even length}}$. Regarding the standard representation, of dimension $n-1=3$, we can compute the its characters from the formula $\chi^{\Gamma_{\text{std}}}(\lambda) = \nu_1(\lambda) - 1$ as described above. Thus far we have found three IRREPs, but there are five classes so two IRREPs are missing. One is formed by taking the product $\Gamma_{\text{std}} \times \Gamma_{\text{sgn}}$. This is also of dimension three. Since $1^2 + 1^2 + 3^2 + 3^2 = 20$, we know that the last IRREP, which we call Γ', is two-dimensional. We arrive at the partial table of Tab. 2.7.

S_4					
N_λ	1	6	3	8	6
Γ_{triv}	1	1	1	1	1
Γ_{sgn}	1	-1	1	1	-1
Γ_{std}	3	1	-1	0	-1
$\Gamma_{\text{std}} \times \Gamma_{\text{sgn}}$	3	-1	-1	0	1
Γ'	2	a	b	c	d

Table 2.7: Partial character table for the symmetric group S_4.

To determine the missing characters, we invoke row orthogonality, which yields the four equations

$$\begin{aligned} 0 &= 2 + 6a + 3b + 8c + 6d \\ 0 &= 2 - 6a + 3b + 8c - 6d \\ 0 &= 6 + 6a - 3b - 6d \\ 0 &= 6 - 6a - 3b + 6d \quad . \end{aligned} \tag{2.119}$$

Solving them is a simple matter and we readily find $a = 0$, $b = 2$, $c = -1$, and $d = 0$.

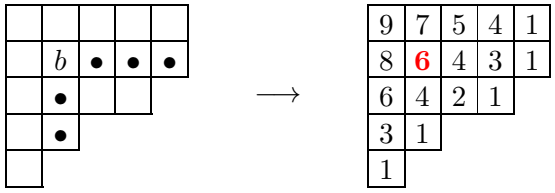
When we get to S_5, we will find that there are seven conjugacy classes, and therefore seven IRREPs. Is there a general way to count the dimensions of the IRREPs of S_n? Funny you should ask.

2.6.3 IRREPs of S_n

Recall that the number of equivalence classes is the number of IRREPs. For the symmetric group, each shape λ corresponds to an IRREP Γ^λ of S_n[24]. What is its dimension $f^\lambda = \dim(\Gamma^\lambda)$? It may be computed from the *hook length formula*,

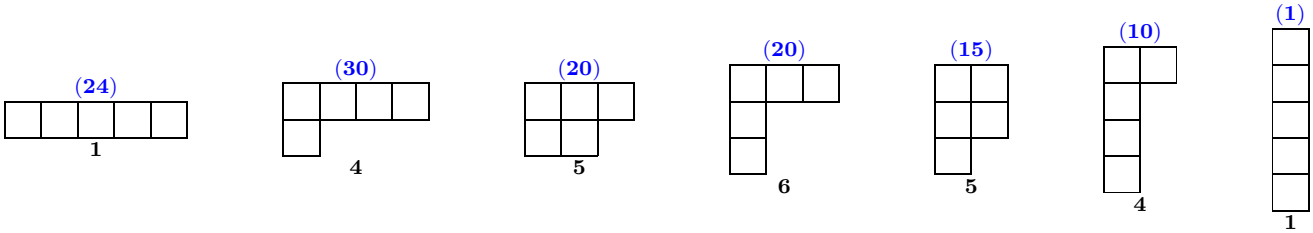
$$f^\lambda = \dim(\Gamma^\lambda) = \frac{n!}{\prod_{b\in\lambda} h_\lambda(b)} \quad , \tag{2.120}$$

where the product in the denominator is over all boxes b of the Young diagram for λ, and $h_\lambda(b)$ is the *hook length* for the box b, which is the total number of boxes in a 'hook' whose vertex is b, with legs extending rightward and downward. For example,



(2.121)

The proof is technical and interested students may consult the book of B. Sagan for details. For our immediate purposes here, let's just see how all this works in practice. Consider the case $n = 5$, for which $|S_n| = 5! = 120$. Behold the seven IRREPs of S_5:



These correspond, respectively, to the shapes $\lambda = (5)$, $(4,1)$, $(3,2)$, $(3,1,1)$, $(2,2,1)$, $(2,1,1,1)$, and $(1,1,1,1,1)$. Each Young diagram is labeled by a subscript which is the dimension dimension $f^\lambda = |\Gamma^\lambda|$

[24] This is perhaps not obvious, but it turns out that the Young tableaux corresponding to a given partition λ may be arranged into a vector space S^λ on which the elements of S_n act, called a *Specht module*. For details, see the books by B. Sagan and W. Fulton listed in chapter 0.

of the corresponding IRREP as computed from the hook length formula, and a superscript $(|\lambda|)$ which is the number of elements in the corresponding equivalence class, as computed from Eqn. 2.115. Note that the sums of the squares of the dimensions of the IRREPs is equal to the sum of the number of elements of each equivalence class is equal to the order of the group S_5:

$$1^2 + 4^2 + 5^2 + 6^2 + 5^2 + 4^2 + 1^2 = 24 + 30 + 20 + 20 + 15 + 10 + 1 = 120 = |S_5| \quad .$$

2.7 Application of Projection onto IRREPs : Triatomic Molecule

Fig. 2.1 shows a planar configuration of three equal masses m connected by identical springs k. Each mass may move in the x and y directions, hence the molecule has six degrees of freedom. As a small oscillations problem in classical mechanics, one solves the equation $\omega^2\,\mathrm{T}\,\boldsymbol{\psi} = \mathrm{V}\boldsymbol{\psi}$, where T and V are the kinetic energy and potential energy matrices, given by the expressions $\mathrm{T}_{nn'} = \left[\partial^2 T(\boldsymbol{q},\dot{\boldsymbol{q}})/\partial\dot{q}_n\partial\dot{q}_{n'}\right]_{\boldsymbol{q}^0}$ and $\mathrm{V}_{nn'} = \left[\partial^2 V(\boldsymbol{q})/\partial q_n \partial q_{n'}\right]_{\boldsymbol{q}^0}$, evaluated at equilibrium, with $\boldsymbol{q}$ the set of generalized coordinates. Here we will find the eigenvectors $\boldsymbol{\psi}_a$ using group theory, without diagonalizing any matrices.

We choose as generalized coordinates the Cartesian x and y positions of each mass relative to the center of the triangle. The equilibrium coordinates of mass #1 are $(0,1)\,\frac{a}{\sqrt{3}}$, of mass #2 $(-\frac{\sqrt{3}}{2},-\frac{1}{2})\,\frac{a}{\sqrt{3}}$, and of mass #3 $(\frac{\sqrt{3}}{2},-\frac{1}{2})\,\frac{a}{\sqrt{3}}$. The symmetry group is D_3, whose character table is provided in Tab. 2.1. Group elements are represented by matrices $D(g)$ acting on the column vector given by the transpose of $\boldsymbol{\psi}^{\mathsf{T}} = (\delta x_1, \delta y_1, \delta x_2, \delta y_2, \delta x_3, \delta y_3)$, the vector of displacements relative to equilibrium. This is a six dimensional representation given by $\Gamma = \Upsilon \times E$, where the Υ and E representations are given in §2.3.1. The reason for this is that the group element R, for example, not only rotates the Cartesian coordinates; it also exchanges the positions of the masses, *i.e.* it switches their labels. This is a six-dimensional representation, and using the decomposition formula we find $\Upsilon = A_1 \oplus E$ and $\Upsilon \times E = A_1 \oplus A_2 \oplus E \oplus E$. The matrices are

$$D(I) = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \qquad D(R) = \begin{pmatrix} 0 & 0 & R \\ R & 0 & 0 \\ 0 & R & 0 \end{pmatrix} \qquad D(W) = \begin{pmatrix} 0 & W & 0 \\ 0 & 0 & W \\ W & 0 & 0 \end{pmatrix}$$

$$D(\sigma) = \begin{pmatrix} \sigma & 0 & 0 \\ 0 & 0 & \sigma \\ 0 & \sigma & 0 \end{pmatrix} \qquad D(\sigma') = \begin{pmatrix} 0 & 0 & \sigma' \\ 0 & \sigma' & 0 \\ \sigma' & 0 & 0 \end{pmatrix} \qquad D(\sigma'') = \begin{pmatrix} 0 & \sigma'' & 0 \\ \sigma'' & 0 & 0 \\ 0 & 0 & \sigma'' \end{pmatrix} \quad . \tag{2.122}$$

where

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad R = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \qquad W = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$\sigma = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \sigma' = \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \qquad \sigma'' = \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \quad . \tag{2.123}$$

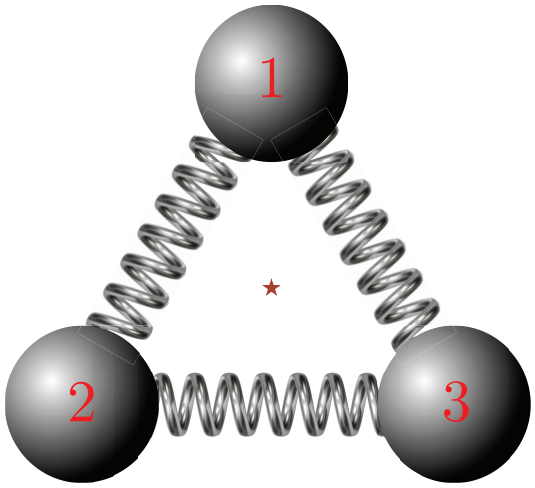


Figure 2.1: A planar molecule modeled as three masses m connected by springs, in the shape of an equilateral triangle. The symmetry is C_{3v}.

We simplify our notation and use g to denote the 2×2 matrix $D^E(g)$ in the E IRREP, and we call the identity I instead of E to obviate any potential confusion with the IRREP E.

Starting with a general rank six vector $\boldsymbol{\psi}^{\mathsf{T}} = \begin{pmatrix} a & b & c & d & e & f \end{pmatrix}$, we find

$$D(I)\,\boldsymbol{\psi} = \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix} \quad , \quad D(R)\,\boldsymbol{\psi} = \frac{1}{2}\begin{pmatrix} -e - \sqrt{3}\,f \\ \sqrt{3}\,e - f \\ -a - \sqrt{3}\,b \\ \sqrt{3}\,a - b \\ -c - \sqrt{3}\,d \\ \sqrt{3}\,c - d \end{pmatrix} \quad , \quad D(W)\,\boldsymbol{\psi} = \frac{1}{2}\begin{pmatrix} -c + \sqrt{3}\,d \\ -\sqrt{3}\,c - d \\ -e + \sqrt{3}\,f \\ -\sqrt{3}\,e - f \\ -a + \sqrt{3}\,b \\ -\sqrt{3}\,a - b \end{pmatrix} \tag{2.124}$$

and

$$D(\sigma)\,\boldsymbol{\psi} = \begin{pmatrix} -a \\ b \\ -e \\ f \\ -c \\ d \end{pmatrix} \quad , \quad D(\sigma')\,\boldsymbol{\psi} = \frac{1}{2}\begin{pmatrix} e + \sqrt{3}\,f \\ \sqrt{3}\,e - f \\ c + \sqrt{3}\,d \\ \sqrt{3}\,c - d \\ a + \sqrt{3}\,b \\ \sqrt{3}\,a - b \end{pmatrix} \quad , \quad D(\sigma'')\,\boldsymbol{\psi} = \frac{1}{2}\begin{pmatrix} c - \sqrt{3}\,d \\ -\sqrt{3}\,c - d \\ a - \sqrt{3}\,b \\ -\sqrt{3}\,a - b \\ e - \sqrt{3}\,f \\ -\sqrt{3}\,e - f \end{pmatrix} \quad . \tag{2.125}$$

Now let's project! We first project onto A_1, where, from Eqn. 2.66,

$$\Pi^{A_1} = \frac{1}{6}\Big\{ D(I) + D(R) + D(W) + D(\sigma) + D(\sigma') + D(\sigma'') \Big\} \quad . \tag{2.126}$$

Adding up the various contributions, we find $\Pi^{A_1}\,\boldsymbol{\psi} = \frac{1}{2\sqrt{3}}\left(2b - \sqrt{3}\,c - d + \sqrt{3}\,e - f\right)\hat{\mathbf{e}}^{A_1}$, where the components of $\hat{\mathbf{e}}^{A_1}$, expressed as a row vector, are

$$\hat{\mathbf{e}}^{A_1} = \tfrac{1}{\sqrt{3}}\begin{pmatrix} 0 & 1 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad . \tag{2.127}$$

Next, we project onto A_2, with

$$\Pi^{A_2} = \frac{1}{6}\Big\{ D(I) + D(R) + D(W) - D(\sigma) - D(\sigma') - D(\sigma'') \Big\} \quad . \tag{2.128}$$

Adding up the various contributions, we find $\Pi^{A_2}\,\boldsymbol{\psi} = \frac{1}{2\sqrt{3}}\left(2a - c + \sqrt{3}\,d - e - \sqrt{3}\,f\right)\hat{\mathbf{e}}^{A_2}$, where the components of $\hat{\mathbf{e}}^{A_2}$ are

$$\hat{\mathbf{e}}^{A_2} = \tfrac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \end{pmatrix} \quad . \tag{2.129}$$

Note that $\hat{\mathbf{e}}^{A_1}\cdot\hat{\mathbf{e}}^{A_2} = 0$ because the A_1 and A_2 IRREPs correspond to orthogonal subspaces.

Note also that $\hat{\mathbf{e}}^{A_1}$ is orthogonal to the following mutually orthogonal vectors:

$$\begin{aligned} \hat{\mathbf{e}}^{x} &= \tfrac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} \\ \hat{\mathbf{e}}^{y} &= \tfrac{1}{\sqrt{3}}\begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix} \\ \hat{\mathbf{e}}^{\phi} &= \tfrac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \end{pmatrix} \quad . \end{aligned} \tag{2.130}$$

These vectors, as you may have guessed, correspond to the three zero modes for our problem: translations along $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$, and rotations about the $\hat{\boldsymbol{z}}$ axis through the center of the triangle. These vectors are obtained by the action of the Lie algebra generators for the continuous translation groups $\mathbb{R}$ and rotation group $\mathsf{SO}(2)$. Infinitesimal translations result in $x_i \to x_i + \varepsilon_x$ and $y_i \to y_i + \varepsilon_y$. To obtain $\hat{\mathbf{e}}^{\phi}$, perform an infinitesimal rotation $\exp(\varepsilon_\phi M)$, where $M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma^y$ upon each of the (x_i^0, y_i^0) pairs of equilibrium coordinates:

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} -\sqrt{3}/2 \\ -1/2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix} \quad , \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} \sqrt{3}/2 \\ -1/2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix} \quad . \tag{2.131}$$

As for $\hat{\mathbf{e}}^{A_2}$, it too is orthogonal to $\hat{\mathbf{e}}^{x,y}$, but we find that $\hat{\mathbf{e}}^{A_2} = \hat{\mathbf{e}}^{\phi}$, which tells us that that the infinitesimal rotation transforms according to the A_2 IRREP of D_3. According to what IRREP do you suppose the two infinitesimal translations transform?

Finally, we come to the E representation, which is two-dimensional. We construct the projectors $\Pi^E_{\mu\nu}$ for $(\mu,\nu) = (1,1)$ and $(\mu,\nu) = (2,1)$:

$$\begin{aligned} \Pi^E_{1,1} &= \frac{1}{3}\Big\{ D(I) - \tfrac{1}{2}\,D(R) - \tfrac{1}{2}\,D(W) - D(\sigma) + \tfrac{1}{2}\,D(\sigma') + \tfrac{1}{2}\,D(\sigma'') \Big\} \\ \Pi^E_{2,1} &= \frac{1}{3}\Big\{ \tfrac{\sqrt{3}}{2}\,D(R) - \tfrac{\sqrt{3}}{2}\,D(W) + \tfrac{\sqrt{3}}{2}\,D(\sigma') - \tfrac{\sqrt{3}}{2}\,D(\sigma'') \Big\} \quad . \end{aligned} \tag{2.132}$$

We find

$$\begin{aligned} \Pi^E_{1,1}\,\boldsymbol{\psi} &= \tfrac{1}{\sqrt{3}}\,(a + c + e)\,\hat{\mathbf{e}}^{x} + \tfrac{1}{\sqrt{3}}\,(a - \tfrac{1}{2}\,c - \tfrac{\sqrt{3}}{2}\,d - \tfrac{1}{2}\,e + \tfrac{\sqrt{3}}{2}\,f)\,\hat{\mathbf{e}}^{E,1} \\ \Pi^E_{2,1}\,\boldsymbol{\psi} &= \tfrac{1}{\sqrt{3}}\,(a + c + e)\,\hat{\mathbf{e}}^{y} + \tfrac{1}{\sqrt{3}}\,(a - \tfrac{1}{2}\,c - \tfrac{\sqrt{3}}{2}\,d - \tfrac{1}{2}\,e + \tfrac{\sqrt{3}}{2}\,f)\,\hat{\mathbf{e}}^{E,2} \quad , \end{aligned} \tag{2.133}$$

where

$$\begin{aligned}\hat{\mathbf{e}}^{E,1} &= \tfrac{1}{\sqrt{3}}\begin{pmatrix}1 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \frac{\sqrt{3}}{2}\end{pmatrix} \\ \hat{\mathbf{e}}^{E,2} &= \tfrac{1}{\sqrt{3}}\begin{pmatrix}0 & -1 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} & \frac{1}{2}\end{pmatrix} \quad .\end{aligned} \tag{2.134}$$

Note that the projection onto the rows of E does not annihilate the components parallel to $\hat{\mathbf{e}}^{x,y}$. The student should pause for contemplation to understand why this is so. We now have derived six mutually orthogonal vectors: $\{\hat{\mathbf{e}}^{A_1}\,,\,\hat{\mathbf{e}}^{A_2}\,,\,\hat{\mathbf{e}}^{E,1}\,,\,\hat{\mathbf{e}}^{E,2}\,,\,\hat{\mathbf{e}}^{x}\,,\,\hat{\mathbf{e}}^{y}\}$, with $\hat{\mathbf{e}}^{\phi} = \hat{\mathbf{e}}^{A_2}$.

Getting back to our small oscillations problem, the potential energy is given by

$$V(\delta x_1,\delta y_1,\delta x_2,\delta y_2,\delta x_3,\delta y_3) = \tfrac{1}{2}k\left(|\boldsymbol{r}_1-\boldsymbol{r}_2|-a\right)^2 + \tfrac{1}{2}k\left(|\boldsymbol{r}_2-\boldsymbol{r}_2|-a\right)^2 + \tfrac{1}{2}k\left(|\boldsymbol{r}_3-\boldsymbol{r}_2|-a\right)^2 \quad . \tag{2.135}$$

To quadratic order in the displacements from equilibrium, we find

$$\begin{aligned}|\boldsymbol{r}_1-\boldsymbol{r}_2|-a &= \tfrac{1}{2}\,\delta x_1 - \tfrac{1}{2}\,\delta x_2 + \tfrac{\sqrt{3}}{2}\,\delta y_1 - \tfrac{\sqrt{3}}{2}\,\delta y_2 + \ldots \\ |\boldsymbol{r}_2-\boldsymbol{r}_3|-a &= \delta x_3 - \delta x_2 + \ldots \\ |\boldsymbol{r}_3-\boldsymbol{r}_1|-a &= \tfrac{1}{2}\,\delta x_3 - \tfrac{1}{2}\,\delta x_1 - \tfrac{\sqrt{3}}{2}\,\delta y_3 + \tfrac{\sqrt{3}}{2}\,\delta y_1 + \ldots \quad .\end{aligned} \tag{2.136}$$

The potential energy is then

$$\begin{aligned}V(\delta x_1,\delta y_1,\delta x_2,\delta y_2,\delta x_3,\delta y_3) = \tfrac{1}{2}k\left[\tfrac{1}{2}\big(\delta x_1-\delta x_2\big)+\tfrac{\sqrt{3}}{2}\big(\delta y_1-\delta y_2\big)\right]^2 + \tfrac{1}{2}k\left(\delta x_2-\delta x_3\right)^2 + \\ \tfrac{1}{2}k\left[\tfrac{1}{2}\big(\delta x_3-\delta x_1\big)-\tfrac{\sqrt{3}}{2}\big(\delta y_3-\delta y_1\big)\right]^2 + \ \ldots\end{aligned} \tag{2.137}$$

and from this one can take the second derivatives by inspection and form the V-matrix. Since we have computed the IRREP projections correctly, we can obtain the eigenvalues of V by performing only one row $\times$ column multiply for each IRREP. One finds that the eigenvalues are $3k$ for the A_1 IRREP and $\frac{3}{2}k$ for the E IRREP. The T-matrix is m times the unit matrix, where m is the mass of each "ion", and therefore the eigenfrequencies are $\omega_{A_1} = \sqrt{3k/m}$ and $\omega_E = \sqrt{3k/2m}$, and of course $\omega_{A_2} = \omega_{E'} = 0$, where E' is a second E doublet corresponding to the translations.

It is instructive to consider the effect of an additional potential,

$$\begin{aligned}V'(\delta x_1,\delta y_1,\delta x_2,\delta y_2,\delta x_3,\delta y_3) &= \tfrac{1}{2}k'\big(|\boldsymbol{r}_1|-\tfrac{1}{\sqrt{3}}a\big)^2 + \tfrac{1}{2}k'\big(|\boldsymbol{r}_2|-\tfrac{1}{\sqrt{3}}a\big)^2 + \tfrac{1}{2}k'\big(|\boldsymbol{r}_3|-\tfrac{1}{\sqrt{3}}a\big)^2 \\ &= \tfrac{1}{2}k'y_1^2 + \tfrac{1}{2}k'\big(\tfrac{\sqrt{3}}{2}x_2+\tfrac{1}{2}y_2\big)^2 + \big(\tfrac{\sqrt{3}}{2}\,x_3-\tfrac{1}{2}y_3\big)^2 + \ldots \quad ,\end{aligned} \tag{2.138}$$

where $a/\sqrt{3}$ is the distance from the center of the triangle to any of the equilibrium points. This potential breaks the translational symmetry but preserves the rotational symmetry, so we expect only one zero mode to remain, corresponding to $\hat{\mathbf{e}}^{A_2} = \hat{\mathbf{e}}^{\phi}$. The energy of the A_1 breathing mode will be shifted due to the new potential. It is a good exercise to work out the effect on the E modes. It turns out that V' leads to a coupling between the two E doublets we have derived. The resulting spectrum will then have two finite frequency doublets each transforming as E. Solve to unlock group theory achievement, level D_3.

2.8 Jokes for Chapter Two

I feel that this chapter was not as funny as the previous one, so I will end with a couple of jokes:

JOKE #1 : A duck walks into a pharmacy and waddles back to the counter. The pharmacist looks down at him and says, "Hey there, little fella! What can I do for you?" "I'd like a box of condoms please," answers the duck. The pharmacist says, "No problem! Would you like me to put that on your bill?" The duck replies, "I'm not that kind of duck."

JOKE #2 : A theorist brings his car to his experimentalist friend and complains that it has been stalling out lately. The experimenter opens the hood and starts poking around. After a few minutes, the engine is idling smoothly. "So what's the story?" asks the theorist. "Meh. Just crap in the carburetor," replies the experimenter. The theorist says, "How often do I have to do that?"

Chapter 3

Group Theory and Quantum Mechanics

As a refresher on various True Facts about linear algebra relevant to quantum mechanics, please review the Appendix §3.3.

3.1 Hilbert Space and Group Symmetries

3.1.1 Classification of the basis states

The realization of symmetries in quantum mechanics is expressed through the action of unitary operator representations $\hat{U}(G)$ of some symmetry group G which act on the Hilbert space $\mathcal{H}$ of states. If $\left[\hat{H}, \hat{U}(g)\right] = 0$ for all $g \in G$, *i.e.* the Hamiltonian commutes with all symmetry operations from G, its eigenspectrum arranges into multiplets, each of which transforms according to some IRREP Γ of G, with corresponding degeneracy d_Γ. Thus, at the outset, one thing group theory can do for us is to provide us with a useful set of basis states $|\, \Gamma\mu,\, l \,\rangle$ in $\mathcal{H}$ which are identified by three labels (Γ, μ, l):

(i) The representation index Γ labels am IRREP of the symmetry group G.

(ii) The basis index $\mu \in \{1, \ldots, d_\Gamma\}$ labels the basis states within the Γ representation.

(iii) The additional index l labels different invariant subspaces transforming according to the same representation. This allows for other quantum numbers not associated with the group symmetry.

Where do these basis states come from? We can generate them via the projection method, which we will discuss in §3.1.5 below.

Such a basis can greatly simplify the diagonalization of our quantum Hamiltonian $\hat{H}$, because, as we shall see,

$$\left\langle\, \Gamma\mu, l \,\middle|\, \hat{H} \,\middle|\, \Gamma'\mu', l' \,\right\rangle = \delta_{\Gamma\Gamma'}\, \delta_{\mu\mu'}\, H^{\Gamma}_{ll'} \quad . \tag{3.1}$$

However, in general the projection method does not guarantee that the basis states $|\,\Gamma\mu,\,l\,\rangle$ are orthogonal. Rather, we have

$$\langle\,\Gamma\mu,l\,|\,\Gamma'\mu',l'\,\rangle = \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,O^{\Gamma}_{ll'} \quad , \tag{3.2}$$

where $O^{\Gamma}_{ll'}$ is the *overlap matrix*. Group theory tells us that basis states which transform according to different IRREPs are necessarily orthogonal, but it says nothing about the overlap of basis states transforming according to two copies of the same IRREP. Thus, we are left with the task of simultaneously diagonalizing the two Hermitian matrices H^{Γ} and O^{Γ}, *i.e.* solving the linear system $H^{\Gamma}_{ll'}\,\phi^{\Gamma s}_{l'} = E_{\Gamma s}\,O^{\Gamma}_{ll'}\,\phi^{\Gamma s}_{l'}$, where s labels the eigenvalue and corresponding eigenfunctions of the $s^{\rm th}$ occurrence of the IRREP Γ. The eigenstates of $\hat H$ then satisfy $\hat H\,\big|\,\Gamma\mu,s\,\big\rangle = E_{\Gamma s}\,\big|\,\Gamma\mu,s\,\big\rangle$ with $\langle\,\Gamma\mu,s\,|\,\Gamma'\mu',s'\,\rangle = \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,\delta_{ss'}$. The index s is necessary because any given IRREP generally occurs several times in the eigenspectrum. This means we can write

$$\hat H = \sum_{\Gamma,s} E_{\Gamma,\,s}\,\hat\Pi^{\Gamma,\,s} \qquad , \qquad \hat\Pi^{\Gamma,\,s} \equiv \sum_{\mu}\big|\,\Gamma\mu,s\,\big\rangle\,\big\langle\,\Gamma\mu,s\,\big| \quad , \tag{3.3}$$

where $\hat\Pi^{\Gamma,\,s}$ is the projector onto the $s^{\rm th}$ occurrence of IRREP Γ.

Example: The Hamiltonian $\hat H = \frac{p^2}{2m} + V(x)$ commutes with the operators $\{1,\mathtt{P}\}$, where $\mathtt{P} = \mathtt{P}^{-1} = \mathtt{P}^\dagger$ is the parity operator, with $\mathtt{P}\,x\,\mathtt{P} = -x$ and $\mathtt{P}\,p\,\mathtt{P} = -p$. Thus, $[\hat H,\mathtt{P}] = 0$ and we can classify all eigenstates of $\hat H$ by representations of $\mathbb{Z}_2$, of which there are only two: Γ_1 (trivial) and Γ_2 (sign). Both IRREPs are one-dimensional, so the μ index is unnecessary. Starting with any set $\big\{\psi_l(x)\big\}$ of L^2-integrable functions on $\mathbb{R}$, we can project onto the trivial (symmetric) and sign (antisymmetric) representations of $\mathbb{Z}_2$, forming $\varphi_{l,\pm} \equiv \psi_l(x) \pm \psi_l(-x)$. While the $\mathbb{Z}_2$ symmetry guarantees that $\langle\,\varphi_{l,\sigma}\,|\,\varphi_{l',\sigma'}\,\rangle$ vanishes if $\sigma \neq \sigma'$, there is no symmetry consideration guaranteeing that basis states within the same IRREP are orthonormal[1].

Diagonalizing $\hat H$ within each of these subspaces yields the *orthonormal* eigenfuntions $\psi^{(\Gamma_1)}_s(x) = \langle\,x\,|\,\Gamma_1 s\,\rangle$ and $\psi^{(\Gamma_2)}_s(x) = \langle\,x\,|\,\Gamma_2 s\,\rangle$ may be taken to be the $s^{\rm th}$ lowest energy eigenfunctions in the even and odd parity sectors, respectively. These energy eigenstates interleave, with the $n^{\rm th}$ energy level having $n-1$ nodes and parity eigenvalue $P = (-1)^{n-1}$.

Example': In later chapters we shall discuss representations of Lie groups, but you already know that for $G = \mathsf{SU}(2)$, the representations are classified by total spin $S \in \frac12\mathbb{Z}$, and that the dimension of each spin-S representation is $d_S = 2S+1$. In a system of N spin-$\frac12$ objects, with N even, one can form representations with integer $S \in \big\{0,1,\ldots,\frac12 N\big\}$. The number of spin-$S$ multiplets is given by[2]

$$M_S = \binom{N}{\frac12 N + S} - \binom{N}{\frac12 N + S + 1} \quad . \tag{3.4}$$

Each of these M_S multiplets is $(2S+1)$-fold degenerate. The Hilbert space basis vectors may be expressed as $|\,S,m,l\,\rangle$, where S labels the representation, $m \in \{-S,\ldots,+S\}$ is the polarization, and l labels the M_S different spin-S multiplets.

[1] For example, we could take $\varphi_{l,+}(x) = A_l x^{2l}\,e^{-x}$ and $\varphi_{l,-}(x) = B_l x^{2l+1}\,e^{-x}$.

[2] This expression counts the difference in the number of states with $S^z = S$ and with $S^z = S+1$. The difference is the number of multiplets in which $S^z = S$ appears but not $S^z = S+1$, and is therefore the number of spin-S multiplets.

3.1.2 Accidental degeneracies

In general,

- ◇ *For a Hamiltonian $\hat{H}$ where $\big[\hat{H}, \hat{U}(G)\big] = 0$, each group of eigenstates transforming according to a representation Γ is d_Γ-fold degenerate. Any degeneracies not associated with the group symmetry are said to be accidental.*

Accidental degeneracies can be removed by varying parameters in the Hamiltonian without breaking the underlying symmetry. As an example, consider the case of a Hilbert space with six states, labeled $\big\{|\,u_1\,\rangle, |\,v_1\,\rangle, |\,u_2\,\rangle, |\,v_2\,\rangle, |\,u_3\,\rangle, |\,v_3\,\rangle\big\}$ and the Hamiltonian

$$\hat{H} = -\sum_{n=1}^{3}\Big[t_0\Big(|\,u_n\,\rangle\langle\,u_{n+1}\,| + |\,u_{n+1}\,\rangle\langle\,u_n\,| + |\,v_n\,\rangle\langle\,v_{n+1}\,| + |\,v_{n+1}\,\rangle\langle\,v_n\,|\Big) + t_1\Big(|\,u_n\,\rangle\langle\,v_n\,| + |\,v_n\,\rangle\langle\,u_n\,|\Big)\Big] \tag{3.5}$$

where $|\,u_4\,\rangle \equiv |\,u_1\,\rangle$ and $|\,v_4\,\rangle \equiv |\,v_1\,\rangle$. The geometry is sketched in Fig. 3.1.

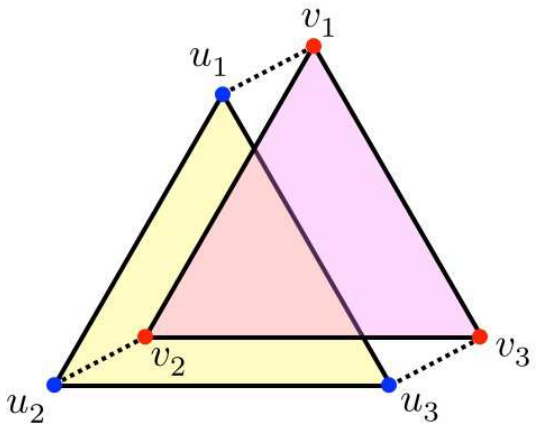


Figure 3.1: Six site cluster with D_{3h} symmetry. Solid bonds between orbitals signify matrix element $-t_0$, while dashed bonds signify matrix element $-t_1$.

The Hamiltonian is symmetric under the symmetry group C_{3v}, which has six elements, corresponding to the symmetries of the equilateral triangle. In fact, this model has an enlarged symmetry, since it is also symmetric under a reflection σ_h in the horizontal plane, which interchanges the orbitals $|\,u_n\,\rangle \leftrightarrow |\,v_n\,\rangle$, corresponding to the group D_{3h}. The group D_{nh} has $4n$ elements and is generated by three elements: a $\frac{2\pi}{n}$ rotation r, a vertical reflection σ_v, and a horizontal reflection σ_h. Its presentation is

$$D_{nh} \;:\; \big\langle\, r\,,\, \sigma_v\,,\, \sigma_h \,\big|\, r^n,\, \sigma_v^2\,,\, \sigma_h^2\,,\, (\sigma_v\, r)^2\,,\, (\sigma_v\,\sigma_h)^2\,,\, \sigma_h\, r\,\sigma_h\, r^{n-1}\,\big\rangle \quad . \tag{3.6}$$

The character table for D_{3h} is given in Tab. 3.1.

The Hamiltonian $\hat{H}$ in Eqn. 3.5 is known as a "tight binding model" and its diagonalization is sufficiently simple that those with a rudimentary background in solid state physics can do so by inspection.

Explicitly, define the states

$$|\,\hat{u}_j\,\rangle = \frac{1}{\sqrt{3}}\sum_{n=1}^{3} e^{-2\pi ijn/3}\,|\,u_n\,\rangle \qquad , \qquad |\,\hat{v}_j\,\rangle = \frac{1}{\sqrt{3}}\sum_{n=1}^{3} e^{-2\pi ijn/3}\,|\,v_n\,\rangle \quad . \tag{3.7}$$

with $j \in \{-1, 0, +1\}$. This is a simple discrete Fourier transform whose inverse is

$$|\,u_n\,\rangle = \frac{1}{\sqrt{3}}\sum_{j=-1}^{1} e^{2\pi ijn/3}\,|\,\hat{u}_j\,\rangle \qquad , \qquad |\,v_n\,\rangle = \frac{1}{\sqrt{3}}\sum_{j=-1}^{1} e^{2\pi ijn/3}\,|\,\hat{v}_j\,\rangle \quad . \tag{3.8}$$

One then has

$$\hat{H} = -\sum_{j=-1}^{1}\Big[2t_0\cos(2\pi j/3)\Big(|\,\hat{u}_j\,\rangle\langle\,\hat{u}_j\,| + |\,\hat{v}_j\,\rangle\langle\,\hat{v}_j\,|\Big) + t_1\Big(|\,\hat{u}_j\,\rangle\langle\,\hat{v}_j\,| + |\,\hat{v}_j\,\rangle\langle\,\hat{u}_j\,|\Big)\Big] \quad . \tag{3.9}$$

Next, define

$$|\,\hat{\psi}_{j,\pm}\,\rangle = \frac{1}{\sqrt{2}}\Big(|\,\hat{u}_j\,\rangle \pm |\,\hat{v}_j\,\rangle\Big) \quad , \tag{3.10}$$

in which case

$$\hat{H} = \sum_{j=-1}^{1}\Big(\varepsilon_{j,+}\,|\,\hat{\psi}_{j,+}\,\rangle\langle\,\hat{\psi}_{j,+}\,| + \varepsilon_{j,-}\,|\,\hat{\psi}_{j,-}\,\rangle\langle\,\hat{\psi}_{j,-}\,|\Big) \quad , \tag{3.11}$$

where the six eigenvalues of H are given by

$$\varepsilon_{j,\pm} = -2t_0\cos(2\pi j/3) \mp t_1 \quad . \tag{3.12}$$

For generic t_0 and t_1, we have that the eigenstates $|\,\hat{\psi}_{0,\pm}\,\rangle$ are each singly degenerate with energies $\varepsilon_{0,\pm} = -2t_0 \mp t_1$, respectively. They transform according to the A_1 and A_2' representations of D_{3h}, respectively. The eigenstates $|\,\hat{\psi}_{\pm1,+}\,\rangle$ are doubly degenerate, with energy $\varepsilon_{\pm1,+} = t_0 - t_1$, and transform according to the E representation. Finally, the states $|\,\hat{\psi}_{\pm1,-}\,\rangle$ are also doubly degenerate, with energy $\varepsilon_{\pm1,-} = t_0 + t_1$, and transform according to E' (see Tab. 3.1).

To elicit an accidental degeneracy, we set $\varepsilon_{0,-} = -2t_0 + t_1$ equal to $\varepsilon_{\pm1,+} = t_0 - t_1$, *i.e.* $t_1 = \frac{3}{2}t_0$. For this special ratio of t_1/t_0, there is a threefold degeneracy, due to a crossing of A_2' and E levels. The multiplicity of this degeneracy is therefore $d_{A_s'} + d_E = 3$, which corresponds to none of the dimensions of the IRREPs of D_{3h}. The degeneracy is accidental and is removed whenever $t_1 \neq \frac{3}{2}t_0$.

Finally, we can break the D_{3h} symmetry back down to C_{3v} by choosing different matrix elements $t_{0,u}$ and $t_{0,v}$ for the two triangles[3]. *Mutatis mutandis*[4], one finds that the degeneracy structure is the same, and the eigenspectrum is given by

$$\varepsilon_{j,\pm} = -(t_{0,u} + t_{0,v})\cos(2\pi j/3) \mp \sqrt{(t_{0,u} - t_{0,v})^2\cos^2(2\pi j/3) + t_1^2} \quad . \tag{3.13}$$

[3]Here we should recall the careful discussion at the end of §1.2.4 regarding the difference between D_n and C_{nv}.
[4]*Vah! Denuone Latine loquebar?*

D_{3h}	E	$2C_3$	$3C_2'$	σ_h	$2S_3$	$3\sigma_v$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E	2	-1	0	2	-1	0
A_1'	1	1	1	-1	-1	-1
A_2'	1	1	-1	-1	-1	1
E'	2	-1	0	-2	1	0

Table 3.1: Character table for the group D_{3h}. The upper left 3×3 block is the character table for D_3. Take care not to confuse the identity element E and its class with the two-dimensional IRREP also labeled E.

The eigenstates are now classified in terms of representations of $C_{3v} \cong D_3$. The two nondegenerate levels each transform according to A_1, and the two sets of doubly degenerate levels each transform according to E.

In general, identical IRREPs cannot be coaxed into degeneracy by terms in the Hamiltonian which preserve the full symmetry group G. This is due to level repulsion. Accidental degeneracy, when it occurs, is in general between distinct IRREPs, and therefore the size of the resulting *supermultiplet* is given by $d_{\Gamma_a} + d_{\Gamma_b}$, where $\Gamma_a \ncong \Gamma_b$. We note that this sort of degeneracy requires the fine tuning of one parameter in the Hamiltonian, such as t_1 (or the dimensionless ratio t_1/t_0) in our above example.

Can we tune further for even greater degeneracy? Yes we can! Mathematically, if $\hat{H} = \hat{H}(\boldsymbol{\lambda})$, where $\boldsymbol{\lambda} = \{\lambda_1, \ldots, \lambda_K\}$ is a set of parameters living in some parameter space manifold $\mathcal{M}$, and $\big[\hat{H}(\boldsymbol{\lambda})\,,\,\hat{U}(g)\big] = 0$ for all $\boldsymbol{\lambda} \in \mathcal{M}$ and all $g \in G$, then requiring that the multiplets for $p > 1$ distinct IRREPs are simultaneously degenerate imposes $p-1$ equations of the form

$$E_{\Gamma_a\,,l_a}(\lambda_1, \ldots, \lambda_K) = E_{\Gamma_b\,,l_b}(\lambda_1, \ldots, \lambda_K) \quad , \tag{3.14}$$

and therefore such a degeneracy, whose multiplicity is $d = \sum_{j=1}^{p} \mathsf{dim}(\Gamma_{a_j})$, has *codimension* $p-1$, meaning that the solution set in $\mathcal{M}$ is of dimension $K - p + 1$. It may be that this value of d corresponds to d_Γ for some other IRREP Γ, but this is not necessarily the case. And of course, it may be that there are no solutions at all. In the above example with symmetry group D_{3h}, we had $\hat{H} = \hat{H}(t_0, t_1)$, so $K = 2$, and degeneracy of the p $(= 2)$ multiplets A_2' and E imposed $p - 1$ $(= 1)$ conditions on $\{t_1, t_2\}$, with a one-dimensional solution set of the form $t_1 = \frac{3}{2} t_0$.

Accidental degeneracy in the C_{60} molecule

Mathematical appetizer: There is a marvelous result in graph theory, due to Euler, which says that for any connected graph on a surface of genus g, the number of faces f, edges e, and vertices v are related according to

$$f - e + v = 2 - 2g \quad . \tag{3.15}$$

The genus g is the number of holes, hence a sphere has genus $g = 0$, a torus $g = 1$, *etc.* It turns out that for the plane we should take $g = \frac{1}{2}$, which we can understand identifying the points at infinity and

thereby compactifying the plane to a sphere. Then the area outside the original graph counts as an extra face. Try sketching some connected graphs on a sheet of paper and see if Euler's theorem holds.

Consider now a threefold coordinated graph on the sphere S^2. Every site is linked to three neighboring sites. Furthermore, let's assume that every face is either a pentagon or a hexagon. The number of faces is then $f = p + h$, where p is the number of pentagons and h the number of hexagons. If we add $5p$ to $6h$, we count every edge twice, so $5p + 6h = 2e$. Similarly, $5p + 6h = 3v$ because the same calculation counts each vertex three times. Thus $e = \frac{5}{2}p + 3h$ and $v = \frac{5}{3}p + 2h$. Now apply Euler's theorem and find that h drops out completely and we are left with $p = 12$. *Any three-fold coordinated graph on the sphere with pentagonal and hexagonal faces will always have twelve pentagons.* Amazing! Take a close look at a soccer ball sometime and you will notice it has 12 pentagonal faces and 20 hexagonal ones, for a total of $f = 32$ faces to go along with $e = 90$ edges and $v = 60$ vertices.

Physics entree : There is a marvelous molecule with chemical formula C_{60}, also known as *Buckminsterfullerene*[5] (colloquially a *buckyball*) which consists of 60 carbon atoms arranged in a soccer ball pattern[6]. See the left panel of Fig. 3.2. Each atom is threefold coordinated, meaning it has three nearest neighbors. As you know, carbon has the electronic structure $1s^2 2s^2 2p^2$. In the planar form graphene, which has the structure of a honeycomb lattice, the $2s$ and $2p_{x,y}$ orbitals engage in sp^2 hybridization. For each carbon atom, three electrons in each atom's sp^2 orbitals are distributed along bonds connecting to its neighbors[7]. Thus each bond gets two electrons (of opposite spin), one from each carbon atom at its ends, which form what chemists call a σ-bond. The 1s orbitals are of course filled, so this leaves one remaining electron from each p_z orbital (the π orbital to our chemist friends) to roam about. The situation is much the same with the buckyball, although unlike graphene it is curved. The single (π) orbital tight binding model is

$$\hat{H} = -\sum_{\langle ij \rangle} \Big(t_{ij} \, | \, \pi_i \, \rangle \langle \, \pi_j \, | + t_{ij}^* \, | \, \pi_j \, \rangle \langle \, \pi_i \, | \Big) \quad , \tag{3.16}$$

where $\langle ij \rangle$ denotes a nearest neighbor bond on the lattice between sites i and j and t_{ij} is the *hopping integral*, which may be complex so long as $\hat{H}$ itself is Hermitian[8].

The eigenspectrum of $\hat{H}$ will be arranged in multiplets whose sizes are given by the dimensions of the IRREPs of the symmetry group of the buckyball. The discrete rotational symmetries of C_{60} belong to the *icosahedral group*, I. You can look up the character table for I and see that it is a nonabelian group with 60 elements, five classes, and five IRREPs A, T_1, T_2, G, and H, with dimensions 1, 3, 3, 4, and 5, respectively. Note that $60 = 1^2 + 3^2 + 3^2 + 4^2 + 5^2$. The icosahedron also has an inversion symmetry, so its full symmetry group, including the improper rotations, has 120 elements and is called I_h.[9] The group I_h has ten classes and ten IRREPs, such that each of the five IRREPs in I is doubled within I_h into

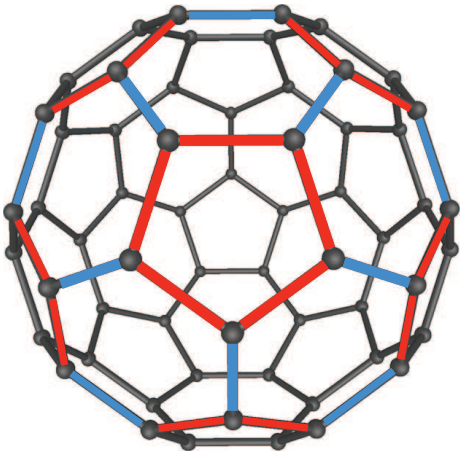
[5] After Buckminster Fuller, the American architect who invented the geodesic dome.

[6] "The icosahedral group ... has no physical interest, since for crystals 5-fold axes cannot occur, and no examples of molecules with this symmetry are known." - M. Hamermesh, *Group Theory and its Application to Physical Problems* (1962), p. 51.

[7] In diamond, the carbon atoms are fourfold coordinated, and the orbitals are sp^3 hybridized.

[8] A local gauge transformation of the orbitals $| \, \pi_i \, \rangle \to e^{i\theta_i} \, | \, \pi_i \, \rangle$ is equivalent to replacing t_{ij} by $t_{ij} \, e^{i(\theta_i - \theta_j)}$. The product $\prod_{\langle ij \rangle \in \kappa} t_{ij}$ of the t_{ij} around a plaquette κ is therefore gauge invariant, and the phase of the product is equal to the total magnetic flux through κ in units of $\hbar c/e$.

[9] Recall that D_n has $2n$ elements, but adding a horizontal reflection plane yields D_{nh} with $4n$ elements. The icosahedron has 15 reflection planes, appearing as class σ in its character tables. Each such reflection can be written as the product of an inversion and a proper rotation. *Fun facts* : $I \cong A_5$ and $I_h \cong \mathbb{Z}_2 \times A_5$, where A_5 is the alternating group with five symbols.



Γ	d_Γ	n_Γ
A_g	1	1
T_{1g}	3	1
T_{2g}	3	1
G_g	4	2
H_g	5	3
A_u	1	0
T_{1u}	3	2
T_{2u}	3	2
G_u	4	2
H_u	5	2

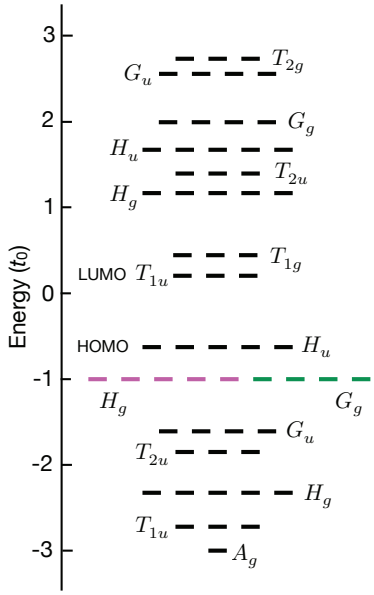


Figure 3.2: Electronic structure of the C_{60} molecule. Left: C_{60} molecule, showing inequivalent bonds. All red bonds lie along pentagons, while all blue bonds do not. Middle: Irreducible representations of the icosahedral group I_h and their dimensions. Right: Tight binding energy spectrum when all bonds have hopping amplitude t_0. Note the accidental degeneracy between G_g and H_g levels, at $E = -t_0$, resulting in a nine-fold degenerate supermultiplet. When the hopping amplitudes along the blue and red bonds differ, icosahedral symmetry is maintained, but the accidental degeneracy is resolved.

an even and an odd version with respect to the inversion[10], sort of like the good and evil versions of Mr. Spock in the original *Star Trek* series episode entitled *"Mirror, Mirror"*. The IRREPs of I_h are labeled with subscripts g and u, for *gerade* and *ungerade*, respectively (from the German for "even" and "odd").

The eigenvalues for the C_{60} tight binding Hamiltonian are shown in Fig. 3.2 for the case $t_{ij} = t_0$ for all nearest neighbor bonds $\langle ij \rangle$. Each of the energy levels accommodates two electrons (spin $\uparrow$ and $\downarrow$), so in the ground state the sixty π electrons fill the lowest 30 levels. HOMO and LUMO respectively refer to "highest occupied molecular orbital" and "lowest unoccupied molecular orbital". The multiplicities of the different energy states correspond to the dimension of the IRREPs, except for a ninefold degenerate level at $E = -t_0$. This is an accidental degeneracy between G_g and H_g IRREPs, whose dimensions are four and five, respectively.

In order for the degeneracy to be accidental, we should be able to remove it by modifying the Hamiltonian while still preserving the I_h symmetry. One physical way to do this is to note that there are actually two inequivalent sets of bonds (edges) on the buckyball: bonds that lie along pentagons (marked red in Fig. 3.2, called 6:5 bonds, 60 in total), and bonds that do not lie along pentagons (marked blue, 6:6 bonds, 30 total). Clearly no symmetry operation can transform a red bond into a blue one, so why should their hopping amplitudes be the same? The answer is that they are not the same. Indeed, the 6:6 bonds are slightly shorter than the 6:5 bonds, and they have a slightly larger value of t_{ij}. By distinguishing

[10] See the discussion in §2.4.7.

$t_0 \equiv t_{(6:6)}$ and $t_1 \equiv t_{(6:5)}$, one retains the I_h symmetry, but the aforementioned degeneracy occurs only for $t_1 = t_0$, precisely in analogy to what we found in our D_{3h} example.

Note that in the tight binding eigenspectrum some IRREPs occur several times. There are three H_g levels, for example, and A_u isn't present anywhere in the spectrum. The eigenfunctions form a reducible 60-dimensional representation of the group I_h whose decomposition is

$$\Gamma^{\text{elec}} = A_g \oplus T_{1g} \oplus T_{2g} \oplus 2G_g \oplus 3H_g \oplus 2T_{1u} \oplus 2T_{2u} \oplus 2G_u \oplus 2H_u \quad . \tag{3.17}$$

The number of times the IRREP Γ appears, n_Γ, is also listed in the table in Fig. 3.2. For singly degenerate atomic orbitals such as the π orbitals of C_{60} , the representation matrices $D^{\text{elec}}(g)$ are *permutation matrices* of the site labels i, with

$$D^{\text{elec}}_{ij}(g) = \langle\, i \,|\, g \,|\, j \,\rangle \equiv \begin{cases} 1 & \text{if } g \text{ takes } j \text{ to } i \\ 0 & \text{otherwise} \quad . \end{cases} \tag{3.18}$$

The character $\chi^{\text{elec}}(g)$ is then simply the number of sites i left invariant by the operation g. We can then find n_Γ using the representation decomposition formula. This will be discussed more fully in §6.4.

3.1.3 Operators and wavefunctions

Here we consider the transformation properties of the Hilbert space vectors $|\, \Gamma\mu,\, l \,\rangle$ for fixed l. Accordingly we suppress these indices throughout this discussion. Recall that

$$\hat{U}(g) \,|\, \Gamma\nu \,\rangle = |\, \Gamma\mu \,\rangle \,\langle\, \Gamma\mu \,|\, \hat{U}(g) \,|\, \Gamma\nu \,\rangle = |\, \Gamma\mu \,\rangle\, D^\Gamma_{\mu\nu}(g) \quad . \tag{3.19}$$

Taking the Hermitian conjugate, one has $\langle\, \Gamma\nu \,|\, U^\dagger(g) = D^{\Gamma^*}_{\mu\nu}(g)\, \langle\, \Gamma\mu \,|$. Thus,

$$D^\Gamma_{\mu\nu}(g) = \langle\, \Gamma\mu \,|\, \hat{U}(g) \,|\, \Gamma\nu \,\rangle \qquad , \qquad D^{\Gamma^*}_{\mu\nu}(g) = \langle\, \Gamma\mu \,|\, \hat{U}(g) \,|\, \Gamma\nu \,\rangle^* = \langle\, \Gamma\nu \,|\, \hat{U}^\dagger(g) \,|\, \Gamma\mu \,\rangle \quad . \tag{3.20}$$

Note that the matrix representation is a group homomorphism:

$$\hat{U}(g_a)\, \hat{U}(g_b) \,|\, \Gamma\nu \,\rangle = \hat{U}(g_a) \,|\, \Gamma\rho \,\rangle\, D^\Gamma_{\rho\nu}(g_b) = |\, \Gamma\mu \,\rangle\, D^\Gamma_{\mu\rho}(g_a)\, D^\Gamma_{\rho\nu}(g_b) = |\, \Gamma\mu \,\rangle\, D^\Gamma_{\mu\nu}(g_a\, g_b) \quad . \tag{3.21}$$

Acting on the state $|\, \boldsymbol{r} \,\rangle$, one has $\hat{U}(g) \,|\, \boldsymbol{r} \,\rangle = |\, g\, \boldsymbol{r} \,\rangle$, and therefore $\langle\, \boldsymbol{r} \,|\, U(g) = \langle\, g^{-1} \boldsymbol{r} \,|$. Therefore, with $\psi(\boldsymbol{r}) = \langle\, \boldsymbol{r} \,|\, \psi \,\rangle$, we then have

$$\hat{U}(g)\, \psi(\boldsymbol{r}) \equiv \langle\, \boldsymbol{r} \,|\, \hat{U}(g) \,|\, \psi \,\rangle = \psi(g^{-1} \boldsymbol{r}) \quad . \tag{3.22}$$

We also have

$$\hat{U}(gh)\, \psi(\boldsymbol{r}) = \hat{U}(g)\, \hat{U}(h)\, \psi(\boldsymbol{r}) = \hat{U}(g)\, \psi(h^{-1} \boldsymbol{r}) = \psi(h^{-1} g^{-1} \boldsymbol{r}) = \psi\big((gh)^{-1} \boldsymbol{r}\big) \quad . \tag{3.23}$$

Acting on a basis function $\psi^\Gamma_\nu(\boldsymbol{r}) = \langle\, \boldsymbol{r} \,|\, \Gamma\nu \,\rangle$, we have

$$\psi^\Gamma_\nu(g^{-1} \boldsymbol{r}) = \hat{U}(g)\, \psi^\Gamma_\nu(\boldsymbol{r}) = \langle\, \boldsymbol{r} \,|\, \hat{U}(g) \,|\, \Gamma\nu \,\rangle = \langle\, \boldsymbol{r} \,|\, \Gamma\mu \,\rangle\, D^\Gamma_{\mu\nu}(g) = \psi^\Gamma_\mu(\boldsymbol{r})\, D^\Gamma_{\mu\nu}(g) \quad . \tag{3.24}$$

Multiplying by $D^{\Gamma^*}_{\nu\alpha}(g)$ and contracting on the index ν, this result entails $\psi^\Gamma_\alpha(\boldsymbol{r}) = D^{\Gamma^*}_{\alpha\nu}(g)\, \psi^\Gamma_\nu(g^{-1} \boldsymbol{r})$.

Fun fact about bras and kets:

◇ While the ket $|\Gamma\mu, l\rangle$ transforms according to Γ, the bra $\langle\Gamma\mu, l|$ transforms according to Γ^*.

Recall also that the product of IRREPs $\Gamma \times \Gamma'$ contains the identity representation if and only if $\Gamma' = \Gamma^*$, with $D^{\Gamma^*}_{\mu\nu}(g) = \big[D^{\Gamma}_{\mu\nu}(g)\big]^*$.

3.1.4 Projection operators

This section recapitulates the results of §2.4.2, now expressed in the form of abstract operators rather than matrices. Consider a unitary representation $D^{\Gamma}(G)$ and define the operators

$$\hat{\Pi}^{\Gamma}_{\mu\nu} \equiv \frac{d_\Gamma}{N_G} \sum_{g\in G} D^{\Gamma^*}_{\mu\nu}(g)\, \hat{U}(g) \quad . \tag{3.25}$$

which project onto the μ basis vector of the Γ representation. They satisfy the following three conditions. First: $\hat{\Pi}^{\Gamma}_{\mu\nu}\, \hat{\Pi}^{\Gamma'}_{\mu'\nu'} = \delta_{\Gamma\Gamma'}\, \delta_{\nu\mu'}\, \hat{\Pi}^{\Gamma}_{\mu\nu'}$. Second: $\big(\hat{\Pi}^{\Gamma}_{\mu\nu}\big)^\dagger = \hat{\Pi}^{\Gamma}_{\nu\mu}$. Third: $\sum_\Gamma \sum_{\mu=1}^{d_\Gamma} \hat{\Pi}^{\Gamma}_{\mu\mu} = \mathbb{1}$. The proof of these relations is left as an exercise to the student.

Starting with an arbitrary collection of initial states $\big\{|\,\psi_l\,\rangle\big\}$, one can form the states

$$\big|\,\Gamma\mu, l\,\big\rangle = \hat{\Pi}^{\Gamma}_{\mu\nu}\,\big|\,\psi_l\,\big\rangle \quad , \tag{3.26}$$

where the index ν is held fixed for each l. One then has $\hat{\Pi}^{\Gamma}_{\mu\nu}\,\big|\,\Gamma'\rho, l\,\big\rangle = \delta_{\Gamma\Gamma'}\,\delta_{\nu\rho}\,\big|\,\Gamma\mu, l\,\big\rangle$. Note that

$$\begin{aligned}
\hat{U}(g)\,\hat{\Pi}^{\Gamma}_{\mu\nu} &= \frac{d_\Gamma}{N_G}\sum_{h\in G} D^{\Gamma^*}_{\mu\nu}(h)\,\hat{U}(g)\,\hat{U}(h) = \frac{d_\Gamma}{N_G}\sum_{h\in G} D^{\Gamma^*}_{\mu\nu}(g^{-1}gh)\,\hat{U}(gh) \\
&= D^{\Gamma^*}_{\mu\rho}(g^{-1})\,\overbrace{\frac{d_\Gamma}{N_G}\sum_{h\in G} D^{\Gamma^*}_{\rho\nu}(gh)\,\hat{U}(gh)}^{\hat{\Pi}^{\Gamma}_{\rho\nu}\ \text{(rearrangement)}} = D^{\Gamma^*}_{\mu\rho}(g^{-1})\,\hat{\Pi}^{\Gamma}_{\rho\nu} = \hat{\Pi}^{\Gamma}_{\rho\nu}\,D^{\Gamma}_{\rho\mu}(g) \quad .
\end{aligned} \tag{3.27}$$

Applying this to $|\psi_l\rangle$, we have

$$\hat{U}(g)\,|\,\Gamma\mu, l\,\rangle = |\,\Gamma\rho, l\,\rangle\,D^{\Gamma}_{\rho\mu}(g) \quad , \tag{3.28}$$

which says that the states $\big\{|\Gamma\mu, l\rangle\big\}$ transform as the Γ IRREP of G. Note further that

$$\begin{aligned}
\big\langle\,\Gamma\mu, l\,\big|\,\Gamma'\mu', l'\,\big\rangle = \big\langle\,\psi_l\,\big|\,\big(\hat{\Pi}^{\Gamma}_{\mu\nu}\big)^\dagger \hat{\Pi}^{\Gamma'}_{\mu'\nu'}\,\big|\,\psi_{l'}\,\big\rangle &= \big\langle\,\psi_l\,\big|\,\hat{\Pi}^{\Gamma}_{\nu\mu}\hat{\Pi}^{\Gamma'}_{\mu'\nu'}\,\big|\,\psi_{l'}\,\big\rangle \\
&= \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,\big\langle\,\psi_l\,\big|\,\hat{\Pi}^{\Gamma}_{\nu\nu'}\,\big|\,\psi_{l'}\,\big\rangle \equiv \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,O^{\Gamma}_{ll'} \quad ,
\end{aligned} \tag{3.29}$$

where $O^{\Gamma}_{ll'} = \big\langle\,\psi_l\,\big|\,\hat{\Pi}^{\Gamma}_{\nu\nu'}\,\big|\,\psi_{l'}\,\big\rangle$. Recall that the column indices are held fixed for each choice of (Γ, l), independent of the row indices. If the choice of ν for each (Γ, l) is considered implicit, we may suppress the indices ν and ν' in the overlap matrix $O^{\Gamma}_{ll'}$. At any rate, we see that the states constructed by projection in eqn. 3.26 are orthogonal only in their representation labels (Γ and Γ') and row labels (μ and μ'), but not in the multiplicity labels l and l'.



Figure 3.3: A projector from the early days of group theory. This projector belonged to Eugene Wigner.

Taking the trace of $\hat{\Pi}^{\Gamma}_{\mu\nu}$, we obtain, for unitary representations, the projection operator

$$\hat{\Pi}^{\Gamma} \equiv \sum_{\mu=1}^{d_\Gamma} \hat{\Pi}^{\Gamma}_{\mu\mu} = \frac{d_\Gamma}{N_G} \sum_{g\in G} \chi^{\Gamma^*}(g)\, \hat{U}(g) \quad . \tag{3.30}$$

If $|\,\psi\,\rangle = \sum_\Gamma \sum_l \sum_{\mu=1}^{d_\Gamma} C^l_{\Gamma\mu}\, |\,\Gamma\mu, l\,\rangle$ is a general sum over Hilbert space basis vectors, then

$$\hat{\Pi}^{\Gamma_a}\,|\,\psi\,\rangle = \sum_l \sum_{\mu=1}^{d_\Gamma} C^l_{\Gamma_a\,\mu}\,\big|\,\Gamma_a\,\mu\,, l\,\big\rangle \tag{3.31}$$

projects $|\,\psi\,\rangle$ onto the IRREP Γ_a.

3.1.5 Projecting arbitrary functions onto IRREPs

Here we describe a straightforward generalization of the method in §2.3.4 of projecting vectors, now applied to functions. For any function $\psi(\boldsymbol{r})$, define

$$\psi^{(\Gamma\nu)}_\mu(\boldsymbol{r}) \equiv \hat{\Pi}^{\Gamma}_{\mu\nu}\,\psi(\boldsymbol{r}) = \frac{d_\Gamma}{N_G} \sum_{g\in G} D^{\Gamma^*}_{\mu\nu}(g)\,\psi(g^{-1}\boldsymbol{r}) \quad . \tag{3.32}$$

Here the representation label Γ as well as the column index ν serve as labels for a set of functions with $\mu \in \{1, \ldots, d_\Gamma\}$. Invoking Eqn. 3.27, we find

$$\hat{U}(g)\,\hat{\Pi}^{\Gamma}_{\mu\nu} = \hat{\Pi}^{\Gamma}_{\rho\nu}\, D^{\Gamma}_{\rho\mu}(g) \tag{3.33}$$

and therefore

$$\hat{U}(g)\,\psi_\mu^{(\Gamma\nu)}(\boldsymbol{r}) = \psi_\rho^{(\Gamma\nu)}(\boldsymbol{r})\,D^\Gamma_{\rho\mu}(g) \quad . \tag{3.34}$$

In other words, suppressing the $(\Gamma\nu)$ label, we have that the functions $\psi_\mu(\boldsymbol{r})$ transform according to the Γ representation of the group. *Thus, we have succeeded in projecting an arbitrary function $\psi(\boldsymbol{r})$ onto any* IRREP *Γ of G we please.* This deserves a celebration with some unusual LaTeX symbols: ☺ 🚲 ⚽ ☕ .

Example: $\mathbb{Z}_2$

Let's see how this marvelous projection machinery works with two examples. The first is rather trivial, from the group $G = \mathbb{Z}_2$, with elements $\{E, P\}$, where $P^2 = E$. We take P to correspond to parity, with $Px = -x$. Thus for any function $\psi(x)$,

$$\hat{U}(E)\,\psi(x) = \psi(x) \qquad , \qquad \hat{U}(P)\,\psi(x) = \psi(P^{-1}x) = \psi(Px) = \psi(-x) \quad . \tag{3.35}$$

$\mathbb{Z}_2$ has two IRREPs, both of which are one-dimensional. In the identity representation Γ_1, the 1×1 matrices are $\hat{U}^{\Gamma_1}(E) = \hat{U}^{\Gamma_1}(P) = 1$. In the sign representation Γ_2, and $\hat{U}^{\Gamma_2}(E) = 1$ while $\hat{U}^{\Gamma_2}(P) = -1$. The projectors are then

$$\hat{\Pi}^{\Gamma_1} = \frac{1}{2}\Big[\hat{U}(E) + \hat{U}(P)\Big] \qquad , \qquad \hat{\Pi}^{\Gamma_2} = \frac{1}{2}\Big[\hat{U}(E) - \hat{U}(P)\Big] \quad . \tag{3.36}$$

Now for the projection:

$$\hat{\Pi}^{\Gamma_1}\,\psi(x) = \tfrac{1}{2}\Big[\psi(x) + \psi(-x)\Big] \qquad , \qquad \hat{\Pi}^{\Gamma_2}\,\psi(x) = \tfrac{1}{2}\Big[\psi(x) - \psi(-x)\Big] \quad . \tag{3.37}$$

Example: C_{3v}

Let's now see how the projection onto basis functions works for a higher-dimensional representation of a nonabelian group. We turn to our old and trusted friend, C_{3v}, which has a two-dimensional representation, E.

Before we project onto E, let's warm up by projecting onto the two one-dimensional representations A_1 and A_2. We have

$$\begin{aligned}\hat{\Pi}^{A_1} &= \frac{1}{6}\Big\{\hat{U}(E) + \hat{U}(R) + \hat{U}(W) + \hat{U}(\sigma) + \hat{U}(\sigma') + \hat{U}(\sigma'')\Big\} \\ \hat{\Pi}^{A_2} &= \frac{1}{6}\Big\{\hat{U}(E) + \hat{U}(R) + \hat{U}(W) - \hat{U}(\sigma) - \hat{U}(\sigma') - \hat{U}(\sigma'')\Big\} \quad .\end{aligned} \tag{3.38}$$

Thus the projection of an arbitrary initial function $\psi(x, y)$ onto A_1 will, according to Eqn. 3.32, be

$$\begin{aligned}\psi^{(A_1)}(x,y) = \frac{1}{6}\Big\{&\psi\big(x,y\big) + \psi\big(-\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\,,\,-\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) + \psi\big(-\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) \\ &+ \psi\big(-x\,,\,y\big) + \psi\big(\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\,,\,\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) + \psi\big(\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,-\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big)\Big\} \,.\end{aligned} \tag{3.39}$$

Similarly, projecting onto A_2 yields

$$\psi^{(A_2)}(x,y) = \frac{1}{6}\Big\{\psi(x,y) + \psi\big(-\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\,,\,-\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) + \psi\big(-\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) \\ - \psi\big(-x\,,\,y\big) + \psi\big(\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) - \psi\big(\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,-\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big)\Big\}\,. \tag{3.40}$$

Note that $\hat{\Pi}^{A_1}$ preserves all constant functions (*e.g.* $\psi = 1$) but annihilates all linear functions of the form $\psi(x,y) = ax + by$.[11] What happens if we take $\psi(x,y) = x^2$? Then we find $\psi^{(A_1)}(x,y) = \frac{1}{2}(x^2+y^2)$, which does indeed transform like the identity, but $\psi^{(A_2)}(x,y) = 0$. What do we need to do to get a nontrivial representation of A_2? Let's try starting with $\psi(x,y) = x^3$. Now we find $\psi^{(A_1)}(x,y) = 0$ but $\psi^{(A_2)}(x,y) = \frac{1}{4}x^3 - \frac{3}{4}xy^2$. Eureka! Note that we may write $\psi^{(A_2)}(x,y) = x\,\big(\frac{1}{2}x + \frac{\sqrt{3}}{2}y\big)\big(\frac{1}{2}x - \frac{\sqrt{3}}{2}y\big)$, which renders its transformation properties more apparent.

Now let's roll up our sleeves and do the projection onto E. Recall the matrices for E:

$$D^E(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^E(R) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \qquad D^E(W) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}$$
$$D^E(\sigma) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^E(\sigma') = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \qquad D^E(\sigma'') = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}\,. \tag{3.41}$$

We now select an arbitrary function $\psi(\boldsymbol{r})$ which itself may have no special symmetry properties. According to Eqn. 3.32, the projection of $\psi(\boldsymbol{r})$ onto the μ row of the E representation is given by

$$\psi_\mu^{(E\nu)}(\boldsymbol{r}) = \frac{1}{3}\Big\{D^E_{\mu\nu}(E)\,\psi(\boldsymbol{r}) + D^E_{\mu\nu}(R)\,\psi(R^{-1}\boldsymbol{r}) + D^E_{\mu\nu}(W)\,\psi(W^{-1}\boldsymbol{r}) \\ + D^E_{\mu\nu}(\sigma)\,\psi(\sigma^{-1}\boldsymbol{r}) + D^E_{\mu\nu}(\sigma')\,\psi(\sigma'^{-1}\boldsymbol{r}) + D^E_{\mu\nu}(\sigma'')\,\psi(\sigma''^{-1}\boldsymbol{r})\Big\}\quad. \tag{3.42}$$

Thus,

$$\psi_\mu^{(E\nu)}(\boldsymbol{r}) = \frac{1}{3}\Bigg\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\psi(x,y) + \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}\psi\big(-\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\,,\,-\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) \\ + \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}\psi\big(-\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) + \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\psi\big(-x\,,\,y\big) \\ + \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}\psi\big(\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\,,\,\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big) + \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}\psi\big(\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\,,\,-\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y\big)\Bigg\}_{\mu\nu}\,. \tag{3.43}$$

Let's take $\nu = 1$, which means we only use the first column of each of the matrices in the above expression. Starting with $\psi(x,y) = x$, we obtain $\psi_1^{(E,1)}(x,y) = x$ and $\psi_2^{(E,1)}(x,y) = y$. Had we chosen instead $\psi(x,y) = y$, we would have found $\psi_1^{(E,1)}(x,y) = \psi_2^{(E,1)}(x,y) = 0$, *i.e.* the projection annihilates the initial state. Generically this will not occur – our choices here have been simple and nongeneric.

Had we chosen instead $\nu = 2$, then taking the second column above we find that $\psi(x,y) = x$ is annihilated by the projection, while for $\psi(x,y) = y$ we obtain $\psi_1^{(E,2)}(x,y) = x$ and $\psi_2^{(E,2)}(x,y) = y$. At any rate, the upshot of this analysis is that $\psi_1(x,y) = x$ and $\psi_2(x,y) = y$ are appropriate basis functions for the E representation of C_{3v}.

[11] Nasty stuff, these projectors.

3.1.6 Partial diagonalization of H

Suppose we have a set of appropriately transforming basis vectors $|\,\Gamma\mu\,\rangle$. One way to obtain such a set is to start with an arbitrary function $f(\boldsymbol{r})$ and then perform the projection onto row μ of representation Γ, forming $f_\mu^{(\Gamma\kappa)}(\boldsymbol{r}) = \hat{\Pi}^\Gamma_{\mu\kappa}\, f(\boldsymbol{r})$, and then defining

$$|\,\Gamma\mu\,\rangle = \mathcal{N}_\mu^\Gamma \int d^d r\; f_\mu^{(\Gamma\kappa)}(\boldsymbol{r})\,|\,\boldsymbol{r}\,\rangle \quad , \tag{3.44}$$

where $\mathcal{N}_\mu^\Gamma$ is a normalization constant. The column index κ is fixed for each Γ and is suppressed. We assume that the projection of $f(\boldsymbol{r})$ onto $f_\mu^{(\Gamma\kappa)}(\boldsymbol{r})$ does not annihilate $f(\boldsymbol{r})$ (else we try again with a different $f(\boldsymbol{r})$ function). We then have[12]

$$\begin{aligned}\langle\,\Gamma\mu\,|\,\Gamma'\mu'\,\rangle &= \mathcal{N}_\mu^{\Gamma^*}\mathcal{N}_{\mu'}^{\Gamma'}\int d^d r\,\left[f_\mu^{(\Gamma\kappa)}(\boldsymbol{r})\right]^* f_{\mu'}^{(\Gamma'\kappa')}(\boldsymbol{r}) = \mathcal{N}_\mu^{\Gamma^*}\mathcal{N}_{\mu'}^{\Gamma'}\int d^d r\; f^*(\boldsymbol{r})\left(\hat{\Pi}^\Gamma_{\mu\kappa}\right)^\dagger \hat{\Pi}^{\Gamma'}_{\mu'\kappa'}\, f(\boldsymbol{r}) \\ &= \mathcal{N}_\mu^{\Gamma^*}\mathcal{N}_{\mu'}^{\Gamma'}\int d^d r\; f^*(\boldsymbol{r})\,\hat{\Pi}^\Gamma_{\kappa\mu}\,\hat{\Pi}^{\Gamma'}_{\mu'\kappa'}\, f(\boldsymbol{r}) = \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,\left|\mathcal{N}_\mu^\Gamma\right|^2\int d^d r\; f^*(\boldsymbol{r})\,\hat{\Pi}^\Gamma_{\kappa\kappa'}\, f(\boldsymbol{r}) \quad ,\end{aligned} \tag{3.45}$$

which confirms that the basis vectors are orthogonal unless their representations (Γ, Γ') and basis indices (μ, μ') agree. We can therefore enforce the normalization $\langle\,\Gamma\mu\,|\,\Gamma'\mu'\,\rangle = \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}$.

Now assuming $\left[\hat{H}, \hat{U}(G)\right] = 0$, we may write $\hat{H} = \hat{U}(g)^\dagger \hat{H}\,\hat{U}(g)$, and therefore

$$\begin{aligned}\langle\,\Gamma\mu\,|\,H\,|\,\Gamma'\mu'\,\rangle &= \frac{1}{N_{\rm G}}\sum_{g\in G}\langle\,\Gamma\mu\,|\,\hat{U}(g)^\dagger\hat{H}\,\hat{U}(g)\,|\,\Gamma'\mu'\,\rangle \\ &= \frac{1}{N_G}\sum_{g\in G} D^{\Gamma^*}_{\nu\mu}(g)\,\langle\,\Gamma\nu\,|\,\hat{H}\,|\,\Gamma'\nu'\,\rangle\, D^{\Gamma'}_{\nu'\mu'}(g) \\ &= \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,\frac{1}{d_\Gamma}\sum_{\nu=1}^{d_\Gamma}\langle\,\Gamma\nu\,|\,\hat{H}\,|\,\Gamma\nu\,\rangle \quad ,\end{aligned} \tag{3.46}$$

where we have invoked the Great Orthogonality Theorem to collapse the sum over the group elements. Thus we see that if we choose our basis functions accordingly, *i.e.* as transforming appropriately under the group operations, the Hamiltonian will automatically be diagonal in the $\Gamma\mu$ indices. Of course this isn't the entire Hilbert space, since in the eigenspectrum of $\hat{H}$, a given representation Γ may occur many times – perhaps even infinitely many. We could, for example, have started by projecting an entire family of arbitrary initial functions, $\{f_l(\boldsymbol{r})\}$, indexed by l, and create their corresponding basis states states, which we would label $|\,\Gamma\mu, l\,\rangle$. The overlaps and the Hamiltonian matrix elements between these two different sectors will in general be nonzero provided the representations and the basis indices agree:

$$\begin{aligned}\langle\,\Gamma\mu, l\,|\,\Gamma'\mu', l'\,\rangle &= \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,\frac{1}{d_\Gamma}\sum_{\nu=1}^{d_\Gamma}\langle\,\Gamma\nu, l\,|\,\Gamma\nu, l'\,\rangle \equiv O^\Gamma_{ll'}\,\delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'} \\ \langle\,\Gamma\mu, l\,|\,\hat{H}\,|\,\Gamma'\mu', l'\,\rangle &= \delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'}\,\frac{1}{d_\Gamma}\sum_{\nu=1}^{d_\Gamma}\langle\,\Gamma\nu, l\,|\,\hat{H}\,|\,\Gamma\nu, l'\,\rangle \equiv H^\Gamma_{ll'}\,\delta_{\Gamma\Gamma'}\,\delta_{\mu\mu'} \quad ,\end{aligned} \tag{3.47}$$

[12] No sum on μ or μ' in Eqn. 3.45.

with no sum on Γ or μ. The first of these comes from the generalized version of Eqn. 3.46 upon replacing $\hat{H}$ by 1. Here $O^\Gamma_{ll'}$ and $H^\Gamma_{ll'}$ are the overlap matrix and Hamiltonian matrix, respectively; note that neither depends on the basis index μ. Our task is then to simultaneously diagonalize these two Hermitian matrices, *i.e.* to solve the linear system $H^\Gamma_{ll'}\,\phi^{\Gamma s}_{l'} = E_{\Gamma s}\,O^\Gamma_{ll'}\,\phi^{\Gamma s}_{l'}$, where a labels the eigenvalue and corresponding eigenfunctions of the $s^{\rm th}$ occurrence of the IRREP Γ. In systems with an infinite number of degrees of freedom, both O^Γ and H^Γ will in general be of infinite rank for each IRREP Γ, *i.e.* each IRREP will in general appear an infinite number of times in the eigenspectrum. Still, we have achieved a substantial simplification by organizing the basis vectors in terms of group symmetry.

3.2 Product Representations

3.2.1 Direct product of two representations

In chapter 2 we discussed the direct product of IRREPs $\Gamma_a \times \Gamma_b$. Recall the action of the group element g on the direct product space $\mathcal{V}_a \otimes \mathcal{V}_b$ is defined in terms of its action on the basis vectors,

$$\hat{U}(g)\,\big|\,{\rm e}^{\Gamma_a\times\Gamma_b}_{\alpha\beta}\,\big\rangle = \big|\,{\rm e}^{\Gamma_a\times\Gamma_b}_{\alpha'\beta'}\,\big\rangle\,D^{\Gamma_a}_{\alpha'\alpha}(g)\,D^{\Gamma_b}_{\beta'\beta}(g) \quad , \tag{3.48}$$

where $\big|\,{\rm e}^{\Gamma_a\times\Gamma_b}_{\alpha\beta}\,\big\rangle \equiv \big|\,{\rm e}^{\Gamma_a}_{\alpha}\,\big\rangle \otimes \big|\,{\rm e}^{\Gamma_b}_{\beta}\,\big\rangle$, where $\big|\,{\rm e}^{\Gamma}_{\mu}\,\big\rangle = \big|\,\Gamma\mu\,\big\rangle$ in our previous notation[13]. Thus the matrix of g in the direct product representation $\Gamma_a \times \Gamma_b$ is given by

$$D^{\Gamma_a\times\Gamma_b}_{\alpha'\beta',\,\alpha\beta}(g) = D^{\Gamma_a}_{\alpha'\alpha}(g)\,D^{\Gamma_b}_{\beta'\beta}(g) \quad , \tag{3.49}$$

where $\alpha\beta$ and $\alpha'\beta'$ on the LHS are composite indices, each taking $d_{\Gamma_a}\times d_{\Gamma_b}$ possible values. The characters in the product representation are given by the product of the individual characters, *viz.*

$$\chi^{\Gamma_a\times\Gamma_b}(g) = \chi^{\Gamma_a}(g)\,\chi^{\Gamma_b}(g) \quad . \tag{3.50}$$

3.2.2 Products of identical representations

Here we discuss three ways of taking the product of identical representations. Since we will be assuming the same representation Γ throughout, might as well suppress the Γ label.

- *Direct product* : This is also called the simple product. Consider an IRREP Γ of a finite group G and construct the tensor product basis $|\,{\rm e}_{\mu\nu}\,\rangle = |\,{\rm e}_\mu\,\rangle \otimes |\,{\rm e}_\nu\,\rangle$, where $\mu,\nu \in \{1,\ldots,d_\Gamma\}$. There are d_Γ^2 linearly independent basis states in the tensor product space $\mathcal{V}\times\mathcal{V}$. In the direct product representation $\Gamma\times\Gamma$, one has

$$\hat{U}(g)\,\big|\,{\rm e}_{\mu\nu}\,\big\rangle = \big|\,{\rm e}_{\mu'\nu'}\,\big\rangle\,D_{\mu'\mu}(g)\,D_{\nu'\nu}(g) \equiv \big|\,{\rm e}_{\mu'\nu'}\,\big\rangle\,D^{\sf D}_{\mu'\nu',\,\mu\nu}(g) \quad . \tag{3.51}$$

[13] When there are multiple occurrences of the IRREP Γ, we will use $|\,{\rm e}^{\Gamma,\,l}_{\mu}\,\rangle$ to always denote an orthonormal basis, with $\langle\,{\rm e}^{\Gamma,l}_{\mu}\,|\,{\rm e}^{\Gamma',\,l'}_{\mu'}\,\rangle = \delta_{\Gamma\Gamma'}\,\delta_{ll'}\,\delta_{\mu\mu'}$.

Therefore the character of g in the direct product representation $\Gamma \times \Gamma$ is

$$\chi^{\mathsf{D}}(g) = \big[\chi^{\Gamma}(g)\big]^2 \quad , \tag{3.52}$$

which is the square of the character in the Γ representation.

- *Symmetrized product* : Consider now the symmetrized basis states,

$$|\,\mathrm{e}^{\mathsf{S}}_{\mu\nu}\,\rangle = \frac{1}{\sqrt{2}}\Big(|\,\mathrm{e}_\mu\,\rangle \otimes |\,\mathrm{e}_\nu\,\rangle + |\,\mathrm{e}_\nu\,\rangle \otimes |\,\mathrm{e}_\mu\,\rangle\Big) \quad . \tag{3.53}$$

Clearly $|\,\mathrm{e}^{\mathsf{S}}_{\mu\nu}\,\rangle = |\,\mathrm{e}^{\mathsf{S}}_{\nu\mu}\,\rangle$, so there are $\frac{1}{2}d_\Gamma(d_\Gamma+1)$ linearly independent basis states in the symmetric product space $(\mathcal{V}\otimes\mathcal{V})^{\mathsf{S}}$. You might worry about the normalization, since

$$\big\langle\,\mathrm{e}^{\mathsf{S}}_{\mu\nu}\,\big|\,\mathrm{e}^{\mathsf{S}}_{\mu'\nu'}\,\big\rangle = \delta_{\mu\mu'}\,\delta_{\nu\nu'} + \delta_{\mu\nu'}\,\delta_{\nu\mu'} \quad , \tag{3.54}$$

and thus the diagonal basis vectors $|\,\mathrm{e}^{\mathsf{S}}_{\mu\mu}\,\rangle$ (no sum on μ) have norm $\sqrt{2}$. It turns out that this doesn't matter, and we can always impose a proper normalization later on. Now let's apply the operator $\hat{U}(g)$:

$$\begin{aligned}\hat{U}(g)\,\big|\,\mathrm{e}^{\mathsf{S}}_{\mu\nu}\,\big\rangle &= \frac{1}{\sqrt{2}}\Big(|\,\mathrm{e}_{\mu'}\,\rangle \otimes |\,\mathrm{e}_{\nu'}\,\rangle\, D_{\mu'\mu}(g)\, D_{\nu'\nu}(g) + |\,\mathrm{e}_{\nu'}\,\rangle \otimes |\,\mathrm{e}_{\mu'}\,\rangle\, D_{\nu'\mu}(g)\, D_{\mu'\nu}(g)\Big) \\ &= \big|\,\mathrm{e}^{\mathsf{S}}_{\mu'\nu'}\,\big\rangle \cdot \frac{1}{2}\Big(D_{\mu'\mu}(g)\, D_{\nu'\nu}(g) + D_{\nu'\mu}(g)\, D_{\mu'\nu}(g)\Big) \equiv \big|\,\mathrm{e}^{\mathsf{S}}_{\mu'\nu'}\,\big\rangle\, D^{\mathsf{S}}_{\mu'\nu',\,\mu\nu}(g) \quad .\end{aligned} \tag{3.55}$$

The character of g in this representation is then

$$\chi^{\mathsf{S}}(g) = D^{\mathsf{S}}_{\mu\nu,\,\mu\nu}(g) = \frac{1}{2}\Big(\big[\chi^{\Gamma}(g)\big]^2 + \chi^{\Gamma}(g^2)\Big) \quad . \tag{3.56}$$

- *Antiymmetrized product* : Consider now the antisymmetrized basis states,

$$|\,\mathrm{e}^{\mathsf{A}}_{\mu\nu}\,\rangle = \frac{1}{\sqrt{2}}\Big(|\,\mathrm{e}_\mu\,\rangle \otimes |\,\mathrm{e}_\nu\,\rangle - |\,\mathrm{e}_\nu\,\rangle \otimes |\,\mathrm{e}_\mu\,\rangle\Big) \quad . \tag{3.57}$$

Now we have $|\,\mathrm{e}^{\mathsf{A}}_{\mu\nu}\,\rangle = -|\,\mathrm{e}^{\mathsf{A}}_{\nu\mu}\,\rangle$, so there are $\frac{1}{2}d_\Gamma(d_\Gamma-1)$ linearly independent basis states in the antisymmetric product space $(\mathcal{V}\otimes\mathcal{V})^{\mathsf{A}}$. We then have

$$\big\langle\,\mathrm{e}^{\mathsf{A}}_{\mu\nu}\,\big|\,\mathrm{e}^{\mathsf{A}}_{\mu'\nu'}\,\big\rangle = \delta_{\mu\mu'}\,\delta_{\nu\nu'} - \delta_{\mu\nu'}\,\delta_{\nu\mu'} \quad . \tag{3.58}$$

Note that the diagonal basis vectors $|\,\mathrm{e}^{\mathsf{A}}_{\mu\mu}\,\rangle = 0$ (no sum on μ) vanish identically. Now let's apply the operator $\hat{U}(g)$:

$$\begin{aligned}\hat{U}(g)\,\big|\,\mathrm{e}^{\mathsf{A}}_{\mu\nu}\,\big\rangle &= \frac{1}{\sqrt{2}}\Big(|\,\mathrm{e}_{\mu'}\,\rangle \otimes |\,\mathrm{e}_{\nu'}\,\rangle\, D_{\mu'\mu}(g)\, D_{\nu'\nu}(g) - |\,\mathrm{e}_{\nu'}\,\rangle \otimes |\,\mathrm{e}_{\mu'}\,\rangle\, D_{\nu'\mu}(g)\, D_{\mu'\nu}(g)\Big) \\ &= \big|\,\mathrm{e}^{\mathsf{A}}_{\mu'\nu'}\,\big\rangle \cdot \frac{1}{2}\Big(D_{\mu'\mu}(g)\, D_{\nu'\nu}(g) - D_{\nu'\mu}(g)\, D_{\mu'\nu}(g)\Big) \equiv \big|\,\mathrm{e}^{\mathsf{A}}_{\mu'\nu'}\,\big\rangle\, D^{\mathsf{A}}_{\mu'\nu',\,\mu\nu}(g) \quad .\end{aligned} \tag{3.59}$$

The character of g in this representation is then

$$\chi^{\mathsf{A}}(g) = D^{\mathsf{A}}_{\mu\nu,\,\mu\nu}(g) = \frac{1}{2}\Big(\big[\chi^{\Gamma}(g)\big]^2 - \chi^{\Gamma}(g^2)\Big) \quad . \tag{3.60}$$

Note that this vanishes whenever Γ is a one-dimensional IRREP, because one-dimensional representations cannot be antisymmetrized!

Note that $\chi(g^2) = \chi\big((h^{-1}gh)^2\big)$, and so the class structure is the same. In other words, if g and g' belong to the same class, then g^2 and g'^2 also belong to the same class. Let's now use the equation

$$n_\Gamma(\Psi) = \frac{1}{N_G}\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^\Gamma(\mathcal{C})^*\,\chi^\Psi(\mathcal{C}) \tag{3.61}$$

to decompose some of these product representations. We'll choose the group D_3, the character table for which is the upper left 3×3 block of the character table for D_{3h} provided in Tab. 3.1. We first work out the direct product $E\times E$, for which $\chi^{\mathsf{D}}(E)=4$, $\chi^{\mathsf{D}}(C_3)=1$, and $\chi^{\mathsf{D}}(C_2')=0$. Applying the decomposition formula, we obtain $E\times E = A_1\oplus A_2\oplus E$. This is consistent with a naïve counting of dimensions, since $2^2 = 1+1+2$.

In order to decompose the symmetrized and antisymmetrized product representations $(E\times E)^{\mathsf{S,A}}$, we must compute the characters $\chi^\Gamma(g^2)$, and for this we need to invoke class relations $[E]^2 = E$, $[C_3]^2 = C_3$, and $[C_2']^2 = E$. These are easy to see, since C_3 contains the rotations R and W, which satisfy $R^2 = W$ and $W^2 = R$. The class C_2' consists of the three two-fold rotations (or mirrors, for C_{3v} elements), each of which squares to the identity. We then have[14]

$$\chi^E\big([E]^2\big) = \chi^E(E) = 2 \quad , \quad \chi^E\big([C_3]^2\big) = \chi^E(C_3) = -1 \quad , \quad \chi^E\big([C_2']^2\big) = \chi^E(E) = 2 \quad . \tag{3.62}$$

According to Eqns. 3.56 and 3.60, we then have

$$\chi^{\mathsf{S}}(E) = 3 \qquad \chi^{\mathsf{S}}(C_3) = 0 \qquad \chi^{\mathsf{S}}(C_2') = 1 \tag{3.63}$$

$$\chi^{\mathsf{A}}(E) = 1 \qquad \chi^{\mathsf{A}}(C_3) = 1 \qquad \chi^{\mathsf{A}}(C_2') = -1 \quad . \tag{3.64}$$

We therefore conclude $(E\times E)^{\mathsf{S}} = A_1\oplus E$ and $(E\times E)^{\mathsf{A}} = A_2$. Can you make sense of the dimensions?

3.2.3 Clebsch-Gordan Coefficients

Recall the decomposition formulae for the product representation $\Gamma_a\times\Gamma_b$ for any finite group G:

$$\Gamma_a\times\Gamma_b = \bigoplus_\Gamma n_\Gamma^{ab}\,\Gamma \tag{3.65}$$

where

$$n_\Gamma^{ab} = \frac{1}{N_G}\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma^*}(\mathcal{C})\,\chi^{\Gamma_a}(\mathcal{C})\,\chi^{\Gamma_b}(\mathcal{C}) \quad . \tag{3.66}$$

We may express the direct product of orthonormal basis states $\big|\,\mathrm{e}_\alpha^{\Gamma_a}\,\big\rangle$ and $\big|\,\mathrm{e}_\beta^{\Gamma_b}\,\big\rangle$, with $1\le\alpha\le d_{\Gamma_a}$ and $1\le\beta\le d_{\Gamma_b}$, in terms of the new orthonormal basis set $\big|\,\mathrm{e}_\gamma^{\Gamma,s}\,\big\rangle$, *viz.*

$$\big|\,\mathrm{e}_\alpha^{\Gamma_a}\,\big\rangle\otimes\big|\,\mathrm{e}_\beta^{\Gamma_b}\,\big\rangle = \sum_\Gamma\sum_{s=1}^{n_\Gamma^{ab}}\sum_{\gamma=1}^{d_\Gamma}\left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma,s\\ \alpha & \beta & \gamma\end{array}\right)\big|\,\mathrm{e}_\gamma^{\Gamma,s}\,\big\rangle \quad . \tag{3.67}$$

[14] Remember that E labels the identity element and its class, as well as the two-dimensional representation. Take care not to confuse the meaning of E in its appropriate context!

Here, the label s indexes possible multiple appearances of the representation Γ in the decomposition of the product $\Gamma_a \times \Gamma_b$. The quantities $\left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle| \begin{smallmatrix} \Gamma, s \\ \gamma \end{smallmatrix}\right)$, known as *Clebsch-Gordan coefficients* (CGCs), are unitary matrices relating the two orthonormal sets of basis vectors. Orthonormality of the bases means

$$\left\langle \mathrm{e}_{\alpha}^{\Gamma_a} \middle| \mathrm{e}_{\alpha'}^{\Gamma_a} \right\rangle = \delta_{\alpha\alpha'} \quad , \quad \left\langle \mathrm{e}_{\beta}^{\Gamma_b} \middle| \mathrm{e}_{\beta'}^{\Gamma_b} \right\rangle = \delta_{\beta\beta'} \quad , \quad \left\langle \mathrm{e}_{\gamma}^{\Gamma, s} \middle| \mathrm{e}_{\gamma'}^{\Gamma', s'} \right\rangle = \delta_{\Gamma\Gamma'}\, \delta_{ss'}\, \delta_{\gamma\gamma'} \quad . \tag{3.68}$$

The inverse basis transformation is

$$\big| \mathrm{e}_{\gamma}^{\Gamma, s} \big\rangle = \sum_{\alpha=1}^{d_a} \sum_{\beta=1}^{d_b} \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma \end{vmatrix}^* \big| \mathrm{e}_{\alpha}^{\Gamma_a} \big\rangle \otimes \big| \mathrm{e}_{\beta}^{\Gamma_b} \big\rangle \quad , \tag{3.69}$$

where we abbreviate $d_a \equiv d_{\Gamma_a}$ and $d_b \equiv d_{\Gamma_b}$. Note that the component IRREPs Γ_a and Γ_b are fixed throughout this discussion.

Relations satisfied by CGCs

Orthonormality and completeness of the CGCs require

$$\sum_{\alpha=1}^{d_a} \sum_{\beta=1}^{d_b} \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma \end{vmatrix}^* \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{vmatrix} \Gamma', s' \\ \gamma' \end{vmatrix} = \delta_{\Gamma\Gamma'}\, \delta_{ss'}\, \delta_{\gamma\gamma'} \tag{3.70}$$

and

$$\sum_{\Gamma} \sum_{s=1}^{n_{\Gamma}^{ab}} \sum_{\gamma=1}^{d_\Gamma} \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma \end{vmatrix}^* \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma \end{vmatrix} = \delta_{\alpha\alpha'}\, \delta_{\beta\beta'} \quad . \tag{3.71}$$

Applying the unitary operators $\hat{U}(g)$ to the basis vectors in their respective representations, one then obtains the relations

$$\sum_{\Gamma} \sum_{s=1}^{n_{\Gamma}^{ab}} \sum_{\gamma=1}^{d_\Gamma} \sum_{\gamma'=1}^{d_\Gamma} \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma \end{vmatrix}^* D^{\Gamma}_{\gamma\gamma'}(g) \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma' \end{vmatrix} = D^{\Gamma_a}_{\alpha\alpha'}(g)\, D^{\Gamma_b}_{\beta\beta'}(g) \tag{3.72}$$

and

$$\sum_{\alpha=1}^{d_a} \sum_{\alpha'=1}^{d_a} \sum_{\beta=1}^{d_b} \sum_{\beta'=1}^{d_b} \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{pmatrix} \begin{vmatrix} \Gamma, s \\ \gamma \end{vmatrix} D^{\Gamma_a}_{\alpha\alpha'}(g)\, D^{\Gamma_b}_{\beta\beta'}(g) \begin{pmatrix} \Gamma_a & \Gamma_b \\ \alpha' & \beta' \end{pmatrix} \begin{vmatrix} \Gamma', s' \\ \gamma' \end{vmatrix}^* = D^{\Gamma}_{\gamma\gamma'}(g)\, \delta_{\Gamma\Gamma'}\, \delta_{ss'} \quad . \tag{3.73}$$

3.2.4 Simply reducible groups

A group G is *simply reducible* if the multiplicities n_{Γ}^{ab} in its IRREP product decompositions are all either $n_{\Gamma}^{ab} = 0$ or $n_{\Gamma}^{ab} = 1$. In this case, we may drop the multiplicity index s. For simply reducible groups, we

can obtain an explicit expression for the CGCs, courtesy of the Great Orthogonality Theorem :

$$\frac{d_\Gamma}{N_G}\sum_{g\in G} D^{\Gamma_a}_{\alpha\alpha'}(g)\,D^{\Gamma_b}_{\beta\beta'}(g)\,D^{\Gamma^*}_{\gamma\gamma'}(g) = \sum_{\Gamma'}\sum_{\sigma,\sigma'}\left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma'\\ \alpha & \beta & \sigma\end{array}\right)^*\left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma'\\ \alpha' & \beta' & \sigma'\end{array}\right)\overbrace{\frac{d_\Gamma}{N_G}\sum_{g\in G} D^{\Gamma'}_{\sigma\sigma'}(g)\,D^{\Gamma^*}_{\gamma\gamma'}(g)}^{=\,\delta_{\Gamma\Gamma'}\,\delta_{\sigma\gamma}\,\delta_{\sigma'\gamma'}}$$
$$= \left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma\\ \alpha & \beta & \gamma\end{array}\right)^*\left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma\\ \alpha' & \beta' & \gamma'\end{array}\right) \quad . \tag{3.74}$$

We now set $\alpha = \alpha' \equiv \alpha_0$, $\beta = \beta' \equiv \beta_0$, and $\gamma = \gamma' \equiv \gamma_0$ in such a way that the LHS of the above equation is nonvanishing[15] to obtain

$$\left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma\\ \alpha_0 & \beta_0 & \gamma_0\end{array}\right) = \sqrt{\frac{d_\Gamma}{N_G}\sum_{g\in G} D^{\Gamma_a}_{\alpha_0\alpha_0}(g)\,D^{\Gamma_b}_{\beta_0\beta_0}(g)\,D^{\Gamma^*}_{\gamma_0\gamma_0}(g)} \quad , \tag{3.75}$$

with no sum on the repeated indices α_0 , β_0, and γ_0 . We can choose $\left(\begin{smallmatrix}\Gamma_a & \Gamma_b & \Gamma\\ \alpha_0 & \beta_0 & \gamma_0\end{smallmatrix}\right)$ to be real and positive, which amounts to a phase convention for the CGCs. The general CGC is then given by

$$\left(\begin{array}{cc|c}\Gamma_a & \Gamma_b & \Gamma\\ \alpha & \beta & \gamma\end{array}\right) = \frac{1}{\left(\begin{smallmatrix}\Gamma_a & \Gamma_b & \Gamma\\ \alpha_0 & \beta_0 & \gamma_0\end{smallmatrix}\right)}\,\frac{d_\Gamma}{N_G}\sum_{g\in G} D^{\Gamma_a}_{\alpha\alpha_0}(g)\,D^{\Gamma_b}_{\beta\beta_0}(g)\,D^{\Gamma^*}_{\gamma\gamma_0}(g) \tag{3.76}$$

When G is not simply reducible and there are multiple appearances of the same representation in the decomposition of the product $\Gamma_a \times \Gamma_b$, the situation is more complicated. Tables of CGCs for physically useful groups are listed in, *e.g.*, Koster *et al.* (1963).

Example : C_{3v}

As an example, consider the case of C_{3v}, with representations A_1, A_2, and E. $A_{1,2}$ are one-dimensional and can be read off from the character table. For the two-dimensional IRREP E, we use the representation matrices in Eqn. 3.41. Since $A_1 \times A_1 = A_2 \times A_2 = A_1$ and $A_1 \times A_2 = A_2$, we have

$$\left(\begin{array}{cc|c}A_1 & A_1 & A_1\\ 1 & 1 & 1\end{array}\right) = \left(\begin{array}{cc|c}A_1 & A_2 & A_2\\ 1 & 1 & 1\end{array}\right) = \left(\begin{array}{cc|c}A_2 & A_2 & A_1\\ 1 & 1 & 1\end{array}\right) = 1 \quad . \tag{3.77}$$

Recall $A_1 \times E = A_2 \times E = E$. We then have

$$\left(\begin{array}{cc|c}A_1 & E & E\\ 1 & \nu & \xi\end{array}\right) = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}_{\nu\xi} \quad , \quad \left(\begin{array}{cc|c}A_2 & E & E\\ 1 & \nu & \xi\end{array}\right) = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}_{\nu\xi} \quad . \tag{3.78}$$

Finally, $E \times E = A_1 \oplus A_2 \oplus E$, and we have

$$\left(\begin{array}{cc|c}E & E & A_1\\ \mu & \nu & 1\end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}_{\mu\nu} \quad , \quad \left(\begin{array}{cc|c}E & E & A_2\\ \mu & \nu & 1\end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}_{\mu\nu} \tag{3.79}$$

and

$$\left(\begin{array}{cc|c}E & E & E\\ \mu & \nu & 1\end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}_{\mu\nu} \quad , \quad \left(\begin{array}{cc|c}E & E & E\\ \mu & \nu & 2\end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_{\mu\nu} \quad . \tag{3.80}$$

[15] See R. Winkler, *Introduction to Group Theory* (2015), p. 84.
Online at http://www.niu.edu/rwinkler/teaching/group-11/g-lecture.pdf

3.2.5 Wigner-Eckart theorem

The transformation properties of basis vectors were defined in Eqn. 3.19: $\hat{U}(g)\,|\,\Gamma\mu\,\rangle = |\,\Gamma\nu\,\rangle\,D^{\Gamma}_{\nu\mu}(g)$. Operators, too, may be classified by their transformation properties under group actions. Since we would like $\langle\,\phi'\,|\,\hat{Q}'\,|\,\psi'\,\rangle = \langle\,\phi\,|\,\hat{Q}\,|\,\psi\,\rangle$, where, dropping representation and basis indices, the primes denote the transformed Hilbert space vectors and operators, the action of a group operation $g \in G$ on a general operator $\hat{Q}$ is $\hat{Q}' = \hat{U}(g)\,\hat{Q}\,\hat{U}^{\dagger}(g)$. We now consider the case of *tensor operators*, which form families which transform among themselves under group operations.

> DEFINITION : A *tensor operator* $\hat{Q}^{\Gamma}_{\mu}$ is a Hilbert space operator which transforms according to an IRREP of some group G. Tensor operators carry representation and basis indices.

The tensor operator $\hat{Q}^{\Gamma}_{\mu}$ transforms as

$$\hat{U}(g)\,\hat{Q}^{\Gamma}_{\mu}\,\hat{U}^{\dagger}(g) = \hat{Q}^{\Gamma}_{\nu}\,D^{\Gamma}_{\nu\mu}(g) \quad . \tag{3.81}$$

We can think of families of tensor operators as invariant subspaces in operator space, $\mathsf{End}(\mathcal{H})$.

Now consider the action of tensor operators on basis vectors, such as $\hat{Q}^{\Gamma_a}_{\alpha}\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle$. We ask how such an object transforms under group operations. We have

$$\begin{aligned}\hat{U}(g)\,\hat{Q}^{\Gamma_a}_{\alpha}\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle &= \hat{U}(g)\,\hat{Q}^{\Gamma_a}_{\alpha}\,\hat{U}^{\dagger}(g)\,\hat{U}(g)\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle \\ &= \hat{Q}^{\Gamma_a}_{\alpha'}\,|\,\mathrm{e}^{\Gamma_b}_{\beta'}\,\rangle\,D^{\Gamma_a}_{\alpha'\alpha}(g)\,D^{\Gamma_b}_{\beta'\beta}(g) = \hat{Q}^{\Gamma_a}_{\alpha'}\,|\,\mathrm{e}^{\Gamma_b}_{\beta'}\,\rangle\,D^{\Gamma_a\times\Gamma_b}_{\alpha'\beta',\,\alpha\beta}(g) \quad .\end{aligned} \tag{3.82}$$

This tells us that $\hat{Q}^{\Gamma_a}_{\alpha}\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle$ transforms according to the product representation $\Gamma_a \times \Gamma_b$. This means that we can expand $\hat{Q}^{\Gamma_a}_{\alpha}\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle$ as a sum over its irreducible components, *viz.*

$$\hat{Q}^{\Gamma_a}_{\alpha}\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle = \sum_{\Gamma,s,\gamma}\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma,s \\ \alpha & \beta & \gamma \end{array}\right)|\,\Psi^{\Gamma,\,s}_{\gamma}\,\rangle \quad , \tag{3.83}$$

where $|\,\Psi^{\Gamma,\,s}_{\gamma}\,\rangle$ transforms according to the Γ IRREP of the symmetry group G, meaning

$$\hat{U}(g)\,|\,\Psi^{\Gamma,\,s}_{\gamma}\,\rangle = |\,\Psi^{\Gamma,\,s}_{\gamma'}\,\rangle\,D^{\Gamma}_{\gamma'\gamma}(g) \quad . \tag{3.84}$$

This will be explicitly demonstrated at the end of this section. Note that, upon invoking orthogonality of the CGCs,

$$|\,\Psi^{\Gamma,\,s}_{\gamma}\,\rangle = \sum_{\alpha,\beta}\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma,s \\ \alpha & \beta & \gamma \end{array}\right)^{*}\hat{Q}^{\Gamma_a}_{\alpha}\,|\,\mathrm{e}^{\Gamma_b}_{\beta}\,\rangle \quad . \tag{3.85}$$

Since states which transform according to different IRREPs are orthogonal, we must have

$$\langle\,\mathrm{e}^{\Gamma_c}_{\gamma}\,|\,\Psi^{\Gamma,\,s}_{\sigma}\,\rangle = \langle\,\Gamma_c\,\|\,Q^{\Gamma_a}\,\|\,\Gamma_b\,\rangle_s\,\delta_{\Gamma\Gamma_c}\,\delta_{\gamma\sigma}\;, \tag{3.86}$$

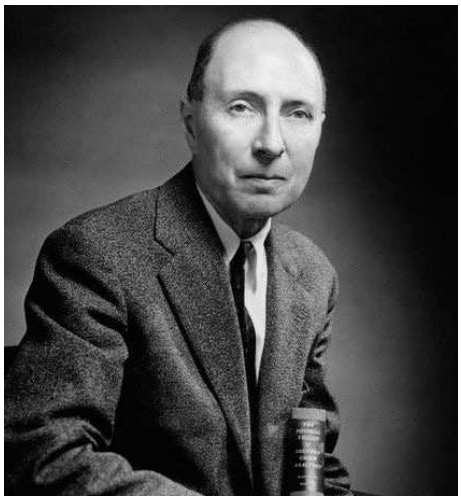


Figure 3.4: Eugene P. Wigner, the Ph.D. thesis supervisor of the Ph.D. thesis supervisor of my Ph.D. thesis supervisor.

where the *reduced matrix element* $\langle\, \Gamma_c \,\|\, Q^{\Gamma_a} \,\|\, \Gamma_b \,\rangle_s$ is independent of the basis indices γ and σ. We therefore have

$$\boxed{\langle\, \mathrm{e}^{\Gamma_c}_{\gamma} \,|\, \hat{Q}^{\Gamma_a}_{\alpha} \,|\, \mathrm{e}^{\Gamma_b}_{\beta} \,\rangle = \sum_s \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c\,, s \\ \alpha & \beta & \gamma \end{array} \right) \langle\, \Gamma_c \,\|\, Q^{\Gamma_a} \,\|\, \Gamma_b \,\rangle_s} \tag{3.87}$$

a result known as the *Wigner-Eckart theorem*. Note that we have assumed that the ket vector $|\, \mathrm{e}^{\Gamma}_{\mu} \,\rangle$ is conjugate to the bra vector $\langle\, \mathrm{e}^{\Gamma}_{\mu} \,|$. In fact, they can come from different copies of each representation corresponding to different quantum numbers[16]. A more general expression of the Wigner-Eckart theorem is then

$$\langle\, \mathrm{e}^{\Gamma_c, l_c}_{\gamma} \,|\, \hat{Q}^{\Gamma_a}_{\alpha} \,|\, \mathrm{e}^{\Gamma_b, l_b}_{\beta} \,\rangle = \sum_s \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c\,, s \\ \alpha & \beta & \gamma \end{array} \right) \langle\, \Gamma_c\,,\, l_c \,\|\, Q^{\Gamma_a} \,\|\, \Gamma_b\,,\, l_b \,\rangle_s \quad . \tag{3.88}$$

Appealing once again to the orthogonality of the CGCs, we obtain the following expression for the Wigner-Eckart reduced matrix elements:

$$\langle\, \Gamma_c\,,\, l_c \,\|\, Q^{\Gamma_a} \,\|\, \Gamma_b\,,\, l_b \,\rangle_s \, \delta_{\Gamma\Gamma_c} \, \delta_{\sigma\gamma} = \sum_{\alpha,\beta} \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma,\, s \\ \alpha & \beta & \sigma \end{array} \right)^* \langle\, \mathrm{e}^{\Gamma_c\,, l_c}_{\gamma} \,|\, \hat{Q}^{\Gamma_a}_{\alpha} \,|\, \mathrm{e}^{\Gamma_b\,, l_b}_{\beta} \,\rangle \quad . \tag{3.89}$$

[16] Note that the multiplicity index s is not the same sort of animal as the index l in the state $|\, \mathrm{e}^{\Gamma,\, l}_{\mu} \,\rangle$. The essential difference is that l labels states according to quantum numbers not associated with the group symmetry. The multiplicity index s, by contrast, knows nothing of the other quantum numbers and arises purely from a group theoretic analysis of the product representations.

If different appearances of the same IRREP are not orthogonal, we still have

$$\begin{aligned}\left\langle\, \Gamma_c\,\gamma\,,\, l_c \,\middle|\, \Gamma_b\,\beta\,,\, l_b\,\right\rangle &= \frac{1}{N_G}\sum_{g\in G}\left\langle\, \Gamma_c\,\gamma\,,\, l_c \,\middle|\, U^\dagger(g)\,U(g)\,\middle|\, \Gamma_b\,\beta\,,\, l_b\,\right\rangle \\ &= \frac{1}{N_G}\sum_{g\in G} D^{\Gamma_c}_{\gamma'\gamma}(g)^*\left\langle\, \Gamma_c\,\gamma'\,,\, l_c \,\middle|\, \Gamma_b\,\beta'\,,\, l_b\,\right\rangle D^{\Gamma_b}_{\beta'\beta}(g) \\ &= \frac{1}{d_{\Gamma_c}}\sum_{\mu=1}^{d_{\Gamma_b}}\left\langle\, \Gamma_c\,\mu\,,\, l_c \,\middle|\, \Gamma_b\,\mu\,,\, l_b\,\right\rangle \delta_{\Gamma_b\Gamma_c}\,\delta_{\alpha\beta} \equiv \left\langle\, \Gamma_c\,,\, l_c \,\middle\|\, \Gamma_b\,,\, l_b\,\right\rangle \delta_{\Gamma_b\Gamma_c}\,\delta_{\alpha\beta}\,.\end{aligned} \tag{3.90}$$

The quantity $\left\langle\, \Gamma\,,\, l_a \,\middle\|\, \Gamma\,,\, l_b\,\right\rangle$ is called the *reduced overlap*, or the overlap matrix $O^{\Gamma}_{l_a l_b}$. Note that it does not depend on the basis indices α and β. By the same token, we also have

$$\left\langle\, \Gamma_c\,\gamma\,,\, l_c \,\middle|\, \Psi^{\Gamma,\,s}_{\sigma}\,\right\rangle = \frac{1}{d_\Gamma}\sum_{\mu=1}^{d_\Gamma}\left\langle\, \Gamma_c\,\mu\,,\, l_c \,\middle|\, \Psi^{\Gamma,\,s}_{\mu}\,\right\rangle \delta_{\Gamma\Gamma_c}\,\delta_{\gamma\sigma} \quad . \tag{3.91}$$

Wigner-Eckart theorem for simply reducible groups

For simply reducible groups, there is no representation multiplicity index s for the direct products, and we have the simpler expression

$$\left\langle\, \mathrm{e}^{\Gamma_c,\,l_c}_{\gamma} \,\middle|\, \hat{Q}^{\Gamma_a}_{\alpha} \,\middle|\, \mathrm{e}^{\Gamma_b,\,l_b}_{\beta}\,\right\rangle = \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha & \beta & \gamma \end{array}\right)\left\langle\, \Gamma_c\,,\, l_c \,\middle\|\, Q^{\Gamma_a} \,\middle\|\, \Gamma_b\,,\, l_b\,\right\rangle \quad . \tag{3.92}$$

In this case, the ratios of matrix elements

$$\frac{\left\langle\, \mathrm{e}^{\Gamma_c,\,l_c}_{\gamma'} \,\middle|\, \hat{Q}^{\Gamma_a}_{\alpha'} \,\middle|\, \mathrm{e}^{\Gamma_b,\,l_b}_{\beta'}\,\right\rangle}{\left\langle\, \mathrm{e}^{\Gamma_c,\,l_c}_{\gamma} \,\middle|\, \hat{Q}^{\Gamma_a}_{\alpha} \,\middle|\, \mathrm{e}^{\Gamma_b,\,l_b}_{\beta}\,\right\rangle} = \frac{\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha' & \beta' & \gamma' \end{array}\right)}{\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma_c \\ \alpha & \beta & \gamma \end{array}\right)} \tag{3.93}$$

are *independent* of all details of the operators $\hat{Q}^{\Gamma_a}_{\alpha}$ other than the representation by which it transforms.

Proof that $\left|\, \Psi^{\Gamma,\,l}_{\gamma}\,\right\rangle$ transforms as advertised

Start with Eqn. 3.83 and apply $\hat{U}(g)$ to both sides. The LHS transforms

$$\hat{U}(g)\,\hat{Q}^{\Gamma_a}_{\alpha}\left|\, \mathrm{e}^{\Gamma_b}_{\beta}\,\right\rangle = \sum_{\alpha',\beta'}\hat{Q}^{\Gamma_a}_{\alpha'}\left|\, \mathrm{e}^{\Gamma_b}_{\beta'}\,\right\rangle D^{\Gamma_a}_{\alpha'\alpha}(g)\,D^{\Gamma_b}_{\beta'\beta}(g) = \sum_{\Gamma,l,\gamma}\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma,l \\ \alpha & \beta & \gamma \end{array}\right)\hat{U}(q)\left|\, \Psi^{\Gamma,\,l}_{\gamma}\,\right\rangle \quad . \tag{3.94}$$

Now multiply by $\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma',l' \\ \alpha & \beta & \gamma' \end{array}\right)^*$ and sum on α and β. Using orthogonality of the CGCs, and dropping primes on the Γ', l', and γ' indices, we obtain

$$\sum_{\alpha,\beta}\sum_{\alpha',\beta'}\hat{Q}^{\Gamma_a}_{\alpha'}\left|\, \mathrm{e}^{\Gamma_b}_{\beta'}\,\right\rangle D^{\Gamma_a}_{\alpha'\alpha}(g)\,D^{\Gamma_b}_{\beta'\beta}(g)\left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma,\,l \\ \alpha & \beta & \gamma \end{array}\right)^* = \hat{U}(g)\left|\, \Psi^{\Gamma,\,l}_{\gamma}\,\right\rangle \quad . \tag{3.95}$$

Finally, reexpress $\hat{Q}^{\Gamma_a}_{\alpha'} \,|\, \mathrm{e}^{\Gamma_b}_{\beta'} \,\rangle$ on the LHS above in terms of the $|\, \Psi^{\Gamma,\,l}_{\gamma} \,\rangle$, to find

$$\begin{aligned}\hat{U}(g) \,|\, \Psi^{\Gamma,\,l}_{\gamma} \,\rangle &= \sum_{\Gamma',l',\gamma'} \sum_{\alpha,\beta} \sum_{\alpha',\beta'} \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma',\,l' \\ \alpha' & \beta' & \gamma' \end{array}\right) D^{\Gamma_a}_{\alpha'\alpha}(g)\, D^{\Gamma_b}_{\beta'\beta}(g) \left(\begin{array}{cc|c} \Gamma_a & \Gamma_b & \Gamma,\,l \\ \alpha & \beta & \gamma \end{array}\right)^* |\, \Psi^{\Gamma',\,l'}_{\gamma'} \,\rangle \\ &= \sum_{\Gamma',l',\gamma'} |\, \Psi^{\Gamma',\,l'}_{\gamma'} \,\rangle\, D^{\Gamma'}_{\gamma'\gamma}(g) \quad ,\end{aligned} \tag{3.96}$$

after invoking the CGC relation Eqn. 3.73.

3.2.6 Level repulsion and degeneracies

Consider a Hamiltonian $\hat{H}_0$ with $\big[\hat{H}_0, \hat{U}(G)\big] = 0$ whose eigenstates are labeled $|\, \Gamma\mu, l \,\rangle \equiv |\, \mathrm{e}^{\Gamma,\,l}_{\mu} \,\rangle$. Suppose two multiplets $|\, \Gamma_a\, \alpha, l_a \,\rangle$ and $|\, \Gamma_b\, \beta, l_b \,\rangle$ are in close proximity, with energies E_a and E_b, respectively. Can they be made degenerate by varying the Hamiltonian in a way which preserves the full symmetry of G? Let's write $\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{V}$, where $\big[\hat{V}, \hat{U}(G)\big] = 0$, and, neglecting all other multiplets which by assumption lie much further away in energy than the gap $|E_a - E_b|$, we compute the Hamiltonian matrix elements in the a, b multiplet basis. Since $\hat{V}$ transforms as the Γ_1 identity IRREP, we have $\Gamma_1 \times \Gamma_b = \Gamma_b$, and therefore

$$\big\langle\, \Gamma_a\, \alpha, l_a \,\big|\, \hat{V} \,\big|\, \Gamma_b\, \beta, l_b \,\big\rangle \;=\; \overbrace{\left(\begin{array}{cc|c} \Gamma_b & \Gamma_1 & \Gamma_a \\ \beta & 1 & \alpha \end{array}\right)}^{= \delta_{\Gamma_a\Gamma_b}\,\delta_{\alpha\beta}} \big\langle\, \Gamma_a, l_a \,\big\|\, \hat{V} \,\big\|\, \Gamma_b, l_b \,\big\rangle \tag{3.97}$$

vanishes unless $\Gamma_a = \Gamma_b$, although we may have $l_a \neq l_b$. When $\Gamma_a = \Gamma_b$,

$$\big\langle\, \Gamma_a, l_a \,\big\|\, \hat{V} \,\big\|\, \Gamma_a, l_b \,\big\rangle = \frac{1}{d_{\Gamma_a}} \sum_{\mu=1}^{d_{\Gamma_a}} \big\langle\, \Gamma_a\, \mu, l_a \,\big|\, \hat{V} \,\big|\, \Gamma_a\, \mu, l_b \,\big\rangle \equiv V_{ab} \quad . \tag{3.98}$$

Consider first the case $\Gamma_a \ncong \Gamma_b$. Then there are no off-diagonal matrix elements in our basis, and the energy shifts are given by

$$\begin{aligned} E_a(\lambda) &= E_a + \lambda V_{aa} \\ E_b(\lambda) &= E_b + \lambda V_{bb} \end{aligned} \tag{3.99}$$

Setting $E_a(\lambda) = E_b(\lambda)$, we obtain a degeneracy of the two multiplets when $\lambda = \lambda_*$, with

$$\lambda_* = \frac{E_b - E_a}{V_{aa} - V_{bb}} \quad . \tag{3.100}$$

The resulting supermultiplet has degeneracy $d = d_{\Gamma_a} + d_{\Gamma_b}$.

When $\Gamma_a = \Gamma_b$, we have nonzero off-diagonal elements. The reduced basis Hamiltonian is given by

$$\hat{H}_{\rm red} = \begin{pmatrix} E_a + \lambda V_{aa} & \lambda V_{ab} \\ \lambda V^*_{ab} & E_b + \lambda V_{bb} \end{pmatrix} \otimes \mathbb{1}_{d_{\Gamma_a} \times d_{\Gamma_a}} \quad . \tag{3.101}$$

Note that we still must distinguish the a and b multiplets, because while they belong to the same representations, they are not identical multiplets, *i.e.* their wavefunctions are different[17]. There are then two d_{Γ_a}-fold degenerate sets of states, with energies

$$E_{ab,\pm} = \tfrac{1}{2}(E_a + \lambda V_{aa} + E_b + \lambda V_{bb}) \pm \tfrac{1}{2}\sqrt{(E_a + \lambda V_{aa} - E_b - \lambda V_{bb})^2 + 4\lambda^2 |V_{ab}|^2} \quad . \tag{3.102}$$

The only way for these multiplets to become degenerate is for the radical to vanish. But there is no choice for λ which will make that happen. Therefore we have an avoided crossing. The best we can do is to minimize the energy difference.

My personal advice: if you are ever caught being degenerate, say that it was an accident.

3.2.7 Example: C_{4v}

Consider the problem of a particle in a two-dimensional $L \times L$ square box, with $\hat{H}_0 = \frac{\boldsymbol{p}^2}{2m} + V(x,y)$ with

$$V(x,y) = \begin{cases} 0 & \text{if } |x| < \frac{1}{2}L \text{ and } |y| < \frac{1}{2}L \\ \infty & \text{otherwise} \quad . \end{cases} \tag{3.103}$$

This problem has a C_{4v} symmetry. Recall $C_{4v} \cong D_4$ is the symmetry group of the square, and is generated by two elements, *i.e.* a counterclockwise rotation through $\frac{1}{2}\pi$ (r) and a reflection in the x-axis (σ). One has $r^4 = \sigma^2 = (r\sigma)^2 = 1$. There are five conjugacyclasses: $\{E\}$, $\{r, r^3\}$, $\{r^2\}$, $\{r\sigma, \sigma r\}$ (diagonal reflections), and $\{\sigma, \sigma r^2\}$ (reflections in the x and y axes). The character table is given in Tab. 3.2.

Note that

$$r\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -y \\ x \end{pmatrix} \quad , \quad \sigma\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ -y \end{pmatrix} \quad , \quad r^2\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ -y \end{pmatrix} \quad , \quad r\sigma\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix} \quad . \tag{3.104}$$

And recall that $\hat{U}(g)\,\Psi(x,y) = \Psi(g^{-1}x, g^{-1}y)$. We define the functions

$$\begin{aligned} \phi_n(u) &= \sqrt{\frac{2}{L}}\,\cos\left(\frac{2\big(n-\frac{1}{2}\big)\pi u}{L}\right) \\ \chi_n(u) &= \sqrt{\frac{2}{L}}\,\sin\left(\frac{2n\pi u}{L}\right) \quad , \end{aligned} \tag{3.105}$$

where $n \in \mathbb{Z}_{>0}$ is a positive integer in either case. Note that the $\{\phi_n(u)\}$ are even under $u \to -u$ whereas the $\{\chi_n(u)\}$ are odd, and that $\phi_n(\pm\frac{1}{2}L) = \chi_n(\pm\frac{1}{2}L) = 0$. We will find it convenient to define the energy unit $\varepsilon_0 \equiv 2\pi^2\hbar^2/mL^2$.

Let's now write down all the possible wavefunctions for this problem. We'll find there are basically five different forms to consider:

[17] Think of the tower of even and odd states for the one-dimensional particle in a symmetric potential. All even states belong to the same Γ_1 representation, but have different wavefunctions.

C_{4v}	E	$\{r, r^3\}$	$\{r^2\}$	$\{r\sigma, \sigma r\}$	$\{\sigma, \sigma r^2\}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

Table 3.2: Character table for the group C_{4v}.

(i) $\Psi^{(\mathrm{i})}_{nn}(x,y) = \phi_n(x)\,\phi_n(y)$: The energy is $E^{(\mathrm{i})}_{nn} = 2n^2\varepsilon_0$. The wavefunction is invariant under all group operations, *i.e.*

$$\hat{U}(r)\,\Psi = \hat{U}(r^2)\,\Psi = \hat{U}(r\sigma)\,\Psi = \hat{U}(\sigma)\,\Psi = \Psi \quad , \tag{3.106}$$

and thus corresponds to the A_1 IRREP.

(ii) $\Psi^{(\mathrm{ii})}_{nn}(x,y) = \chi_n(x)\,\chi_n(y)$: The energy is $E^{(\mathrm{ii})}_{nn} = 2(n-\frac{1}{2})^2\varepsilon_0$. We find

$$\hat{U}(r)\,\Psi = \hat{U}(\sigma)\,\Psi = -\Psi \quad , \quad \hat{U}(r^2)\,\Psi = \hat{U}(r\sigma)\,\Psi = \Psi \quad , \tag{3.107}$$

corresponding to the B_1 IRREP.

(iii) $\Psi^{(\mathrm{iii})}_{mn,\pm}(x,y) = \frac{1}{\sqrt{2}}\big[\phi_m(x)\,\phi_n(y) \pm \phi_m(y)\,\phi_n(x)\big]$ with $m < n$. The energy for both states is given by $E^{(\mathrm{iii})}_{mn} = (m^2+n^2)\varepsilon_0$. Is this a two-dimensional representation? We have

$$\hat{U}(r)\,\Psi_\pm = \hat{U}(r\sigma)\,\Psi_\pm = \pm\,\Psi_\pm \quad , \quad \hat{U}(r^2)\,\Psi_\pm = \hat{U}(\sigma)\,\Psi_\pm = \Psi_\pm \quad , \tag{3.108}$$

which tells us that Ψ_+ transforms according to A_1 and Ψ_- according to B_2. So we have two one-dimensional IRREPs and no sign of the two-dimensional E IRREP yet.

(iv) $\Psi^{(\mathrm{iv})}_{mn,\pm}(x,y) = \frac{1}{\sqrt{2}}\big[\chi_m(x)\,\chi_n(y) \pm \chi_m(y)\,\chi_n(x)\big]$ with $m < n$. The energy for both states is given by $E^{(\mathrm{iv})}_{mn} = \big((m-\frac{1}{2})^2 + (n-\frac{1}{2})^2\big)\varepsilon_0$. We find

$$\hat{U}(r)\,\Psi_\pm = \mp\,\Psi_\pm \quad , \quad \hat{U}(r^2)\,\Psi_\pm = \Psi_\pm \quad , \quad \hat{U}(r\sigma)\,\Psi_\pm = \pm\Psi_\pm \quad , \quad \hat{U}(\sigma)\,\Psi_\pm = -\Psi_\pm \quad . \tag{3.109}$$

which tells us that Ψ_+ transforms as B_1 according and Ψ_- according to A_2. So again two one-dimensional IRREPs and still no sign of the elusive E.

(v) $\Psi^{(\mathrm{v})}_{mn,\pm}(x,y) = \frac{1}{\sqrt{2}}\big[\phi_m(x)\,\chi_n(y) \pm \phi_m(y)\,\chi_n(x)\big]$ with $m \le n$. The energy for both states is given by $E^{(\mathrm{v})}_{mn} = \big(m^2 + (n-\frac{1}{2})^2\big)\varepsilon_0$. We find

$$\hat{U}(r)\,\Psi_\pm = \pm\,\Psi_\mp \quad , \quad \hat{U}(r^2)\,\Psi_\pm = -\Psi_\pm \quad , \quad \hat{U}(r\sigma)\,\Psi_\pm = \pm\Psi_\pm \quad , \quad \hat{U}(\sigma)\,\Psi_\pm = -\Psi_\mp \quad . \tag{3.110}$$

At long last, the E representation has shown itself! Note how in this basis,

$$D^E(r) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad , \quad D^E(r^2) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad D^E(r\sigma) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad D^E(\sigma) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad . \tag{3.111}$$

Now suppose we add a perturbation which transforms as the identity IRREP Γ_1. For example, we could take $\hat{H} = \hat{H}_0 + \hat{V}$ with $\hat{V}(x,y) = \lambda x^2 y^2$. According to the Wigner-Eckart theorem, this won't split any of the E multiplets, but rather will simply lead to an equal energy shift for both E states. One only need compute one matrix element, per Eqn. 3.97.

3.3 Appendix : Random True Facts About Linear Algebra

Normal matrices and eigenspectra : Quantum mechanical Hamiltonians can be represented as Hermitian matrices. In elementary school linear algebra class, we all learned that any Hermitian matrix H is diagonalizable by a unitary transformation, its eigenvalues are real, and eigenvectors corresponding to different eigenvalues are necessarily orthogonal. In the case of degenerate eigenvalues, their associated eigenvectors may be chosen to be mutually orthogonal via the Gram-Schmidt process.

Any complex square matrix A which satisfies $A^\dagger A = AA^\dagger$ is called *normal*. Hermitian matrices are normal, but so are antihermitian and unitary matrices[18]. Real symmetric, antisymmetric, and orthogonal matrices satisfy $A^{\mathsf{T}}A = AA^{\mathsf{T}}$. The *Schur decomposition theorem* guarantees that any $n \times n$ matrix A may be decomposed as $A = VTV^\dagger$, where $V \in \mathsf{U}(n)$ and T is upper triangular. Now if A is normal, $[A, A^\dagger] = V\,[T, T^\dagger]\,V^\dagger = 0$, hence T is normal. However, it is easy to show that any normal upper triangular matrix must be diagonal[19], so $A = VDV^\dagger$, which means $D = V^\dagger AV$ is the diagonal matrix of eigenvalues of A. Conversely, if $A = VDV^\dagger$ is unitarily equivalent to a diagonal matrix, it is trivial to show that A is normal. Thus *any $n \times n$ matrix A is diagonalizable by a unitary transformation if and only if A is normal.*

There is a real version of Schur decomposition whereby a real matrix B satisfying $B^{\mathsf{T}}B = BB^{\mathsf{T}}$ may be decomposed as $B = RSR^{\mathsf{T}}$, where R is a real orthogonal matrix, and S is *block upper triangular*. The diagonal blocks of S are either 1×1, corresponding to real eigenvalues, or 2×2, corresponding to complex eigenvalues. One eventually concludes that real symmetric matrices have real eigenvalues, real antisymmetric matrices have pure imaginary (or zero) eigenvalues, and real orthogonal matrices have unimodular complex eigenvalues.

Now let's set $A = VDV^\dagger$ and consider different classes of matrix A. If A is Hermitian, $A = A^\dagger$ immediately yields $D = D^\dagger$, which says that all the eigenvalues of A must be real. If $A^\dagger = -A$, then $D^\dagger = -D$ and all the eigenvalues are purely imaginary. And if $A^\dagger = A^{-1}$, then $D^\dagger = D^{-1}$ and we conclude that all the eigenvalues are unimodular, *i.e.* of the form $e^{i\omega_j}$. This analysis also tells us that any unitary matrix U can be written in the form $U = \exp(iH)$ for some Hermitian matrix H.

Jordan blocks : What happens when an $n \times n$ matrix A is not normal? In this case A is not diagonalizable by a unitary transformation, and while the sum of the dimensions of its eigenspaces is generically equal to the matrix dimension $\dim(A) = n$, this is not guaranteed; it may be less than n. For example, consider

[18] There are many examples of normal matrices which are neither Hermitian, antihermitian, nor unitary. For example, any diagonal matrix with arbitrary complex diagonal entries is normal.

[19] $T^\dagger T = TT^\dagger$ says that $\sum_j |T_{ij}|^2 = \sum_j |T_{ji}|^2$, *i.e.* the sum of the square moduli of the elements in the $i^{\rm th}$ row is the same as that for the $i^{\rm th}$ column. Starting with $i = 1$, the only possible nonzero entry in the first column is $T_{1,1}$, hence all the remaining entries in the first row must vanish. Filling in all these zeros, proceed to $i = 2$. Since we just showed $T_{1,2} = 0$, we conclude that the only possible nonzero entry in the second column is $T_{2,2}$, hence all remaining entries in the second row must vanish. Continuing in this manner, we conclude that T is diagonal if it is both normal and upper triangular.

the matrix

$$A = \begin{pmatrix} r & 1 \\ 0 & r \end{pmatrix} \quad . \tag{3.112}$$

The eigenvalues are solutions to $\det(\lambda I - A) = 0$, hence $\lambda = r$, but there is only one eigenvector, $\psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. What is always true for any complex matrix A is that it can be brought to *Jordan canonical form* by a similarity transformation $J = P^{-1}AP$, where P is invertible, and

$$J = \begin{pmatrix} J_1 & & \\ & \ddots & \\ & & J_b \end{pmatrix} \quad , \tag{3.113}$$

where b is the number of *Jordan blocks* and where each block J_s is of the form

$$J_s = \begin{pmatrix} \lambda_s & 1 & & \\ & \lambda_s & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_s \end{pmatrix} \quad . \tag{3.114}$$

Thus each J_s is tridiagonal, with diagonal elements all given by λ_s and each element directly above the diagonal equal to one. Clearly J_s has only one eigenvalue, λ_s, and writing the corresponding *right* eigenvector as $\vec{\psi}$, the condition $J_s\vec{\psi} = \lambda_s\vec{\psi}$ yields the equations

$$\lambda_s\,\psi_1 + \psi_2 = \lambda_s\,\psi_1 \quad , \quad \lambda_s\,\psi_2 + \psi_3 = \lambda_s\,\psi_2 \quad \ldots \quad \lambda_s\,\psi_{n-1} + \psi_{n_s} = \lambda_s\,\psi_{n_s-1} \quad , \tag{3.115}$$

where $n_s = \dim(J_s)$. These equations entail $\psi_2 = \psi_3 = \cdots = \psi_{n_s} = 0$, which says that there is only one such eigenvector, whose components are $\psi_j = \delta_{j,1}$. Note that the corresponding *left* eigenvector $\vec{\chi}^{\,\mathsf{T}}$ is then $\chi_j = \delta_{j,n_s}$. If $n_s > 1$ we then have $\vec{\chi}\cdot\vec{\psi} = 0$, which means that the left and right eigenvectors of A which correspond to the Jordan blocks with $n_s > 1$ are orthogonal. *Nota bene*: It may be the case that there are degeneracies among the eigenvalues $\{\lambda_s\}$.

To summarize[20], for every general complex $n \times n$ matrix A,

- A may be brought to Jordan canonical form by a similarity transformation $J = P^{-1}AP$, where $J = \mathrm{bdiag}(J_1, \ldots, J_b)$ is block diagonal, with each $(J_s)_{ij} = \lambda_s\,\delta_{ij} + \delta_{i,j-1}$ for $s \in \{1, \ldots, b\}$.
- There are $b \leq n$ eigenvalues $\{\lambda_1, \ldots, \lambda_b\}$ (again, not necessarily all distinct) and b corresponding eigenvectors $\{\vec{\psi}_1, \ldots, \vec{\psi}_b\}$. If $b = n$ then the matrix is diagonalizable.
- The dimension n of the matrix A satisfies $n = n_1 + \ldots + n_b$, *i.e.* it is the sum of the dimensions of all its Jordan blocks.
- Let $\lambda \in \{\lambda_1, \ldots, \lambda_b\}$ be an eigenvalue, and define

  $$\mathsf{t}_k(\lambda) = \dim\ker(A - \lambda)^k \quad , \tag{3.116}$$

  which is the *dimension of the null space* of the matrix $A - \lambda I$. Then

[20] See https://en.wikipedia.org/wiki/Jordan_normal_form.

- $\diamond$ $t_k(\lambda)$ is the number of Jordan blocks corresponding to the eigenvalue λ.
- $\diamond$ The number of Jordan blocks of size greater than k is $\mathsf{t}_{k+1}(\lambda) - \mathsf{t}_k(\lambda)$. Thus the number of Jordan blocks of size k for the eigenvalue λ is

$$\mathsf{N}_k(\lambda) = 2\,\mathsf{t}_k(\lambda) - \mathsf{t}_{k+1}(\lambda) - \mathsf{t}_{k-1}(\lambda) \quad . \tag{3.117}$$

Singular value decomposition : Note the difference between the decomposition into Jordan canonical form and singular value decomposition (SVD), in which we write an $m \times n$ matrix A as $A = USV^\dagger$, where U is $m \times k$, V is $n \times k$ (hence $V^\dagger$ is $k \times n$), $U^\dagger U = V^\dagger V = \mathbb{I}_{k\times k}$, and $S = \mathsf{diag}(s_1, \ldots, s_k)$ is $k \times k$ with $k \le \mathsf{min}(m, n)$ and each $s_j > 0$. The elements s_j are the singular values and the rows of U and V are the singular vectors. Note that $A^\dagger A = VS^2V^\dagger$ is $n \times n$ and $AA^\dagger = US^2U^\dagger$ is $m \times m$. If we define

$$R(\lambda) = \prod_{j=1}^{k} \left(\lambda - s_j^2\right) \quad , \tag{3.118}$$

Then

$$P(\lambda) \equiv \mathsf{det}(\lambda - A^\dagger A) = \lambda^{n-k} R(\lambda) \qquad , \qquad Q(\lambda) \equiv \mathsf{det}(\lambda - AA^\dagger) = \lambda^{m-k} R(\lambda) \quad . \tag{3.119}$$

For any square $n \times n$ complex matrix A we therefore have two decompositions, via JCF and SVD, *viz.*

$$A = PJP^{-1} = USV^\dagger \quad , \tag{3.120}$$

where J is the Jordan canonical form of A. When A is normal, $k = n$ and $U = V = P$, *i.e.* the two decompositions are equivalent.

Selection rules : Suppose $[H, A] = 0$ where $H = H^\dagger$ and A is general. Then in the basis of H eigenstates, $\langle n|A|n\rangle = 0$ if $E_m \neq E_n$. The proof is elementary. In the eigenbasis of H,

$$0 = \langle\, m \,|\, [H, A] \,|\, n \,\rangle = (E_m - E_n) \,\langle\, m \,|\, A \,|\, n \,\rangle \quad . \tag{3.121}$$

This result helps us establish that H and A can be simultaneously diagonalized, for expressed in the eigenbasis of H, the operator A must be block diagonal, where the sizes of each of the blocks correspond to the degrees of degeneracy in the eigenspectrum of H. But then a separate unitary transformation can be applied to each of these blocks in order to bring each to diagonal form, without any effect on H.

Degeneracies and nonabelian symmetries : Suppose $[H, A] = [H, B] = 0$ but $[A, B] \neq 0$, where H is a Hamiltonian, and A, B are general operators. A and B might represent different generators of a nonabelian symmetry, for example, such as the components of the total spin operator $\boldsymbol{S}$, which satisfy $[S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma} S^\gamma$. We conclude that the spectrum of H must be degenerate. The reason is that in the eigenbasis of H, both A and B are block diagonal, with the dimensions of the blocks corresponding to the degree of degeneracy in the spectum of H. If H had a nondegenerate spectrum, then A and B would also be diagonal in the H eigenbasis, which would contradict the fact that $[A, B] \neq 0$. When degeneracies are present, the A blocks and B blocks occur in the same locations, and cannot in general be simultaneously diagonalized. So nonabelian symmetries entail degenerate energy eigenvalues. We will study this in great detail in subsequent chapters.

Polar decomposition : Any matrix A may be decomposed in the form $A = HU$, where H is Hermitian and U is unitary. This is reminiscent of writing any complex number z as $z = r\,e^{i\theta}$. The proof is surprisingly simple. First, note that the matrix $AA^\dagger$ is nonnegative definite. Therefore one can write $AA^\dagger = VD^2V^\dagger$ where D is a real diagonal matrix and V is unitary. Now define $H \equiv VDV^\dagger$, in which case $AA^\dagger = H^2$. This must mean $U = H^{-1}A$. We just need to check that U is unitary: $UU^\dagger = H^{-1}AA^\dagger H^{-1} = H^{-1}H^2H^{-1} = E$, so we are done.

Matrix direct product : Given the $n \times n$ matrix A and the $r \times r$ matrix Θ, the direct product matrix $M \equiv A \otimes \Theta$ is defined by its matrix elements $M_{ia,jb} = A_{ij}\,\Theta_{ab}$. Multiplication is a snap:

$$(A \otimes \Theta)(A' \otimes \Theta') = AA' \otimes \Theta\Theta' \quad . \tag{3.122}$$

Expressed as a single matrix, we can write the composite indices ia and jb as $\mu \equiv (i-1)r + a$ and $\nu \equiv (j-1)r + b$. Note $\mu, \nu \in \{1, \ldots, nr\}$ as i, j, a, b range over their allowed values. Thus i, j refer to the larger block structure and a, b to the structure within the blocks. The general structure is then

$$A \otimes \Theta = \begin{pmatrix} A_{11}\,\Theta & \cdots & A_{1n}\,\Theta \\ \vdots & \ddots & \vdots \\ A_{n1}\,\Theta & \cdots & A_{nn}\,\Theta \end{pmatrix} \quad , \tag{3.123}$$

where each Θ is an $r \times r$ matrix.

As an example, consider the matrices

$$\Gamma^1 = \sigma^x \otimes E \quad , \quad \Gamma^2 = \sigma^y \otimes E \quad , \quad \Gamma^3 = \sigma^z \otimes \sigma^x \quad , \quad \Gamma^4 = \sigma^z \otimes \sigma^y \quad , \quad \Gamma^5 = \sigma^z \otimes \sigma^z \quad . \tag{3.124}$$

We can express these in 4×4 form as

$$\Gamma^1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad , \quad \Gamma^2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \quad , \quad \Gamma^3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \tag{3.125}$$

and

$$\Gamma^4 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix} \quad , \quad \Gamma^5 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad . \tag{3.126}$$

These matrices form a *Clifford algebra*, defined by the anticommutator $\{\Gamma^a, \Gamma^b\} = 2\delta^{ab}$. Note that for any Hamiltonian $H = \sum_a d_a\,\Gamma^a$ that $H^2 = \sum_a d_a^2\,\mathbb{1}$. If H is of rank $2k$, then its eigenspectrum consists of two k-fold degenerate levels with $\lambda = \pm|\boldsymbol{d}|$.

3.4 Jokes for Chapter Three

I feel I am running out of math/physics-related jokes, and soon I may have to draw upon my inexhaustible supply of rabbi jokes.

PHILOSOPHER JOKE : Jean-Paul Sartre is sitting in a coffeeshop. A waitress comes by and asks, "What can I get for you today, Professor Sartre?" "Coffee. Black. No cream," comes the reply. A few minutes later the waitress returns. "I'm very sorry, Professor, but we are all out of cream," she says, "Can I bring your coffee with no milk instead?"

RABBI JOKE : (Actually this is something of a math riddle appropriate for children and, sadly, certain undergraduates, but it happens to involve a rabbi.) An old Jew named Shmuel died in the *shtetl* and his will gave his estate to his three sons. It specified that the eldest son should get one half, the middle son one third, and the youngest one ninth. The problem was that Shmuel's entire estate consisted of seventeen chickens, and, well, seventeen is a prime number.

So the sons met to discuss what they should do and the eldest says, "let's ask the rabbi - he is very wise and he will tell us how best to proceed." So they go to the rabbi, who starts to think and think and finally he says, "this is a very difficult problem. But I'll tell you what. Your father was a very good man who always helped out at the *shul*[21], and it just so happens that I have an extra chicken which I am willing to donate to his estate. Now you have eighteen chickens and can execute his will properly. *Zei gezunt!*[22]"

The sons were overjoyed and agreed that the rabbi was indeed wise, and generous as well. So they divided the eighteen chickens. The eldest got half, or nine chickens. The middle got a third, which is six. And the youngest got a ninth, which is two. But nine plus six plus two is seventeen, so they had a chicken left over.

So they gave it back to the rabbi.

[21] *I.e.* the local synagogue.
[22] A Yiddish benediction meaning "be healthy".

Chapter 4

Continuous Translations and Rotations

4.1 Translations and their Representations

4.1.1 Discrete translations and their continuum limit

Consider an infinite one-dimensional lattice of points $x_n = na$, where $n \in \mathbb{Z}$ and a is the lattice spacing. If all sites are equivalent, the relevant symmetry group is $\mathbb{Z}$, *i.e.* the group of the integers under addition. The unitary representations are labeled by a *wavevector* k, with dimensions of inverse length, such that $D^k(n) = \exp(-ikna)$. Then $D^k(n)\, D^k(n') = D^k(n+n')$ yadda yadda yadda. Clearly the representation matrices are periodic under $k \to k + \frac{2\pi}{a}$, hence k may be restricted to the interval $k \in \left[-\frac{\pi}{a}\,,\,+\frac{\pi}{a}\right]$, with the endpoints identified. Alternatively, we could define $z \equiv \exp(-ika)$ and say that the unitary representations are labeled by a unimodular complex number $z \in S^1$. This interval over which k may be restricted (without loss of generality) is called the *first Brillouin zone* in condensed matter physics.

In d space dimensions, the unitary IRREPs of the group $\mathbb{Z}^d$ are labeled by a d-component wavevector[1] $\boldsymbol{k} = \{k_1, \ldots, k_d\}$, with $D^{\boldsymbol{k}}(\boldsymbol{n}) = \exp(-i\boldsymbol{k}\cdot\boldsymbol{n}a)$, where $\boldsymbol{n} = \{n_1, \ldots, n_d\} \in \mathbb{Z}^d$. The Brillouin zone becomes a d-dimensional product of intervals of the $d = 1$ type, or, equivalently, a d-dimensional torus T^d, with $\boldsymbol{z} = \{z_1, \ldots, z_d\} \in T^d$. The set of points $\boldsymbol{R} = a\sum_{j=1}^d n_j\, \hat{\boldsymbol{e}}_j$ in d-dimensional space describes a d-dimensional cubic lattice.

In general, we can choose a set of linearly independent vectors $\{\boldsymbol{a}_j\}$ with $j \in \{1, \ldots, d\}$ and define the lattice position $\boldsymbol{R} = \sum_j n_j \boldsymbol{a}_j$. This is the construction for a d-dimensional *Bravais lattice*. The representations are given by $D^{\boldsymbol{k}}(\boldsymbol{R}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$. The unit cell volume is given by

$$\Omega = \epsilon_{\mu_1\cdots\mu_d}\, a_1^{\mu_1}\cdots a_d^{\mu_d} \quad , \tag{4.1}$$

and is by definition positive[2]. The $\{\boldsymbol{a}_j\}$ are called the *elementary direct lattice vectors* and by convention one chooses them to have the shortest possible lengths. One can then define the *elementary reciprocal*

[1] For $d = 1$, the wave*vector* is in fact a scalar. Ain't that a kick in the head?

[2] If the expression in Eqn. 4.1 is negative, swap the labels of two of the elementary direct lattice vectors $\boldsymbol{a}_j$.

lattice vectors,

$$b_k^\nu \equiv \frac{2\pi}{\Omega}\,\epsilon_{\mu_1\cdots\mu_{k-1}\,\nu\,\mu_{k+1}\cdots\mu_d} a_1^{\mu_1}\cdots a_{k-1}^{\mu_{k-1}}\,a_{k+1}^{\mu_{k+1}}\cdots a_d^{\mu_d} \quad , \tag{4.2}$$

which satisfy

$$\boldsymbol{a}_i\cdot\boldsymbol{b}_j = 2\pi\delta_{ij} \quad . \tag{4.3}$$

For example, with $d=3$ we have $\Omega = \boldsymbol{a}_1\cdot\boldsymbol{a}_2\times\boldsymbol{a}_3$ and

$$\boldsymbol{b}_1 = \frac{2\pi}{\Omega}\,\boldsymbol{a}_2\times\boldsymbol{a}_3 \quad , \quad \boldsymbol{b}_2 = \frac{2\pi}{\Omega}\,\boldsymbol{a}_3\times\boldsymbol{a}_1 \quad , \quad \boldsymbol{b}_3 = \frac{2\pi}{\Omega}\,\boldsymbol{a}_1\times\boldsymbol{a}_2 \quad . \tag{4.4}$$

The Brillouin zone volume is $\hat\Omega = (2\pi)^d/\Omega$. The first Brillouin zone is the set of wavevectors $\boldsymbol{k}$ such that

$$\boldsymbol{k} = \sum_{j=1}^d \frac{\theta_j}{2\pi}\,\boldsymbol{b}_j \quad , \tag{4.5}$$

with $\theta_j\in[-\pi,\pi]$ for all $j\in\{1,\ldots,d\}$.

For example, the triangular lattice is described by

$$\boldsymbol{a}_1 = a\Big(\tfrac{1}{2}\hat{\boldsymbol{x}} - \tfrac{\sqrt{3}}{2}\,\hat{\boldsymbol{y}}\Big) \quad , \quad \boldsymbol{a}_2 = a\Big(\tfrac{1}{2}\hat{\boldsymbol{x}} + \tfrac{\sqrt{3}}{2}\,\hat{\boldsymbol{y}}\Big) \tag{4.6}$$

with $\Omega = \frac{\sqrt{3}}{2}\,a^2$. The elementary reciprocal lattice vectors are then

$$\boldsymbol{b}_1 = \frac{4\pi}{a\sqrt{3}}\Big(\tfrac{\sqrt{3}}{2}\,\hat{\boldsymbol{x}} - \tfrac{1}{2}\,\hat{\boldsymbol{y}}\Big) \quad , \quad \boldsymbol{b}_2 = \frac{4\pi}{a\sqrt{3}}\Big(\tfrac{\sqrt{3}}{2}\,\hat{\boldsymbol{x}} + \tfrac{1}{2}\,\hat{\boldsymbol{y}}\Big) \quad . \tag{4.7}$$

In the continuum limit, $\boldsymbol{R}\to\boldsymbol{r}$ becomes continuous and $D^{\boldsymbol{k}}(\boldsymbol{r}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$.

4.1.2 The cyclic group and its continuum limit

Recall how the cyclic group C_N, describing a single n-fold axis, is isomorphic to $\mathbb{Z}_N$, the group of integer clock arithmetic modulo N. The group elements are $\{1,\omega,\ldots,\omega^{N-1}\}$, with $\omega\equiv\exp(-2\pi i/N)$, and the representations Γ_j are labeled by integers $j\in\{0,\ldots,N-1\}$, with the 1×1 representation matrices $D^j(\omega^l)=\omega^{jl}$. In the continuum limit $N\to\infty$, we define $\theta\equiv 2\pi l/N$, and $D^j(\theta)=e^{-ij\theta}$ with $j\in\mathbb{Z}$. Note the periodicity under $\theta\to\theta+2\pi$. These are the IRREPs of the group $C_\infty\cong\mathsf{SO}(2)$. Note that there are an infinite number of IRREPs, as there must be upon consideration of the $N\to\infty$ limit of the formula $N_G=\sum_\Gamma d_\Gamma^2$.

Note that $\mathsf{SO}(2)$ is also the group of continuous *translations* in one dimension when *periodic boundary conditions* (PBCs) are imposed. PBCs mean that x is equivalent to $x+L$, where L is the length of the system. This is equivalent to placing our one-dimensional system on a circle. One must then have $D^k(x)=e^{-ikx}=e^{-ik(x+L)}$, *i.e.* $e^{-ikL}=1$ for all k, which requires $k=2\pi j/L$ with $j\in\mathbb{Z}$. Equivalently, define $\theta\equiv 2\pi x/L$, and label the IRREPs by j, in which case we recover $D^j(\theta)=e^{-ij\theta}$.

For discrete translations, we may still implement PBCs, equivalencing sites n and $n+N$, where $L = Na$ is the size of the system. We then have $\exp(ikNa) = 1$, in which case k is among a discrete set,

$$k \in \frac{2\pi}{Na}\left\{-\tfrac{1}{2}N\,,\,\ldots\,,\,\tfrac{1}{2}N\right\} \tag{4.8}$$

where we have assumed N even for simplicity. In the $N \to \infty$ limit, with a remaining finite, this discrete set becomes the interval $ka \in [-\pi, \pi]$.

4.1.3 Consequences of parity symmetry on the eigenspectrum

One might ask, as I did during a moment of intellectual weakness at 2 am, how it is then that the dispersion relation $\varepsilon(k)$ for a free particle in one dimension satisfies $\varepsilon(k) = \varepsilon(-k) = \hbar^2k^2/2m$, *i.e.* the states other than $k = 0$ are all doubly degenerate. Where are the two-dimensional IRREPs? Now if you are going to ask this question, you should make sure that you ask a very smart person, like my colleague John McGreevy, who will tell you that the symmetries of the free particle are not just continuous translations along the real line, *i.e.* the group $\mathbb{R}$ under addition (or $\mathbb{Z}$ for a discrete infinite chain), but rather $\mathbb{R} \rtimes \mathbb{Z}_2$, where $\mathbb{Z}_2$ is due to parity, and where, as we discussed in chapter 1, the symbol $\rtimes$ denotes the *semidirect product*. If we denote the parity operation σ and translation through u by $t(u)$ (rather than u itself, which is slightly awkward notation in this context), then the elements of $\mathbb{R} \times \mathbb{Z}_2$ are $t(u)$ and $s(u)$, where $s(u) \equiv \sigma\, t(u) = t(-u)\, \sigma$. The multiplication table for $\mathbb{R} \rtimes \mathbb{Z}_2$ is as follows:

$$\begin{aligned} t(u_1)\, t(u_2) &= t(u_1 + u_2) \\ t(u_1)\, s(u_2) &= s(u_2 - u_1) \\ s(u_1)\, t(u_2) &= s(u_1 + u_2) \\ s(u_1)\, s(u_2) &= t(u_2 - u_1) \quad . \end{aligned} \tag{4.9}$$

Now for the IRREPs, which are still labeled by a real scalar k. The one-dimensional IRREPs are given by

$$D^{(k)}\big(t(u)\big) = e^{-iku} \qquad , \qquad D^{(k)}\big(s(u)\big) = 1 \quad . \tag{4.10}$$

However, now there are also two-dimensional IRREPs, given by

$$D^{(k)}\big(t(u)\big) = \begin{pmatrix} e^{-iku} & 0 \\ 0 & e^{iku} \end{pmatrix} \qquad , \qquad D^{(k)}\big(s(u)\big) = \begin{pmatrix} 0 & e^{iku} \\ e^{-iku} & 0 \end{pmatrix} \quad . \tag{4.11}$$

The student should verify that the group multiplication law is satisfied by each of these IRREPs. The above results directly generalize to the case where $\mathbb{R}$ is replaced in d dimensions by $\mathbb{R}^d$ (continuous and infinite), $\mathbb{T}^d$ (continuous and periodic) or $\mathbb{Z}^d$ (discrete and infinite) or $\mathbb{Z}_n^d$ (discrete and periodic). Note that in §1.5.3 we discussed how $D_n = \mathbb{Z}_n \rtimes \mathbb{Z}_2$. For all $n \geq 2$, the dihedral groups D_n have two-dimensional IRREPs. And as John notes, $\mathbb{R}$ is essentially indistinguishable from a very large circle $\mathbb{S}^1$, which is the continuum limit of a periodic chain.

4.1.4 Invariant measure for SO(2)

Recall the orthogonality and completeness theorems for finite groups:

$$\begin{aligned}\frac{1}{N_G}\sum_{g\in G} D^{\Gamma}_{ik}(g)^*\, D^{\Gamma'}_{i'k'}(g) &= \frac{1}{d_\Gamma}\,\delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'} \\ \sum_{\Gamma,i,k} d_\Gamma\, D^{\Gamma}_{ik}(g)^*\, D^{\Gamma}_{ik}(g') &= N_G\,\delta_{gg'} \quad .\end{aligned} \tag{4.12}$$

How do these generalize for continuous (Lie) groups? A natural guess might be

$$\begin{aligned}\int_G d\mu(g)\; D^{\Gamma}_{ik}(g)^*\, D^{\Gamma'}_{i'k'}(g) &\sim \frac{1}{d_\Gamma}\,\delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'} \\ \sum_{\Gamma,i,k} d_\Gamma\, D^{\Gamma}_{ik}(g)^*\, D^{\Gamma}_{ik}(g') &\sim \delta(g-g') \quad .\end{aligned} \tag{4.13}$$

Here we assume that while the number of IRREPs is infinite, the dimension d_Γ of each IRREPs is finite. The expression $d\mu(g)$ is an integration measure on the group manifold G, and $\delta(g-g')$ is a generalization of the Dirac delta function[3]. An important feature of the measure is that it should be invariant under replacement of g by gh, where h is any element in G. *I.e.* $d\mu(g) = d\mu(gh)$ for all $g, h \in G$. This is because the group integration is the continuum limit of a sum over all the elements of a finite group, and by rearrangement we know that $\sum_{g\in G} F(g)$ is the same as $\sum_{g\in G} F(gh^{-1})$ for all h. For $G = \mathsf{SO}(2)$, the group elements $g = g(\phi)$ are parameterized by the angle variable $\phi \in [0, 2\pi]$. We then have

$$d\mu(g) = \rho(\phi)\, d\phi \quad , \tag{4.14}$$

where $\rho(\phi)$ is a weighting function. The condition that $d\mu(g)$ be an invariant measure means that it is unchanged under group multiplication $g \to gh$ for all fixed h. This means $\rho(\phi) = \rho(\phi+\alpha)$ for all $\alpha \in [0, 2\pi)$, hence $\rho(\phi) = C$, a constant. Normalizing $\int_G d\mu(g) \equiv 1$, we have $\rho(\phi) = \frac{1}{2\pi}$. The completeness and orthonormality relations then become

$$\begin{aligned}\int_0^{2\pi} \frac{d\phi}{2\pi}\,\big[D^j(\phi)\big]^* D^{j'}(\phi) &= \delta_{jj'} \\ \sum_{j=-\infty}^{\infty} \big[D^j(\phi)\big]^* D^j(\phi') &= 2\pi\,\delta(\phi-\phi') \quad .\end{aligned} \tag{4.15}$$

with $D^j(\phi) = e^{-ij\phi}$.

[3]The formal statement of completeness is known as the *Peter-Weyl theorem*, which we shall discuss in §4.3.5. Since we do not add elements of the group itself, the notation $\delta(g-g')$ is problematic, and we shall see further below how to make proper sense of all this.

4.2 Remarks about SO(N) and SU(N)

4.2.1 How SO(N) acts on vectors, matrices, and tensors

SO(2) is abelian and while important in physics, it is rather trivial from the point of view of group theory. We've just classified all its unitary representations. On to SO(N), which is nonabelian for $N > 2$.

SO(N) $\subset$ GL($N, \mathbb{R}$) is the group of proper rotations in N Euclidean dimensions, *i.e.* the group of $N \times N$ real matrices R satisfying $RR^{\mathsf{T}} = R^{\mathsf{T}}R = \mathbb{1}$. Acting on the vector space $\mathbb{R}^N$, rotation matrices act on basis vectors in the following manner:

$$\hat{\boldsymbol{e}}^a \to \hat{\boldsymbol{e}}'^a = \hat{\boldsymbol{e}}^b \, R_{ba} \quad . \tag{4.16}$$

Thus with $\boldsymbol{x} = x_a \, \hat{\boldsymbol{e}}^a$, we have

$$\boldsymbol{x}' = x_a \, \hat{\boldsymbol{e}}^b \, R_{ba} \quad \Rightarrow \quad x'_a = R_{ab} \, x_b \quad . \tag{4.17}$$

The group also acts on $N \times N$ matrices, with $M' = RMR^{\mathsf{T}}$, *i.e.*

$$M'_{ij} = R_{ia} \, R_{jb} \, M_{ab} = (RMR^{\mathsf{T}})_{ij} \quad . \tag{4.18}$$

A matrix M_{ij} may be generalized to an object with more indices, called a *tensor*. A p-tensor carries p indices $\{i_1, \ldots, i_p\}$, with each $i_p \in \{1, \ldots, N\}$,, and is denoted $M_{i_1 i_2 \cdots i_p}$. Under elements of SO(N), an n-tensor transforms thusly:

$$M'_{i_1 \cdots i_p} = R_{i_1 a_1} \cdots R_{i_p a_p} \, M_{a_1 \cdots a_p} \quad . \tag{4.19}$$

The transformation coefficients $C^{i_1 \cdots i_p}_{a_1 \cdots a_p}(R) \equiv R_{i_1 a_1} \cdots R_{i_p a_p}$ form a representation of SO(N) because

$$C^{i_1 \cdots i_p}_{a_1 \cdots a_p}(S) \, C^{a_1 \cdots a_p}_{j_1 \cdots j_p}(R) = C^{i_1 \cdots i_p}_{j_1 \cdots j_p}(SR) \quad . \tag{4.20}$$

What is the dimension of this representation? It is given by the dimension of the space on which the transformation coefficients act, *i.e.* the space of p-tensors M, where each index runs over N possible values. Thus, we have obtained a representation of dimension N^p.

But is this representation reducible? To address this question, let's first think about the case $n = 2$, *i.e.* good old matrices. Our representation is then of dimension N^2. But any matrix M^{ik} can be written as

$$M^{ik} = \overbrace{\frac{1}{N} \, \mathsf{Tr}\, M \, \delta^{ik}}^{c \, \delta^{ik}} + \overbrace{\frac{1}{2}\Big(M^{ik} - M^{ki}\Big)}^{A^{ik}} + \overbrace{\frac{1}{2}\Big(M^{ik} + M^{ki}\Big) - \frac{1}{N} \, \mathsf{Tr}\, M \, \delta^{ik}}^{S^{ik}} \tag{4.21}$$

where $c = \frac{1}{N} \mathsf{Tr}\, M$, $A = -A^{\mathsf{T}}$ is an antisymmetric matrix, and $S = S^{\mathsf{T}}$ is a traceless symmetric matrix. Orthogonal transformations preserve all these forms: RR^{T} is the identity, RAR^{T} is itself antisymmetric, and RSR^{T} is itself traceless and symmetric. Note that A has $\frac{1}{2}N(N-1)$ independent components, and S has $\frac{1}{2}N(N+1) - 1$ independent components. Thus, our representation, which is N^2-dimensional, reduces as

$$N^2 = 1 \oplus \tfrac{1}{2}N(N-1) \oplus \big[\tfrac{1}{2}N(N+1) - 1\big] \quad . \tag{4.22}$$

For $N = 3$, this says $9 = 1 \oplus 3 \oplus 5$. Note that the dimension of the antisymmetric tensor representation is the same as that of the vector representation. This is because an three component vector is *dual* to a 3×3 antisymmetric 2-tensor (*i.e.* matrix).

4.2.2 Invariant symbols, dual tensors, and up/down index notation

Any matrix $R \in \mathsf{SO}(3)$ preserves the Kronecker delta symbol δ^{ab} as well as the totally antisymmetric symbol ϵ^{abc}. Recall that

$$\epsilon_{i_1 \cdots i_N} = \mathsf{sgn} \begin{pmatrix} 1 & 2 & \cdots & N \\ i_1 & i_2 & \cdots & i_N \end{pmatrix} \quad . \tag{4.23}$$

and that $\epsilon_{i_1 \cdots i_N} = 0$ if any of the indices i_p are repeated. Note that for any matrix R, one has

$$\begin{aligned} R^i{}_a \, R^j{}_b \, \delta^{ab} &= (R R^{\mathsf{T}})_{ij} \\ R^{i_1}{}_{a_1} \cdots R^{i_N}{}_{a_N} \, \epsilon^{a_1 \cdots a_N} &= \mathsf{det}(R) \, \epsilon^{i_1 \cdots i_N} \quad . \end{aligned} \tag{4.24}$$

Hence if $R \in \mathsf{SO}(N)$, the Kronecker and epsilon symbols remain invariant under an orthogonal transformation. The raised and lowered indices don't do anything but aid us in identifying which pairs are to be contracted, *i.e.* $R^i{}_j = R_i{}^j = R_{ij}$. We always contract an upper index with a lower index[4].

True facts about the epsilon symbol:

$$\begin{aligned} \epsilon^{i_1 \cdots i_N} \, \epsilon_{i_1 \cdots i_N} &= N! \\ \epsilon^{i_1 \cdots i_N} \, \epsilon_{j_1 i_2 \cdots i_N} &= (N-1)! \, \delta^{i_1}_{j_1} \\ \epsilon^{i_1 \cdots i_N} \, \epsilon_{j_1 j_2 i_3 \cdots i_N} &= (N-2)! \left(\delta^{i_1}_{j_1} \, \delta^{i_2}_{j_2} - \delta^{i_1}_{j_2} \, \delta^{i_2}_{j_1} \right) \quad . \end{aligned} \tag{4.25}$$

The general case:

$$\epsilon^{i_1 \cdots i_N} \, \epsilon_{j_1 \cdots j_K i_{K+1} \cdots i_N} = (N-K)! \sum_{\sigma \in S_K} \mathsf{sgn}(\sigma) \, \delta^{i_1}_{j_{\sigma(1)}} \cdots \delta^{i_K}_{j_{\sigma(K)}} \quad . \tag{4.26}$$

Given a totally antisymmetric K-tensor $A^{a_1 \cdots a_K}$, we may use the ϵ-symbol to construct its *dual*, which is a totally antisymmetric $(N-K)$-tensor $\widetilde{A}^{i_1 \cdots i_{N-K}}$, *viz.*

$$\widetilde{A}_{i_1 \cdots i_{N-K}} \equiv \frac{1}{K!} \, \epsilon_{i_1 \cdots i_{N-K} a_1 \cdots a_K} \, A^{a_1 \cdots a_K} \quad . \tag{4.27}$$

What is the dual of the dual? We have

$$\begin{aligned} \widetilde{\widetilde{A}}^{b_1 \cdots b_K} &= \frac{1}{(N-K)!} \, \epsilon^{b_1 \cdots b_K i_1 \cdots i_{N-K}} \widetilde{A}_{i_1 \cdots i_{N-K}} \\ &= \frac{1}{K! \, (N-K)!} \, \epsilon^{b_1 \cdots b_K i_1 \cdots i_{N-K}} \, \epsilon_{i_1 \cdots i_{N-K} a_1 \cdots a_K} \, A^{a_1 \cdots a_K} \\ &= \frac{(-1)^{K(N-K)}}{K!} \sum_{\sigma \in S_K} \mathsf{sgn}(\sigma) \, \delta^{b_1}_{a_1} \cdots \delta^{b_K}_{a_K} \, A^{a_1 \cdots a_K} = (-1)^{K(N-K)} \, A^{b_1 \cdots b_K} \quad . \end{aligned} \tag{4.28}$$

[4]Since R is not necessarily a symmetric matrix, we offset the upper and lower indices to indicate which is the row and which is the column index, *i.e.* $R^i{}_j = R_{ij}$ but $R_j{}^i = R_{ji}$. For diagonal matrices like the δ-symbol, we don't need to do this, and we write $\delta^a_b = \delta_{ab} = \delta_{ba}$. We can use the δ-symbol to raise and lower indices, *viz.* $\delta^{ij} M_{jk} = M^i{}_k$. In relativistic theories, the metric tensor $g_{\mu\nu} = \mathsf{diag}(+,-,-,-)$ is used to raise and lower indices, which introduces sign changes.

Thus, up to a sign, the dual of the dual tensor is the original tensor. We see that for $N = 3$, the dual of a vector V^a is the antisymmetric tensor

$$\widetilde{V}_{ab} = \epsilon_{abc}\, V^c = \begin{pmatrix} 0 & +V^3 & -V^2 \\ -V^3 & 0 & +V^1 \\ +V^2 & -V^1 & 0 \end{pmatrix} \quad . \tag{4.29}$$

This establishes the equivalence between vector and antisymmetric matrix representations of $\mathsf{SO}(3)$. For $N = 4$, we have

$$F^{\mu\nu} = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix} \quad \Rightarrow \quad \widetilde{F}_{\mu\nu} = \tfrac{1}{2}\,\epsilon_{\mu\nu\rho\sigma}\,F^{\rho\sigma} = \begin{pmatrix} 0 & -B_x & -B_y & -B_z \\ B_x & 0 & -E_z & E_y \\ B_y & E_z & 0 & -E_x \\ B_z & -E_y & E_x & 0 \end{pmatrix} \quad . \tag{4.30}$$

One can also readily establish that if

$$B^{b_1 \cdots b_K} = R^{\,b_1}_{\;a_1} \cdots R^{\,b_K}_{\;a_K}\, A^{a_1 \cdots a_K} \quad , \tag{4.31}$$

then

$$\widetilde{B}_{j_1 \cdots j_{N-K}} = R_{j_1}^{\;\;i_1} \cdots R_{j_{N-K}}^{\;\;i_{N-K}}\, \widetilde{A}_{i_1 \cdots i_{N-K}} \quad , \tag{4.32}$$

i.e. the dual of the orthogonal transform is the orthogonal transform of the dual.

4.2.3 Tensor representations of SU(N)

Let $U \in \mathsf{SU}(N)$. Thus, $U_{ia}\,U^\dagger_{aj} = U_{ia}U^*_{ja} = \delta_{ij}$. Let Q be a rank $(p+q)$ tensor, with components $Q_{a_1 \cdots a_p\,,\,b_1 \cdots b_q}$. We define

$$Q'_{a_1 \cdots a_p\,,\,b_1 \cdots b_q} = C^{a_1 \cdots a_p\,,\,b_1 \cdots b_q}_{a'_1 \cdots a'_p\,,\,b'_1 \cdots b'_q}\,(U)\; Q_{a'_1 \cdots a'_p\,,\,b'_1 \cdots b'_q} \tag{4.33}$$

where

$$C^{a_1 \cdots a_p\,,\,b_1 \cdots b_q}_{a'_1 \cdots a'_p\,,\,b'_1 \cdots b'_q}(U) = U_{a_1 a'_1} \cdots U_{a_p a'_p} U^*_{b_1 b'_1} \cdots U^*_{b_q b'_q} \quad . \tag{4.34}$$

This forms a representation of $\mathsf{SU}(N)$ because

$$C^{a_1 \cdots a_p\,,\,b_1 \cdots b_q}_{a'_1 \cdots a'_p\,,\,b'_1 \cdots b'_q}\,(U)\; C^{a'_1 \cdots a'_p\,,\,b'_1 \cdots b'_q}_{a''_1 \cdots a''_p\,,\,b''_1 \cdots b''_q}\,(V) = C^{a_1 \cdots a_p\,,\,b_1 \cdots b_q}_{a''_1 \cdots a''_p\,,\,b''_1 \cdots b''_q}\,(UV) \quad . \tag{4.35}$$

As with the special orthogonal group, the Levi-Civita ϵ symbol is an invariant tensor:

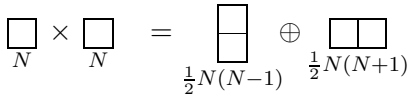
$$U_{a_1 b_1} U_{a_2 b_2} \cdots U_{a_N b_N}\, \epsilon^{b_1 \cdots b_N} = \overbrace{\det(U)}^{=\,1}\, \epsilon^{a_1 \cdots a_N} \quad . \tag{4.36}$$

Consider the tensor representation of $\mathsf{SU}(N)$ with $C^{a_1 a_2}_{a'_1 a'_2}\,(U) = U_{a_1 a'_1} U_{a_2 a'_2}$. For $\mathsf{SO}(N)$, there is always a one-dimensional IRREP where the tensor $M_{a_1 a_2} = A\,\delta_{a_1 a_2}$, because $R_{a_1 a'_1} R_{a_2 a'_2}\,\delta_{a'_1 a'_2} = (RR^{\mathsf{T}})_{a_1 a_2} = \delta_{a_1 a_2}$.

Not so for SU(N), because $UU^{\intercal} \neq 1$ in general. Still, symmetric and antisymmetric tensors transform among their respective kinds, hence rather than eqn. 4.22, we have

$$N^2 = \tfrac{1}{2}N(N-1) \oplus \tfrac{1}{2}N(N+1) \quad . \tag{4.37}$$

Thus, the trivial IRREP in SO(N) adjoins in SU(N) to the symmetric matrix IRREP to form a larger symmetric matrix IRREP of dimension $\frac{1}{2}N(N+1)$. The general classification scheme for IRREPs of SO(N) and SU(N) is facilitated by the use of Young tableaux similar to those encountered in our study of the symmetric group. The rules for counting IRREPs and their dimensions are different, however. In the language of Young diagrams,



. (4.38)

Next, consider the tensor representation of SU(N) with $C^{a_1 a_2}_{a_1' a_2'}(U) = U_{a_1 a_1'} U^*_{a_2 a_2'}$. Now we find that the Kronecker matrix $\delta_{a_1 a_2}$ does indeed remain invariant, hence there is a trivial one-dimensional representation in the decomposition of this representation. However, one can also see that symmetric and antisymmetric matrices will in general mix under this transformation, hence the symmetric and antisymmetric IRREPs of SO(N) adjoin in SU(N) to yield an IRREP of dimension $N^2 - 1$, which is the adjoint representation:

$$N \times \overline{N} = \mathsf{id} \oplus \mathsf{adj} \quad . \tag{4.39}$$

Here we denote by N the fundamental IRREP of SU(N), and by $\overline{N}$ the *antifundamental* (*i.e.* complex conjugate) IRREP.

4.3 SO(3) and SU(2)

Recall that SO(3) is the matrix Lie group of rotations in Euclidean 3-space. Its elements can be represented as $R(\xi, \hat{\boldsymbol{n}})$, meaning a (right-handed) rotation by ξ about $\hat{\boldsymbol{n}}$, with $\xi \in [0, \pi]$. As discussed in chapter 1, topologically this means that each element of SO(3) can be associated with a point $\xi\hat{\boldsymbol{n}}$ in a filled sphere of radius π. Since $R(\pi, \hat{\boldsymbol{n}}) = R(\pi, -\hat{\boldsymbol{n}})$, points on the surface of this sphere are identified with their antipodes, resulting in $\pi_1\big(\mathsf{SO}(3)\big) \cong \mathbb{Z}_2$.

The Lie algebra so(3) consists of real antisymmetric 3×3 matrices. We can define a basis for this algebra,

$$\Sigma^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & +1 & 0 \end{pmatrix} \quad , \quad \Sigma^y = \begin{pmatrix} 0 & 0 & +1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad , \quad \Sigma^z = \begin{pmatrix} 0 & -1 & 0 \\ +1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{4.40}$$

Note that $\Sigma^a_{ij} = -\epsilon_{aij}$, from which one easily establishes the commutation relations $\big[\Sigma^a, \Sigma^b\big] = \epsilon_{abc}\,\Sigma^c$. Then with $\boldsymbol{\xi} = \xi\hat{\boldsymbol{n}}$, we have $R(\xi, \hat{\boldsymbol{n}}) = \exp(\boldsymbol{\xi} \cdot \boldsymbol{\Sigma}) = \exp(\xi\, \hat{\boldsymbol{n}} \cdot \boldsymbol{\Sigma})$. Note that

$$\big(\hat{\boldsymbol{n}} \cdot \boldsymbol{\Sigma}\big)_{ab} = \begin{pmatrix} 0 & -n^z & +n^y \\ +n^z & 0 & -n^x \\ -n^y & +n^x & 0 \end{pmatrix}_{ab} = -\epsilon_{abc}\, n^c \quad . \tag{4.41}$$

Squaring this, we obtain

$$\big[(\hat{\boldsymbol{n}}\cdot\boldsymbol{\Sigma})^2\big]_{ac} = \epsilon_{abd}\,n^d\,\epsilon_{bce}\,n^e = n^a n^c - \delta^{ac} \equiv -Q^{ac}_{\hat{\boldsymbol{n}}} \quad , \tag{4.42}$$

where $Q^{ab}_{\hat{\boldsymbol{n}}} = \delta^{ab} - n^a n^c$ is the orthogonal projector with respect to $\hat{\boldsymbol{n}}$. The projector onto $\hat{\boldsymbol{n}}$ is of course $P^{ab}_{\hat{\boldsymbol{n}}} = n^a n^b$. Defining $\Sigma_{\hat{\boldsymbol{n}}} \equiv \hat{\boldsymbol{n}}\cdot\boldsymbol{\Sigma}$, it is now easy to show that

$$P_{\hat{\boldsymbol{n}}}Q_{\hat{\boldsymbol{n}}} = Q_{\hat{\boldsymbol{n}}}P_{\hat{\boldsymbol{n}}} = 0 \quad , \quad P_{\hat{\boldsymbol{n}}}\Sigma_{\hat{\boldsymbol{n}}} = \Sigma_{\hat{\boldsymbol{n}}}P_{\hat{\boldsymbol{n}}} = 0 \quad , \quad Q_{\hat{\boldsymbol{n}}}\Sigma_{\hat{\boldsymbol{n}}} = \Sigma_{\hat{\boldsymbol{n}}}Q_{\hat{\boldsymbol{n}}} = \Sigma_{\hat{\boldsymbol{n}}} \quad , \tag{4.43}$$

as well as the projector relations $P^2_{\hat{\boldsymbol{n}}} = P_{\hat{\boldsymbol{n}}}$ and $Q^2_{\hat{\boldsymbol{n}}} = Q_{\hat{\boldsymbol{n}}}$ and our previous result $\Sigma^2_{\hat{\boldsymbol{n}}} = -Q_{\hat{\boldsymbol{n}}}$.

From these relations, we may sum the exponential series for $R(\xi,\hat{\boldsymbol{n}})$ to obtain

$$R_{ab}(\xi,\hat{\boldsymbol{n}}) = \exp(\xi\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\Sigma}) = n^a n^b + \big(\delta^{ab} - n^a n^b\big)\cos\xi - \epsilon_{abc}\,n^c\sin\xi \quad . \tag{4.44}$$

It is also a simple matter to show that if $S\in\mathsf{SO}(3)$, then

$$S\,R(\xi,\hat{\boldsymbol{n}})\,S^{-1} = R(\xi,\hat{\boldsymbol{n}}') \tag{4.45}$$

where $\hat{\boldsymbol{n}}' = S\hat{\boldsymbol{n}}$. This means that rotations through a fixed angle ξ form an equivalence class. Recall from chapter 1 how $\mathsf{SO}(3)$ is topologically equivalent to a three-dimensional sphere of radius π, with radial coordinate ξ and angular coordinates given by the unit vector $\hat{\boldsymbol{n}}$. The condition $R(\pi,\hat{\boldsymbol{n}}) = R(\pi,-\hat{\boldsymbol{n}})$ means that $\mathsf{SO}(3)$ is multiply connected, with $\pi_1\big(\mathsf{SO}(3)\big)\simeq\mathbb{Z}_2$. Thus the equivalence classes of $\mathsf{SO}(3)$ correspond to concentric two-dimensional spheres, with antipodes identified on the surface $\xi=\pi$.

In the physics literature, the $\mathsf{so}(3)$ generators are Hermitian, and we write $J^a = i\Sigma^a = D(\hat{J}^a)$ is a 3×3 matrix representation of the *operator* $\hat{J}^a$, where the familiar commutation relations $\big[\hat{J}^a,\hat{J}^b\big] = i\epsilon_{abc}\hat{J}^c$ hold for both the angular momentum operator $\hat{J}^a$ as well as its representation matrices J^a. Thus,

$$R(\xi,\hat{\boldsymbol{n}}) = \exp\big(-i\xi\,\hat{\boldsymbol{n}}\cdot\boldsymbol{J}\big) = D\big[\exp(-i\xi\,\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{J}})\big] \quad , \tag{4.46}$$

is the matrix representation of the rotation operator $\hat{R}(\xi,\hat{\boldsymbol{n}}) = \exp(-i\xi\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{J}})$. Rather than the $(\xi,\hat{\boldsymbol{n}})$ parameterization, we could also choose to parameterize a general $R\in\mathsf{SO}(3)$ by the Euler angles (α,β,γ) familiar from the classical mechanics of rotating bodies[5], where $\alpha,\gamma\in[\,0,2\pi)$ and $\beta\in[\,0,\pi\,]$. The general rotation operation in terms of the Euler angles is depicted in Fig. 4.1 and is given by

$$R(\alpha,\beta,\gamma) = \exp(-i\gamma J^{z''})\,\exp(-i\beta J^{y'})\,\exp(-i\alpha J^z) \quad . \tag{4.47}$$

Here $\exp(-i\alpha J^z)$ rotates by α about the original $\hat{\boldsymbol{z}} = \hat{\boldsymbol{e}}^0_3$ axis, $\exp(-i\beta J^{y'})$ by β about the new $\hat{\boldsymbol{y}}' = \hat{\boldsymbol{e}}'_2$ axis, and $\exp(-i\gamma J^{z''})$ by γ about the new $\hat{\boldsymbol{z}}'' = \hat{\boldsymbol{e}}''_3$ axis. Then

$$\begin{aligned}\exp(-i\gamma J^{z''}) &= \exp(-i\beta J^{y'})\exp(-i\gamma J^z)\exp(i\beta J^{y'})\\ \exp(-i\beta J^{y'}) &= \exp(-i\alpha J^z)\exp(-i\beta J^y)\exp(i\alpha J^z)\end{aligned} \tag{4.48}$$

and so we find

$$R(\alpha,\beta,\gamma) = \exp(-i\alpha J^z)\,\exp(-i\beta J^y)\,\exp(-i\gamma J^z) \quad . \tag{4.49}$$

[5]Since we reflexively parameterize the unit vector $\hat{\boldsymbol{n}}$ in terms of its polar angle θ and azimuthal angle ψ, we'll call the Euler angles (α,β,γ) rather than the also common (ϕ,θ,ψ) to obviate any confusion.

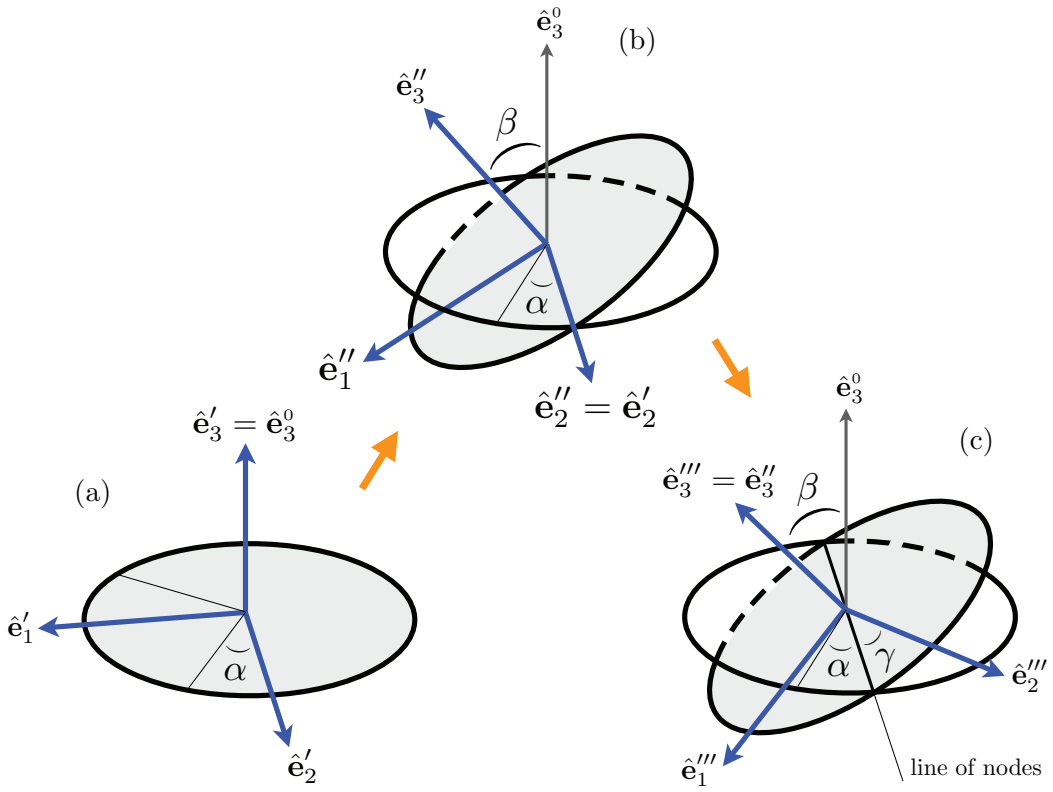


Figure 4.1: Definition of Euler angles and their order of operations in Eqn. 4.47.

Thus, we obtain an expression which looks very much like that in Eqn. 4.47, except (i) the rotations are now about lab-fixed axes and (ii) the order of operations is reversed. Identifying $R(\alpha,\beta,\gamma) \equiv R(\xi,\hat{\boldsymbol{n}})$, one obtains a relation[6]

$$\phi = \tfrac{1}{2}(\pi+\alpha-\gamma) \quad , \quad \tan\theta = \frac{\tan\left(\frac{1}{2}\beta\right)}{\sin\left(\frac{1}{2}\alpha+\frac{1}{2}\gamma\right)} \quad , \quad \cos^2\left(\tfrac{1}{2}\xi\right) = \cos^2\left(\tfrac{1}{2}\beta\right)\cos^2\left(\tfrac{1}{2}\alpha+\tfrac{1}{2}\gamma\right) \quad . \tag{4.50}$$

Note that

$$\big[R(\alpha,\beta,\gamma)\big]^{-1} = \exp(i\gamma J^z)\,\exp(i\beta J^y)\,\exp(i\alpha J^z) \quad . \tag{4.51}$$

Explicitly, we may write

$$\begin{aligned} R(\alpha,\beta,\gamma) &= \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix} \quad . \end{aligned} \tag{4.52}$$

For future reference, we note that

$$\mathrm{Tr}\, R(\alpha,\beta,\gamma) = \cos(\alpha+\gamma)\cos\beta + \cos(\alpha+\gamma) + \cos\beta \quad . \tag{4.53}$$

[6]See Wu-Ki Tung, *Group Theory in Physics*, p. 99.

4.3.1 Irreducible representations of SO(3)

We now promote the generators and group elements to operators acting on Hilbert space, writing $\hat{R}(\alpha,\beta,\gamma)$, $\hat{J}^a$, *etc.*, and we seek representations of SO(3) which can be used to classify the eigenstates of a rotationally invariant Hamiltonian, *i.e.* one for which $\big[\hat{H},\hat{R}(\xi,\hat{\boldsymbol{n}})\big]=0$ for all rotations $\hat{R}(\xi,\hat{\boldsymbol{n}})$. Clearly it is enough that $\big[\hat{H},J^a\big]=0$ for all the generators J^a, so we will seek a representation of the Lie algebra so(3). This will yield a representation of the group SO(3) itself, provided global conditions such as $\hat{R}(\pi,\hat{\boldsymbol{n}})=\hat{R}(\pi,-\hat{\boldsymbol{n}})$ are met. As we shall soon see, we will be led naturally to a set of projective representations, which you already know correspond to half-odd integer total angular momentum, as well as proper representations, corresponding to integer angular momentum.

We will seek finite-dimensional representations in which the generators $\hat{J}^a$ are all represented by Hermitian matrices. In general we can pull this off for compact Lie groups like SO(3). We'll follow a general point of attack outlined by Élie Cartan, whose work in the first half of the 20$^{\rm th}$ century laid the foundations for the theory of Lie groups. Cartan's approach was to start with a standard vector $|\,\psi_0\,\rangle\in\mathcal{H}$ and to generate the remaining vectors in an irreducible basis by iteratively applying various generators. One important entity which helps us label the IRREPs is the existence of a *Casimir operators*. A Casimir is an operator $\hat{C}$ which commutes with all elements of the group, and hence with all operators in the Lie algebra. For so(3), this is $\hat{C}=\hat{\boldsymbol{J}}^2$. By Schur's first lemma, this means $\hat{C}$ is a multiple of the identity, hence the individual IRREPs may be labeled by the eigenvalues $\{C_1,\ldots,C_K\}$ of all the Casimirs, where K is the total number of Casimirs[7].

For so(3), following Cartan's method, it is useful to define the ladder operators $\hat{J}^\pm=\hat{J}^x\pm i\hat{J}^y$. Then

$$\big[\hat{J}^z,\hat{J}^\pm\big]=\pm\hat{J}^\pm\qquad,\qquad\big[\hat{J}^+,\hat{J}^-\big]=2\hat{J}^z \tag{4.54}$$

as well as $\hat{\boldsymbol{J}}^2=(\hat{J}^z)^2+\hat{J}^z+\hat{J}^-\hat{J}^+$ and $(\hat{J}^\pm)^\dagger=\hat{J}^\mp$. In the vector space $\mathcal{V}$ of our representation, we label the basis vectors by the eigenvalues of the Hermitian operator $\hat{J}^z$ as write them as $|\,m\,\rangle$, with $\hat{J}^z|\,m\,\rangle=m\,|\,m\,\rangle$. We then apply $\hat{J}^+$, and from the commutation relations we have

$$\hat{J}^z\hat{J}^+\,\big|\,m\,\big\rangle=(m+1)\,\hat{J}^+\,\big|\,m\,\big\rangle\quad. \tag{4.55}$$

We can keep applying $\hat{J}^+$, but eventually, if the representation is finite, we must reach a state $|\,j\,\rangle$ for which $\hat{J}^z\,|\,j\,\rangle=j\,|\,j\,\rangle$ but $\hat{J}^+\,|\,j\,\rangle=0$. We then have $\hat{\boldsymbol{J}}^2|\,j\,\rangle=j(j+1)|\,j\,\rangle$. The eigenvalue of our Casimir is thus $j(j+1)$, and $|\,j\,\rangle$, our "standard vector", is called the *highest weight state*.

We now work downward from $|\,j\,\rangle$, successively applying $\hat{J}^-$. Note that for any normalized state $|\,m\,\rangle$ with $m\le j$,

$$\begin{aligned}\big\langle\,m\,\big|\,(\hat{J}^-)^\dagger\hat{J}^-\,\big|\,m\,\big\rangle&=\big\langle\,m\,\big|\,\hat{J}^+\hat{J}^-\,\big|\,m\,\big\rangle=\big\langle\,m\,\big|\,\big(\hat{\boldsymbol{J}}^2-(\hat{J}^z)^2+\hat{J}^z\big)\,\big|\,m\,\big\rangle\\&=j(j+1)-m(m-1)\quad.\end{aligned} \tag{4.56}$$

We also have $\hat{J}^z\hat{J}^-|\,j,m\,\rangle=(m-1)\hat{J}^-|\,j,m\,\rangle$, hence we may take

$$\hat{J}^-\big|\,m\,\big\rangle=\sqrt{j(j+1)-m(m-1)}\,\big|\,m-1\,\big\rangle\quad. \tag{4.57}$$

[7] A Lie group can have several Casimirs. For example, SU(3) has two and in general SU(N) has $N-1$ Casimirs.

If the representation is finite, eventually one must reach a state where $\hat{J}^-|\,m\,\rangle = 0$, which requires $m = -j$. As this state is achieved by an integer number of applications of the lowering operator $\hat{J}^-$, we must have $j - (-j) = 2j \in \mathbb{N}$, where $\mathbb{N}$ denotes the natural numbers $\{0, 1, 2, \ldots\}$. Thus, $j \in \frac{1}{2}\mathbb{N}$, which is to say j may be a positive integer or a half odd positive integer. We now include the label j on all states, in order to label the representation, and we have

$$\begin{aligned}
\hat{\boldsymbol{J}}^2 \,\big|\, j,m\,\big\rangle &= j(j+1)\,\big|\, j,m\,\big\rangle \\
\hat{J}^z \,\big|\, j,m\,\big\rangle &= m\,\big|\, j,m\,\big\rangle \\
\hat{J}^\pm \,\big|\, j,m\,\big\rangle &= \sqrt{j(j+1) - m(m\pm 1)}\,\big|\, j,m\pm 1\,\big\rangle \quad ,
\end{aligned} \tag{4.58}$$

where $m \in \{-j, \ldots, j\}$. When we refer to the matrix elements of $\hat{J}^a$, we will respectfully remove the hats from the operators, *i.e.* J^a is the matrix whose elements are $J^a_{mm'} = \langle\, j,m\,|\,\hat{J}^a\,|\,j,m'\,\rangle$.

4.3.2 Rotation matrices

Rotation matrices are the matrices corresponding to a particular group element, and are specific to each representation. By definition,

$$\hat{R}(\alpha,\beta,\gamma)\,|\,j,m'\,\rangle = |\,j,m\,\rangle\,D^{(j)}_{mm'}(\alpha,\beta,\gamma) \quad . \tag{4.59}$$

Since $\hat{R}(\alpha,\beta,\gamma) = \exp(-i\alpha\hat{J}^z)\exp(-i\beta\hat{J}^y)\exp(-i\gamma\hat{J}^z)$, we have

$$D^{(j)}_{mm'}(\alpha,\beta,\gamma) = e^{-i\alpha m}\,e^{-i\gamma m'}\,d^{(j)}_{mm'}(\beta) \quad , \tag{4.60}$$

with

$$d^{(j)}_{mm'}(\beta) = \big\langle\, j,m\,\big|\,\exp(-i\beta\hat{J}^y)\,\big|\,j,m'\,\big\rangle \quad . \tag{4.61}$$

As the matrices of $\hat{J}^\pm$ are real[8], iJ^y is real, and we conclude $d^{(j)}_{mm'}(\beta)$ is a real-valued matrix of rank $2j+1$. For all j we have $\big[d^{(j)}(\beta)\big]^{\mathsf{T}} = d^{(j)}(-\beta) = \big[d^{(j)}(\beta)\big]^{-1}$, as well as

$$d^{(j)}_{-m,-m'}(\beta) = (-1)^{2j-m-m'}d^{(j)}_{m,m'}(\beta) = (-1)^{m-m'}d^{(j)}_{m,m'}(\beta) \quad . \tag{4.62}$$

Note that we could have stuck with the $(\xi,\hat{\boldsymbol{n}})$ parameterization, and written

$$\hat{R}(\xi,\hat{\boldsymbol{n}})\,|\,j,m'\,\rangle = |\,j,m\,\rangle\,D^{(j)}_{mm'}(\xi,\hat{\boldsymbol{n}}) \quad , \tag{4.63}$$

but clearly the Euler angle parameterization is advantageous due to the particularly simple way in which the α and γ angles appear in the rotation matrices.

[8]This was actually a convention that we chose, by taking the prefactor on the RHS of the last of Eqn. 4.58 to be real, and is originally due to Condon and Shortley.

Characters

Recall that rotations through a fixed angle ξ form a class within $\mathsf{SO}(3)$. What is the character of this class? Since the axis doesn't matter, we choose $\hat{\boldsymbol{n}} = \hat{\boldsymbol{z}}$, in which case

$$\chi^{(j)}(\xi) = \mathsf{Tr}\exp(-i\xi J^z) = \sum_{m=-j}^{j} e^{-im\xi} = \frac{\sin\left[(j+\frac{1}{2})\xi\right]}{\sin(\frac{1}{2}\xi)} \quad . \tag{4.64}$$

Using the Euler angle parameterization,

$$\chi^{(j)}(\alpha,\beta,\gamma) = \sum_{m=-j}^{j} e^{-im(\alpha+\gamma)}\, d^{(j)}_{mm}(\beta) \quad . \tag{4.65}$$

Examples

The simplest example of course is $j = \frac{1}{2}$, where $\boldsymbol{J} = \frac{1}{2}\boldsymbol{\sigma}$ are the Pauli matrices. Then

$$d^{(1/2)}(\beta) = \exp(-i\beta\sigma^y/2) = \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix} \quad . \tag{4.66}$$

For $j = 1$, we need to exponentiate the 3×3 matrix $i\beta J^y$. Let's first find the normalized eigenvalues and eigenvectors of J^y:

$$\boldsymbol{\psi}^{+} = \frac{1}{2}\begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} \quad . \quad \boldsymbol{\psi}^{0} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad , \quad \boldsymbol{\psi}^{-} = \frac{1}{2}\begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix} \quad , \tag{4.67}$$

with corresponding eigenvalues $+1$, 0, and -1, respectively. From these we construct the projectors

$$P^{\pm}_{ij} = \psi^{\pm}_i\,\psi^{\pm *}_j = \frac{1}{4}\begin{pmatrix} 1 & \mp i\sqrt{2} & -1 \\ \pm i\sqrt{2} & 2 & \mp i\sqrt{2} \\ -1 & \pm i\sqrt{2} & 1 \end{pmatrix} \quad , \quad P^{0}_{ij} = \psi^{0}_i\,\psi^{0*}_j = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad . \tag{4.68}$$

The projectors are mutually orthogonal and complete: $P^a P^b = \delta^{ab} P^a$ (no sum) and $\sum_a P^a = \mathbb{1}$. We can decompose J^y into its projectors, writing $J^y = P^+ - P^-$, in which case

$$\begin{aligned} \exp(-i\beta J^y) &= \mathbb{1} - i\beta\,(P^+ - P^-) - \tfrac{1}{2}\beta^2\,(P^+ - P^-)^2 + \ldots \\ &= P^0 + \cos\beta\,(P^+ + P^-) - i\sin\beta\,(P^+ - P^-) \quad . \end{aligned} \tag{4.69}$$

since $(P^+ - P^-)^{2n} = P^+ + P^-$ and $(P^+ - P^-)^{2n+1} = P^+ - P^-$, allowing us to sum the Taylor series. Thus, we have

$$d^{(1)}(\beta) = \exp(-i\beta J^y) = \frac{1}{2}\begin{pmatrix} 1+\cos\beta & -\sqrt{2}\,\sin\beta & 1-\cos\beta \\ \sqrt{2}\,\sin\beta & 2\,\cos\beta & -\sqrt{2}\,\sin\beta \\ 1-\cos\beta & \sqrt{2}\,\sin\beta & 1+\cos\beta \end{pmatrix} \quad . \tag{4.70}$$

For a general Hermitian matrix M, we can always decompose M into its orthogonal projectors, *viz.*

$$M = \sum_l \lambda_k \, P^{(k)} \quad , \tag{4.71}$$

where $P^{(k)}$ projects onto the $k^{\rm th}$ eigenspace and λ_k is the associated eigenvalue. We can always orthogonalize projectors associated with degenerate eigenspaces, and so

$$\exp(-i\theta M) = \sum_k \exp(-i\theta\lambda_k) \, P^{(k)} \quad , \tag{4.72}$$

where λ_k is the $k^{\rm th}$ eigenvalue of M. Therefore

$$d^{(j)}(2\pi) = \sum_{m=-j}^{j} e^{-2\pi i m} \, P^{(m)} = (-1)^{2j} \, \mathbb{1} \quad . \tag{4.73}$$

This immediately tells us that the IRREPs we have found with $j \in \mathbb{Z} + \frac{1}{2}$ are not proper IRREPs, but rather are *projective* IRREPs.

The general expression for the $d^{(j)}(\beta)$ matrices is

$$d^{(j)}_{mm'}(\beta) = \sum_{k=0}^{2j} (-1)^k \, \frac{\big[(j+m)!\,(j-m)!\,(j+m')!\,(j-m')!\big]^{1/2}}{k!\,(j+m-k)!\,(j-m'+k)!\,(k-m+m')!} \, \big[\cos(\tfrac{1}{2}\beta)\big]^{2j+m-m'-2k} \big[\sin(\tfrac{1}{2}\beta)\big]^{2k-m+m'} \quad , \tag{4.74}$$

where it is to be understood that values of k which make the arguments of any of the factorials negative are excluded from the sum.

Parameterizations of SU(2)

$\mathsf{SU}(2) \in \mathsf{GL}(2,\mathbb{C})$ is the group of unitary 2×2 complex matrices with determinant 1. We have met up with $\mathsf{SU}(2)$ along the way several times already. Let's recall some of its parameterizations. Any matrix $U \in \mathsf{SU}(2)$ may be written as

$$U(w,x) = \begin{pmatrix} w & x \\ -x^* & w^* \end{pmatrix} \tag{4.75}$$

where $w, x \in \mathbb{C}$ and $\det U = |w|^2 + |x|^2 = 1$. Thus, $\mathsf{SU}(2) \cong S^3$, the three dimensional sphere. We may also write

$$U(\xi, \hat{\boldsymbol{n}}) = \exp\big(-\tfrac{i}{2}\,\xi\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}\big) = \cos\big(\tfrac{1}{2}\xi\big)\mathbb{1} - i\sin\big(\tfrac{1}{2}\xi\big)\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} \quad , \tag{4.76}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices and $\hat{\boldsymbol{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is a unit vector. The ranges of the parameters (ξ, θ, ϕ) are $\xi \in [0, 2\pi)$, $\theta \in [0, \pi]$, and $\phi \in [0, 2\pi)$. This parameterization carries the interpretation of a rotation by an angle ξ about the axis $\hat{\boldsymbol{n}}$. We've seen how $\mathsf{SU}(2)$ is a double cover of $\mathsf{SO}(3)$, for if $U = \exp\big(-\frac{i}{2}\,\xi\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}\big)$, then

$$R_{ab} = \tfrac{1}{2}\mathsf{Tr}\big(U\sigma^a\,U^\dagger\sigma^b\big) = n^a n^b + \big(\delta^{ab} - n^a n^b\big)\cos\xi - \epsilon_{abc}\,n^c\,\sin\xi \tag{4.77}$$

where $R \in \mathsf{SO}(3)$. Note that $R(2\pi - \xi, \hat{\boldsymbol{n}}) = R(\xi, -\hat{\boldsymbol{n}})$, so the coordinates (ξ, θ, ϕ) cover $\mathsf{SO}(3)$ twice, and for a unique expression of $\mathsf{SO}(3)$ matrices we restrict $\xi \in [0, \pi]$ and identify $R(\pi, \hat{\boldsymbol{n}}) \equiv R(\pi, -\hat{\boldsymbol{n}})$, as we have discussed before. Finally, we have the Euler angle parameterization,

$$U(\alpha, \beta, \gamma) = \exp\left(-\tfrac{i}{2}\,\alpha\,\sigma^z\right) \exp\left(-\tfrac{i}{2}\,\beta\,\sigma^y\right) \exp\left(-\tfrac{i}{2}\,\gamma\,\sigma^z\right) \tag{4.78}$$

where $\alpha \in [0, 2\pi)$, $\beta \in [0, \pi]$, and $\gamma \in [0, 4\pi)$.

4.3.3 Guide for the perplexed

The action of rotation operators on wavefunctions can be confusing when it comes to active *versus* passive rotations. To set the record straight, consider the action of a rotation operator $\hat{U}(R)$ where $R(\xi, \hat{\boldsymbol{n}}) \in \mathsf{SO}(3)$. When there is no *intrinsic* spin, we have

$$\hat{U}(R)\,\psi(\boldsymbol{r}) \equiv \big\langle\, \boldsymbol{r} \,\big|\, \hat{U}(R) \,\big|\, \psi \,\big\rangle = \big\langle\, \boldsymbol{r}R \,\big|\, \psi \,\big\rangle = \psi(\boldsymbol{r}R) = \psi(R^{\mathsf{T}}\boldsymbol{r}) \quad , \tag{4.79}$$

where $R \equiv D^{\mathsf{def}}(R)$ is the 3×3 matrix representation of the rotation R in the defining representation of $\mathsf{SO}(3)$[9]. Now suppose there is intrinsic spin j. We assume the structure of Hilbert space is such that spatial and spin degrees of freedom enter as a direct product, *i.e.* that the wavefunction can be written

$$\big|\, \Psi \,\big\rangle = \big|\, \psi_{m'} \,\big\rangle \otimes \big|\, m' \,\big\rangle \quad . \tag{4.80}$$

with an implied sum on m' from over the range $\{-j\,,\,\ldots\,,\,j\}$. We then have

$$\hat{U}(R) \,\big|\, \Psi \,\big\rangle = \Big[\hat{U}_{\rm rot}(R) \,\big|\, \psi_{m'} \,\big\rangle\Big] \otimes \big|\, m \,\big\rangle\, D^{(j)}_{mm'}(R) \tag{4.81}$$

so that

$$\begin{aligned} \big\langle\, \boldsymbol{r} \,\big|\, \hat{U}(R) \,\big|\, \Psi \,\big\rangle &= \big\langle\, \boldsymbol{r} \,\big|\, \hat{U}_{\rm rot}(R) \,\big|\, \psi_{m'} \,\big\rangle \,\big|\, m \,\big\rangle\, D^{(j)}_{mm'}(R) \\ &= \psi_{m'}(\boldsymbol{r}R) \,\big|\, m \,\big\rangle\, D^{(j)}_{mm'}(R) = \big[\hat{U}(R)\,\Psi(\boldsymbol{r})\big]_m \,\big|\, m \,\big\rangle \quad , \end{aligned} \tag{4.82}$$

where $\hat{U}_{\rm rot}(R) = \exp(-i\xi \boldsymbol{L}\cdot\hat{\boldsymbol{n}}/\hbar)$ is the spatial rotation part of $\hat{U}(R)$. We can also write this as

$$\hat{U}(R) \begin{pmatrix} \psi_{+j}(\boldsymbol{r}) \\ \vdots \\ \psi_{-j}(\boldsymbol{r}) \end{pmatrix} = D^{(j)}(R) \begin{pmatrix} \psi_{+j}(\boldsymbol{r}R) \\ \vdots \\ \psi_{-j}(\boldsymbol{r}R) \end{pmatrix} \quad . \tag{4.83}$$

Attend to the order of operations here or you may lead an unhappy life: $R = D^{\mathsf{def}}(R)$ multiplies the row vector $\boldsymbol{r}$ on the *right*, while $D^{(j)}(R)$ multiplies the column vector $\boldsymbol{\Psi}$ on the *left*.

[9] Recall that in the defining representation of any matrix Lie group $G \subset \mathsf{GL}(n, \mathbb{F})$, each element g is represented by itself.

4.3.4 Invariant measure for Lie groups

How does one sum over all the elements of a continuous group? Since the group space G is a manifold, we may integrate over G if we have an appropriate *measure* $d\mu(g)$. Integrating with respect to this measure should be the equivalent of summing over all elements of a discrete group. But then, by rearrangement, we must have

$$\int\limits_G d\mu(g)\,\phi(gh^{-1}) = \int\limits_G d\mu(g)\,\phi(g) \tag{4.84}$$

for any function $\phi(g)$ and any fixed $h \in G$. Thus, we require $d\mu(gh) = d\mu(g)$ in order that the integral remain invariant under rearrangement. A measure which satisfies this desideratum is called an *invariant* (or *Haar*) *measure*.

Let each group element $g \in G$ be parameterized by a set of coordinates $\boldsymbol{x} = \{x_1, \ldots, x_{\mathsf{dim}(G)}\}$. We define $\boldsymbol{x}_g$ to be the coordinates corresponding to the group element g. The coordinates $\boldsymbol{x}_{gh}$ for the product gh must depend on those of the components g and h, and accordingly we write

$$\boldsymbol{x}_{gh} = \boldsymbol{f}(\boldsymbol{x}_g\,,\,\boldsymbol{x}_h) \quad , \tag{4.85}$$

where $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{y})$ is the *group composition function*. Any group composition function must satisfy the following consistency relations:

$$\begin{aligned} \boldsymbol{f}\big(\boldsymbol{f}(\boldsymbol{x},\boldsymbol{y})\,,\boldsymbol{z}\big) &= \boldsymbol{f}\big(\boldsymbol{x}\,,\boldsymbol{f}(\boldsymbol{y},\boldsymbol{z})\big) \\ \boldsymbol{f}(\boldsymbol{x}_E,\boldsymbol{y}) &= \boldsymbol{f}(\boldsymbol{y},\boldsymbol{x}_E) = \boldsymbol{y} \\ \boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}^{-1}) &= \boldsymbol{f}(\boldsymbol{x}^{-1},\boldsymbol{x}) = \boldsymbol{x}_E \quad , \end{aligned} \tag{4.86}$$

where $\boldsymbol{x}_E$ are the coordinates of the identity E, *i.e.* $g(\boldsymbol{x}_E) = E$, and $\boldsymbol{x}^{-1}$ are the coordinates of the inverse of $g(\boldsymbol{x})$, *i.e.* $g(\boldsymbol{x}^{-1}) = \big[g(\boldsymbol{x})\big]^{-1}$. We can use the composition functions to construct an invariant measure, by writing

$$d\mu\big(g(\boldsymbol{x})\big) = \rho(\boldsymbol{x}) \prod_{j=1}^{\mathsf{dim}(G)} dx_j \tag{4.87}$$

with

$$\rho_0 = \rho(\boldsymbol{x}) \left| \det\left(\frac{\partial f_j(\boldsymbol{\epsilon},\boldsymbol{x})}{\partial \epsilon_k} \right)_{\boldsymbol{\epsilon}=\boldsymbol{\epsilon}_E} \right| \quad , \tag{4.88}$$

where $\rho_0 = \rho(\boldsymbol{x}_E)$. An equivalent and somewhat more convenient definition is the following. For any $g(\boldsymbol{x})$, express $g^{-1}\frac{\partial g}{\partial x_i}$ in terms of the Lie algebra generators T^a, *i.e.*

$$g^{-1}(\boldsymbol{x})\,\frac{\partial g(\boldsymbol{x})}{\partial x_i} = \sum_{a=1}^{\mathsf{dim}(G)} M_{ia}(\boldsymbol{x})\,T^a \quad , \tag{4.89}$$

where $\{T^a\}$ are the generators of the Lie algebra $\mathfrak{g}$. Then[10]

$$\rho(\boldsymbol{x}) = \rho_0\,\big|\det M(\boldsymbol{x})\big| \quad . \tag{4.90}$$

[10]Since we are taking the absolute value of the determinant, it doesn't matter whether we use the math or physics convention for the generators, since the difference is only a power of i, which is unimodular.

Note that

$$\big[h\,g(\boldsymbol{x})\big]^{-1}\,\frac{\partial\big[h\,g(\boldsymbol{x})\big]}{\partial x_i} = g^{-1}(\boldsymbol{x})\,h^{-1}\,h\,\frac{\partial g(\boldsymbol{x})}{\partial x_i} = M_{ia}(\boldsymbol{x})\,T^a \tag{4.91}$$

and therefore the measure is invariant under left multiplication of g. The student should check that it is also right-invariant. For *compact, semisimple* Lie groups, we will always be able to choose a normalization of the generators $\mathsf{Tr}\,(T^aT^b) = c\,\delta^{ab}$, in which case we may write

$$M_{ia}(\boldsymbol{x}) = c^{-1}\,\mathsf{Tr}\left(T^a\,g^{-1}(\boldsymbol{x})\,\frac{\partial g(\boldsymbol{x})}{\partial x_i}\right) \quad . \tag{4.92}$$

It is conventional to normalize the invariant measure according to

$$\int\limits_G d\mu(g) \equiv 1 \quad . \tag{4.93}$$

Let's implement these formulae for the cases of $\mathsf{SO}(2)$ and $\mathsf{SU}(2)$ (and $\mathsf{SO}(3)$). For $\mathsf{SO}(2)$,

$$U(\phi) = \begin{pmatrix}\cos\phi & -\sin\phi\\ \sin\phi & \cos\phi\end{pmatrix} \quad , \quad U^{-1}(\phi) = g(-\phi) \quad , \quad \frac{\partial U}{\partial\phi} = \begin{pmatrix}-\sin\phi & -\cos\phi\\ \cos\phi & -\sin\phi\end{pmatrix} \quad , \tag{4.94}$$

and thus

$$U^{-1}(\phi)\,\frac{\partial U}{\partial\phi} = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \quad . \tag{4.95}$$

The RHS is $-i\sigma^y$, and σ^y is the generator of $\mathsf{SO}(2)$ (physics convention). Thus, $\rho(\phi)$ is a constant, and normalizing over the group manifold, we have $\rho(\phi) = \frac{1}{2\pi}$.

The analysis for $\mathsf{SU}(2)$ is not quite so trivial, but still straightforward. Let's choose the parameterization $U(\xi,\hat{\boldsymbol{n}}) = \exp\big(-\frac{i}{2}\,\xi\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}\big)$. Then $U^{-1}(\xi,\hat{\boldsymbol{n}}) = U(\xi,\hat{\boldsymbol{n}})$ and

$$dU(\xi,\hat{\boldsymbol{n}}) = -\tfrac{1}{2}\sin\big(\tfrac{1}{2}\xi\big)\,d\xi - \tfrac{1}{2}\cos\big(\tfrac{1}{2}\xi\big)\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}\,d\xi - i\sin\big(\tfrac{1}{2}\xi\big)\,d\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} \tag{4.96}$$

and one readily obtains

$$U^{-1}(\xi,\hat{\boldsymbol{n}})\,dU(\xi,\hat{\boldsymbol{n}}) = -\tfrac{i}{2}\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}\,d\xi - \tfrac{i}{2}\sin\xi\,d\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} + \tfrac{i}{2}\,(1-\cos\xi)\,\hat{\boldsymbol{n}}\times d\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} \quad . \tag{4.97}$$

It is convenient to define vectors $\hat{\boldsymbol{e}}_{1,2}$ such that $\{\hat{\boldsymbol{e}}_1,\hat{\boldsymbol{e}}_2,\hat{\boldsymbol{n}}\}$ forms an orthonormal triad for all (θ,ϕ). Explicitly,

$$\begin{aligned}\hat{\boldsymbol{e}}_1 &= (\cos\theta\cos\phi\,,\,\cos\theta\sin\phi\,,\,-\sin\theta)\\ \hat{\boldsymbol{e}}_2 &= (-\sin\phi\,,\,\cos\phi\,,\,0)\\ \hat{\boldsymbol{n}} &= (\sin\theta\cos\phi\,,\,\sin\theta\sin\phi\,,\,\cos\theta) \quad .\end{aligned} \tag{4.98}$$

One then finds

$$\begin{aligned}d\hat{\boldsymbol{n}} &= \hat{\boldsymbol{e}}_1\,d\theta + \hat{\boldsymbol{e}}_2\,\sin\theta\,d\phi\\ \hat{\boldsymbol{n}}\times d\hat{\boldsymbol{n}} &= -\hat{\boldsymbol{e}}_1\,\sin\theta\,d\phi + \hat{\boldsymbol{e}}_2\,d\theta \quad ,\end{aligned} \tag{4.99}$$

and we have

$$U^{-1}(\xi,\hat{\boldsymbol{n}})\,dU(\xi,\hat{\boldsymbol{n}}) = -\frac{i}{2}\begin{pmatrix} d\xi & d\theta & d\phi \end{pmatrix}\begin{pmatrix} \hat{\boldsymbol{n}} \\ \sin\xi\,\hat{\boldsymbol{e}}_1 + (1-\cos\xi)\,\hat{\boldsymbol{e}}_2 \\ (1-\cos\xi)\,\sin\theta\,\hat{\boldsymbol{e}}_1 - \sin\xi\,\sin\theta\,\hat{\boldsymbol{e}}_2 \end{pmatrix}\cdot\boldsymbol{\sigma} \quad . \tag{4.100}$$

Thus, we have

$$\rho(\xi,\theta,\phi) \propto \hat{\boldsymbol{n}}\cdot\big[\sin\xi\,\hat{\boldsymbol{e}}_1 + (1-\cos\xi)\,\hat{\boldsymbol{e}}_2\big]\times\big[(1-\cos\xi)\,\hat{\boldsymbol{e}}_1 - \sin\xi\,\hat{\boldsymbol{e}}_2\big]\sin\theta = -4\sin^2(\tfrac{1}{2}\xi) \quad , \tag{4.101}$$

where $\xi\in[0,2\pi]$. Normalizing, we have the invariant measure

$$d\mu(\xi,\theta,\phi) \;=\; \overbrace{\frac{1}{8\pi^2}\,(1-\cos\xi)\sin\theta}^{\rho(\xi,\theta,\phi)}\,d\xi\,d\theta\,d\phi = \frac{(1-\cos\xi)\,d\xi}{2\pi}\,\frac{d\hat{\boldsymbol{n}}}{4\pi} \quad . \tag{4.102}$$

We can also compute the invariant measure using the Euler angle parameterization,

$$U(\alpha,\beta,\gamma) = \exp\big(-\tfrac{i}{2}\,\alpha\,\sigma^z\big)\exp\big(-\tfrac{i}{2}\,\beta\,\sigma^y\big)\exp\big(-\tfrac{i}{2}\,\gamma\,\sigma^z\big) \quad . \tag{4.103}$$

One finds

$$\begin{aligned} U^{-1}\,\frac{\partial U}{\partial\alpha} &= -\frac{i}{2}\,\big[-\sin\beta\cos\gamma\,\sigma^x + \sin\beta\sin\gamma\,\sigma^y + \cos\beta\,\sigma^z\big] \\ U^{-1}\,\frac{\partial U}{\partial\beta} &= -\frac{i}{2}\,\big[\sin\gamma\,\sigma^x + \cos\gamma\,\sigma^y\big] \\ U^{-1}\,\frac{\partial U}{\partial\gamma} &= -\frac{i}{2}\,\sigma^z \quad , \end{aligned} \tag{4.104}$$

and so

$$M = -\frac{i}{2}\begin{pmatrix} -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \\ -\sin\gamma & -\cos\gamma & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad . \tag{4.105}$$

Thus, $\det(M) = \frac{i}{8}\sin\beta$ and the normalized invariant measure in the Euler angle representation is

$$d\mu(\alpha,\beta,\gamma) = \frac{\sin\beta\,d\alpha\,d\beta\,d\gamma}{\mathsf{vol}(G)} \quad , \tag{4.106}$$

where $\mathsf{vol}(G)$ is the group volume, *i.e.* the integral of the numerator over the allowed range of the angles (α,β,γ). Remember that $\alpha\in[0,2\pi)$, $\beta\in[0,\pi]$, and $\gamma\in[0,4\pi)$ for $\mathsf{SU}(2)$, hence $\mathsf{vol}\big(\mathsf{SU}(2)\big) = 16\pi^2$, but for $\mathsf{SO}(3)$,

$$R(\alpha,\beta,\gamma) = \exp\big(-i\alpha J^z\big)\exp\big(-i\beta J^y\big)\exp\big(-i\gamma J^z\big) \quad , \tag{4.107}$$

we have $\gamma\in[0,2\pi)$, and accordingly $\mathsf{vol}\big(\mathsf{SO}(3)\big) = 8\pi^2$.

4.3.5 Peter-Weyl theorem

Armed with the invariant measure, we can now express the Great Orthogonality Theorem for Lie groups. It goes by the name of the *Peter-Weyl theorem*, and says that the functions

$$V_{\Gamma ik}(g) = \sqrt{d_\Gamma}\, D^\Gamma_{ik}(g) \tag{4.108}$$

form a complete and orthonormal basis in the space of square-integrable functions on the group manifold. This means

$$\boxed{\begin{aligned} \int\limits_G d\mu(g)\; V^*_{\Gamma ik}(g)\, V_{\Gamma' i'k'}(g) &= \sqrt{d_\Gamma\, d_{\Gamma'}} \int\limits_G d\mu(g)\; D^{\Gamma^*}_{ik}(g)\, D^{\Gamma'}_{i'k'}(g) = \delta_{\Gamma\Gamma'}\,\delta_{ii'}\,\delta_{kk'} \\ \sum_{\Gamma,i,k} V_{\Gamma ik}(g)\, V^*_{\Gamma ik}(g') &= \sum_{\Gamma ik} d_\Gamma\, D^\Gamma_{ik}(g)\, D^{\Gamma^*}_{ik}(g') = \delta(g,g') \end{aligned}} \tag{4.109}$$

where the symbol $\delta(g,g')$ satisfies

$$\int\limits_G d\mu(g')\;\delta(g,g')\,F(g') = \sum_{\Gamma,i,k} \big\langle\, V_{\Gamma ik}\,\big|\,F\,\big\rangle\, V_{\Gamma ik}(g) = F(g) \quad , \tag{4.110}$$

where $\langle\, V_{\Gamma ik}\,|\,F\,\rangle = \int\limits_G d\mu(g)\, V^*_{\Gamma ik}(g)\, F(g)$, and where the last inequality must be understood in terms of "convergence in the L^2 norm". In other words, the convergence is in the norm, and not necessarily pointwise, just like in the analogous case of the Fourier transform. For any function $F(g)$ which can be expanded in terms of the basis functions $V_{\Gamma ik}(g)$, one has

$$\int\limits_G d\mu(g')\;\delta(g,g')\;\overbrace{\sum_{\Gamma,i,k} C_{\Gamma ik}\, V_{\Gamma ik}(g')}^{F(g')} = \overbrace{\sum_{\Gamma ik} C_{\Gamma ik}\, V_{\Gamma ik}(g)}^{F(g)} \quad . \tag{4.111}$$

4.3.6 Projection operators

In analogy with the case for discrete groups, we can construct projectors onto the μ row of the Γ IRREP for any compact Lie group G, *viz.*

$$\hat\Pi^\Gamma_{\mu\nu} = d_\Gamma \int\limits_G d\mu(g)\; D^{\Gamma^*}_{\mu\nu}(g)\,\hat U(g) \quad . \tag{4.112}$$

Again, these satisfy

$$\hat\Pi^\Gamma_{\mu\nu}\hat\Pi^{\Gamma'}_{\mu'\nu'} = \delta_{\Gamma\Gamma'}\,\delta_{\nu\mu'}\,\hat\Pi^\Gamma_{\mu\nu'} \quad , \tag{4.113}$$

and

$$\hat U(g)\,\hat\Pi^\Gamma_{\mu\nu} = \hat\Pi^\Gamma_{\rho\nu}\, D^\Gamma_{\rho\mu}(g) \quad . \tag{4.114}$$

Projection matrices are defined in analogous fashion, with

$$\Pi^{\Gamma}_{\mu\nu} = d_{\Gamma} \int\limits_{G} d\mu(g)\; D^{\Gamma^*}_{\mu\nu}(g)\, \Delta(g) \tag{4.115}$$

satisfying $\Pi^{\Gamma}_{\mu\nu}\, \Pi^{\Gamma'}_{\mu'\nu'} = \delta_{\Gamma\Gamma'}\, \delta_{\nu\mu'}\, \Pi^{\Gamma}_{\mu\nu'}$ and $\Delta(g)\, \Pi^{\Gamma}_{\mu\nu} = \Pi^{\Gamma}_{\rho\nu}\, D^{\Gamma}_{\rho\mu}(g)$. Here $\Delta(G)$ is a matrix representation of the Lie group.

As an example, consider the group $\mathsf{SO}(2)$. To project an arbitrary periodic function $f(\phi)$ onto the j IRREP, we use $D^{(j)}(\alpha) = \exp(-ij\alpha)$ and $\hat{U}(\alpha) = \exp(-i\alpha L^z) = \exp(-\alpha\,\partial_\phi)$. The IRREPs are all one-dimensional. We then have

$$\hat{\Pi}^{(j)} f(\phi) = \int\limits_0^{2\pi} \frac{d\alpha}{2\pi}\, e^{ij\alpha}\, e^{-\alpha\,\frac{\partial}{\partial\phi}}\, f(\phi) = \int\limits_0^{2\pi} \frac{d\alpha}{2\pi}\, e^{ij\alpha}\, f(\phi-\alpha) = \hat{f}_j\, e^{ij\phi} \quad , \tag{4.116}$$

where

$$\hat{f}_j = \int\limits_0^{2\pi} \frac{d\alpha}{2\pi}\, e^{-ij\alpha}\, f(\alpha) \quad . \tag{4.117}$$

is the discrete Fourier transform of the function $f(\alpha)$. Note that $\hat{U}(\alpha)$ has eigenvalue $e^{-ij\alpha} = D^{(j)}(\alpha)$ when acting on the projected function $\hat{f}_j\, e^{ij\phi}$.

4.3.7 Product representations for $\mathsf{SU}(2)$

In the product basis, we have

$$\hat{U}(g)\,\Big[\,\big|\,j_1, m_1\,\big\rangle \otimes \big|\,j_2\,, m_2\,\big\rangle\,\Big] = \sum_{m_1', m_2'} \big|\,j_1, m_1'\,\big\rangle \otimes \big|\,j_2\,, m_2'\,\big\rangle\; \overbrace{D^{j_1}_{m_1', m_1}(g)\, D^{j_2}_{m_2', m_2}(g)}^{D^{j_1\times j_2}_{m_1' m_2', m_1 m_2}(g)} \quad . \tag{4.118}$$

Taking traces, we have

$$\chi^{j_1\times j_2}(g) = \chi^{(j_1)}(g)\, \chi^{(j_2)}(g) \quad . \tag{4.119}$$

Generalizing the decomposition formula to the case of continuous groups,

$$n_{\Gamma}(\Psi) = \int\limits_{G} d\mu(g)\; \chi^{\Gamma^*}(g)\, \chi^{\Psi}(g) \quad . \tag{4.120}$$

For $\mathsf{SU}(2)$, the invariant measure is $d\mu(\xi, \hat{\boldsymbol{n}}) = \frac{1}{\pi}\sin^2(\frac{1}{2}\xi)\, d\xi \cdot \frac{d\hat{\boldsymbol{n}}}{4\pi}$.

Recall that $\chi^{(j)}(\xi) = \sin\big[(j+\frac{1}{2})\,\xi\big]\big/\sin(\frac{1}{2}\xi)$. Thus, according to the decomposition rule,

$$\begin{aligned} n_j^{j_1\times j_2} &= \frac{2}{\pi}\int_0^\pi d\xi\ \sin^2\!\big(\tfrac{1}{2}\xi\big)\,\chi^{(j)}(\xi)\,\chi^{j_1}(\xi)\,\chi^{j_2}(\xi) \\ &= \frac{2}{\pi}\int_0^\pi d\xi \sum_{m=-j}^{j} e^{-im\xi}\,\sin\big((j_1+\tfrac{1}{2})\,\xi\big)\,\sin\big((j_2+\tfrac{1}{2})\,\xi\big) \\ &= \frac{1}{\pi}\int_0^\pi d\xi \sum_{m=-j}^{j} e^{-im\xi}\,\Big\{\cos\big[(j_1-j_2)\,\xi\big]-\cos\big[(j_1+j_2+1)\,\xi\big]\Big\} = \begin{cases} 1 & \text{if } |j_1-j_2|\le j\le (j_1+j_2) \\ 0 & \text{otherwise} \end{cases} . \end{aligned} \tag{4.121}$$

Thus, for each j with $|j_1-j_2|\le j\le (j_1+j_2)$, there is one representation within the direct product $j_1\times j_2$. Note that

$$\begin{aligned} \sum_{|j_1-j_2|}^{j_1+j_2}(2j+1) &= \tfrac{1}{2}(j_1+j_2)(j_1+j_2+1)-\tfrac{1}{2}\big(|j_1-j_2|-1\big)|j_1-j_2|+(j_1+j_2)-|j_1-j_2| \\ &= (2j_1+1)(2j_2+1) \quad , \end{aligned} \tag{4.122}$$

which says that the dimension of the product representation is the product of the dimensions of its factors.

The direct product of two representations j_1 and j_2 is expanded as

$$\big|\,j_1,m_1\,\big\rangle\otimes\big|\,j_2\,,m_2\,\big\rangle = \sum_{j,m}\begin{pmatrix} j_1 & j_2 \\ m_1 & m_2 \end{pmatrix}\begin{vmatrix} j \\ m \end{vmatrix}\big|\,j,m\,\big\rangle \quad . \tag{4.123}$$

The CGCs are nonzero only if $|j_1-j_2|\le j\le (j_1+j_2)$ and $m=m_1+m_2$. They are tabulated in various publications (*e.g.*, see *Wikipedia*). To derive the CGCs, one starts with the state with $m_1=j_1$ and $m_2=j_2$, which corresponds to $j=j_1+j_2$ and $m=m_1+m_2$. Since

$$\big|\,j_1+\mathrm{J}_2,j_1+j_2\,\big\rangle = \big|\,j_1,j_1\,\big\rangle\otimes\big|\,j_2\,,j_2\,\big\rangle \quad , \tag{4.124}$$

we have, trivially, that

$$\begin{pmatrix} j_1 & j_2 \\ m_1 & m_2 \end{pmatrix}\begin{vmatrix} j_1+j_2 \\ j_1+j_2 \end{vmatrix} = \delta_{m_1\,,j_1}\,\delta_{m_2\,,j_2} \quad . \tag{4.125}$$

Now apply the lowering operator $\hat{J}^-$ to get

$$\begin{aligned} \hat{J}^-\,\big|\,j_1+j_2\,,\,j_1+j_2\,\big\rangle &= \big[2(j_1+j_2)\big]^{1/2}\,\big|\,j_1+j_2\,,\,j_1+j_2-1\,\big\rangle \\ &= \Big[\,\hat{J}^-\,\big|\,j_1,j_1\,\big\rangle\Big]\otimes\big|\,j_2,j_2\,\big\rangle+\big|\,j_1,j_1\,\big\rangle\otimes\Big[\,\hat{J}^-\,\big|\,j_2,j_2\,\big\rangle\Big] \\ &= \sqrt{2j_1}\,\big|\,j_1\,,\,j_1-1\,\big\rangle\otimes\big|\,j_2\,,\,j_2\,\big\rangle+\sqrt{2j_2}\,\big|\,j_1\,,\,j_1\,\big\rangle\otimes\big|\,j_2\,,\,j_2-1\,\big\rangle \quad . \end{aligned} \tag{4.126}$$

Thus,

$$\big|\,j_1+j_2\,,\,j_1+j_2-1\,\big\rangle = \sqrt{\frac{j_1}{j_1+j_2}}\,\big|\,j_1,j_1-1\,\big\rangle\otimes\big|\,j_2,j_2\,\big\rangle+\sqrt{\frac{j_2}{j_1+j_2}}\,\big|\,j_1,j_1\,\big\rangle\otimes\big|\,j_2,j_2-1\,\big\rangle \quad . \tag{4.127}$$

Taking the inner product with eqn. 4.123 then gives

$$\left(\begin{array}{cc|c} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & j_1+j_2-1 \end{array}\right) = \sqrt{\frac{j_1}{j_1+j_2}}\,\delta_{m_1,j_1-1}\,\delta_{m_2,j_2} + \sqrt{\frac{j_2}{j_1+j_2}}\,\delta_{m_1\,,\,j_1}\,\delta_{m_2\,,\,j_2-1} \quad . \tag{4.128}$$

Continue to apply $\hat{J}^-$ to generate all the states $|\,j_1+j_2\,,\,m\,\rangle$ for $m \in \{-j_1-j_2\,,\,\ldots\,,\,j_1+j_2\}$.

Next, consider the state

$$|\,j,m\,\rangle = \sqrt{\frac{j_2}{j_1+j_2}}\,|\,j_1,j_1-1\,\rangle\otimes|\,j_2,j_2\,\rangle - \sqrt{\frac{j_1}{j_1+j_2}}\,|\,j_1,j_1\,\rangle\otimes|\,j_2,j_2-1\,\rangle \quad , \tag{4.129}$$

which clearly has $m = j_1+j_2-1$ but which is orthogonal to the state in Eqn. 4.127. We conclude that the above state is none other than $|\,j_1+j_2-1\,,\,j_1+j_2-1\,\rangle$, and consequently

$$\left(\begin{array}{cc|c} j_1 & j_2 & j_1+j_2-1 \\ m_1 & m_2 & j_1+j_2-1 \end{array}\right) = \sqrt{\frac{j_2}{j_1+j_2}}\,\delta_{m_1\,,\,j_1-1}\,\delta_{m_2\,,\,j_2} - \sqrt{\frac{j_1}{j_1+j_2}}\,\delta_{m_1\,,\,j_1}\,\delta_{m_2\,,\,j_2-1} \quad . \tag{4.130}$$

Applying the lowering operator to this state, one creates a state with $j = j_1+j_2-1$ and $m = j_1+j_2-2$, and one may continue to apply $\hat{J}^-$ to generate the entire family of basis states for the $j = j_1+j_2-1$ representation. One then constructs a new state ψ with $m = j_1+j_2-2$ which is normalized and orthogonal to both $|\,j_1+j_2\,,\,j_1+j_2-2\,\rangle$ and $|\,j_1+j_2-1\,,\,j_1+j_2-2\,\rangle$. This must be $|\,j_1+j_2-2\,,\,j_1+j_2-2\,\rangle$. Continuing in this manner, one eventually constructs all the basis states $|\,j,m\,\rangle$ in terms of the product states, from which one can read off the CGCs.

4.3.8 Spherical harmonics

The angular momentum operators,

$$\hat{L}^x = i\left(z\,\frac{\partial}{\partial y} - y\,\frac{\partial}{\partial z}\right) \quad , \quad \hat{L}^y = i\left(x\,\frac{\partial}{\partial z} - z\,\frac{\partial}{\partial x}\right) \quad , \quad \hat{L}^z = i\left(y\,\frac{\partial}{\partial x} - x\,\frac{\partial}{\partial y}\right) \quad , \tag{4.131}$$

satisfy the SO(3) algebra $\big[\hat{L}^a,\hat{L}^b\big] = i\epsilon_{abc}\,\hat{L}^c$. Clearly $L^a f(r) = 0$ when acting on a spherically symmetric function. Therefore we may express the $\hat{L}^a$ in terms of derivatives with respect to θ and ϕ, *viz.*

$$L^\pm = e^{\pm i\phi}\left(i\,\mathrm{ctn}\,\theta\,\frac{\partial}{\partial\phi} \pm \frac{\partial}{\partial\theta}\right) \quad , \quad L^z = -i\,\frac{\partial}{\partial\phi} \quad , \quad \hat{\boldsymbol{L}}^2 = -\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\,\sin\theta\,\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\phi^2} \quad . \tag{4.132}$$

We then have

$$\hat{\boldsymbol{L}}^2\,Y_{lm}(\hat{\boldsymbol{n}}) = l(l+1)\,Y_{lm}(\hat{\boldsymbol{n}}) \qquad , \qquad \hat{L}^z\,Y_{lm}(\hat{\boldsymbol{n}}) = m\,Y_{lm}(\hat{\boldsymbol{n}}) \quad , \tag{4.133}$$

with $l \in \mathbb{N}$, where $Y_{lm}(\hat{\boldsymbol{n}})$ is the *spherical harmonic*. The spherical harmonics are related to the rotation matrices. If we define

$$|\,\hat{\boldsymbol{n}}\,\rangle \equiv \hat{R}(\phi,\theta,0)\,|\,\hat{\boldsymbol{z}}\,\rangle \quad , \tag{4.134}$$

where $|\,\hat{\boldsymbol{z}}\,\rangle$ is the ket vector corresponding to an orientation along $\hat{\boldsymbol{z}}$[11], then

$$\langle\, l,m \,|\, \hat{\boldsymbol{n}} \,\rangle = \sum_{m'=-l}^{l} \langle\, l,m \,|\, \hat{R}(\phi,\theta,0) \,|\, l,m' \,\rangle \langle\, l,m' \,|\, \hat{\boldsymbol{z}} \,\rangle \quad . \tag{4.135}$$

We then have $Y_{lm}(\hat{\boldsymbol{n}}) = \langle\, \hat{\boldsymbol{n}} \,|\, l,m \,\rangle$. Now

$$\langle\, l,m \,|\, \hat{\boldsymbol{z}} \,\rangle = Y_{lm}(\hat{\boldsymbol{z}}) = \sqrt{\frac{2l+1}{4\pi}}\,\delta_{m,0} \tag{4.136}$$

and therefore

$$Y_{lm}(\hat{\boldsymbol{n}}) = \sqrt{\frac{2l+1}{4\pi}}\,\big[D^{(l)}_{m0}(\phi,\theta,0)\big]^* = \sqrt{\frac{2l+1}{4\pi}}\,d^{(l)}_{m0}(\theta)\,e^{im\phi} \quad . \tag{4.137}$$

Note that $Y_{l,-m}(\hat{\boldsymbol{n}}) = (-1)^m\,Y^*_{lm}(\hat{\boldsymbol{n}})$ and that $D^{(l)}_{m0}(\phi,\theta,\psi) = D^{(l)}_{m0}(\phi,\theta,0)$ because $e^{-im'\gamma} = 1$ for $m' = 0$. The spherical harmonics are normalized according to

$$\int\! d\hat{\boldsymbol{n}}\; Y^*_{lm}(\hat{\boldsymbol{n}})\,Y_{l'm'}(\hat{\boldsymbol{n}}) = \delta_{ll'}\,\delta_{mm'} \quad . \tag{4.138}$$

Note that there is no factor of 4π in the denominator of the measure, which is $d\hat{\boldsymbol{n}} = \sin\theta\,d\theta\,d\phi$. The *associated Legendre polynomials*[12] $P_{lm}(\cos\theta)$ are related to the $d^{(l)}$ matrices by

$$P_{lm}(\cos\theta) = (-1)^m\sqrt{\frac{(l+m)!}{(l-m)!}}\,d^{(l)}_{m0}(\theta) \quad , \tag{4.139}$$

and therefore we have

$$Y_{lm}(\hat{\boldsymbol{n}}) = \sqrt{\frac{2l+1}{4\pi}\,\frac{(l-m)!}{(l+m)!}}\,P_{lm}(\cos\theta)\,e^{im\phi} \quad . \tag{4.140}$$

See https://en.wikipedia.org/wiki/Table_of_spherical_harmonics for explicit expressions of $Y_{lm}(\hat{\boldsymbol{n}})$ for low orders of the angular momentum l. Finally, note that

$$\langle\, \hat{\boldsymbol{n}} \,|\, \hat{R}(\xi,\hat{\boldsymbol{\xi}}) \,|\, l,m \,\rangle = \sum_{m'=-l}^{l} Y_{lm}(\hat{\boldsymbol{n}})\,D^{(l)}_{m'm}(\phi_{\boldsymbol{\xi}},\theta_{\boldsymbol{\xi}},\psi_{\boldsymbol{\xi}}) \quad , \tag{4.141}$$

where $(\phi_{\boldsymbol{\xi}},\theta_{\boldsymbol{\xi}},\psi_{\boldsymbol{\xi}})$ are the Euler angles corresponding to the rotation $\hat{R}(\xi,\hat{\boldsymbol{\xi}})$. Writing $|\,\hat{\boldsymbol{n}}'\,\rangle = \hat{R}(-\xi,\hat{\boldsymbol{\xi}})\,|\,\hat{\boldsymbol{n}}\,\rangle$ as the ket vector $|\,\hat{\boldsymbol{n}}\,\rangle$ rotated by $-\xi$ about the direction $\hat{\boldsymbol{\xi}}$, and taking $m = 0$, we obtain the *spherical harmonic addition formula*,

$$Y_{l0}(\hat{\boldsymbol{n}}') = \sqrt{\frac{4\pi}{2l+1}}\sum_{m=-l}^{l} Y_{lm}(\hat{\boldsymbol{n}})\,Y^*_{lm}(\hat{\boldsymbol{n}}_{\boldsymbol{\xi}}) \quad , \tag{4.142}$$

[11] That is, we suppress the radial coordinate in $|\,\boldsymbol{r}\,\rangle \equiv |\,r,\hat{\boldsymbol{n}}\,\rangle$.

[12] Wisconsin Senator Joseph McCarthy was famous for his aggressive questioning of witnesses before the U.S. Senate Subcommittee on Investigations in 1954, theatrically haranguing them by demanding, "Are you now or have you ever been associated with the Legendre polynomials?" Those who answered in the affirmative or refused to answer were blacklisted and forbidden from working on special functions. A similar fate befell those who associated with Laguerre, Jacobi, or Gegenbauer polynomials.

where $\hat{\boldsymbol{n}}_{\boldsymbol{\xi}}$ is the unit vector whose polar and azimuthal angles are $(\theta_{\boldsymbol{\xi}}, \phi_{\boldsymbol{\xi}})$. Note that $\hat{\boldsymbol{n}}_{\boldsymbol{\xi}} \neq \hat{\boldsymbol{\xi}}$ in general! Since $P_{l0}(\cos\theta) = P_l(\cos\theta)$, we have

$$P_l(\cos\vartheta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\hat{\boldsymbol{n}})\, Y^*_{lm}(\hat{\boldsymbol{n}}_{\boldsymbol{\xi}}) \quad , \tag{4.143}$$

where, as the student should confirm, ϑ is the angle between $\hat{\boldsymbol{n}}$ and $\hat{\boldsymbol{n}}_{\boldsymbol{\xi}}$.

4.3.9 Tensor operators and the Wigner-Eckart theorem for SU(2)

An *irreducible tensor operator* $\hat{Q}^J_M$ is one which transforms according to the J IRREP of $\mathsf{SU}(2)$, meaning

$$\hat{R}\,\hat{Q}^J_M\,\hat{R}^\dagger = \sum_{M'=-J}^{J} \hat{Q}^J_{M'}\, D^{(J)}_{M'M}(R) \quad , \tag{4.144}$$

where $\hat{R}$ is the unitary operator corresponding to the group element R. Writing $\hat{R} = \exp(i\boldsymbol{\epsilon}\cdot\hat{\boldsymbol{J}})$ where $\hat{\boldsymbol{J}}$ are the operator generators of $\mathsf{su}(2)$, and expanding for infinitesimal $\boldsymbol{\epsilon}$, one finds

$$\big[\hat{J}^a\,,\,\hat{Q}^J_M\big] = \sum_{M'=-J}^{J} \hat{Q}^J_{M'} \left\langle\, J, M' \,\middle|\, J^a \,\middle|\, J, M \,\right\rangle \quad . \tag{4.145}$$

Mercifully, as we have seen, $\mathsf{SU}(2)$ is simply reducible, meaning that the product representation $j_1 \times j_2$ contains representations with $j \in \big\{|j_1 - j_2|\,, \ldots,\, j_1 + j_2\big\}$ where each j IRREP occurs only once. This means that we can decompose the state $\hat{Q}^J_m \,|\, j', m'; \lambda' \,\rangle$ as

$$\hat{Q}^J_M \,|\, j', m'; \lambda' \,\rangle = \sum_{j,m} \left(\begin{array}{cc|c} J & j' & j \\ M & m' & m \end{array} \right) |\, \Psi^{j,\lambda'}_m \,\rangle \quad . \tag{4.146}$$

Here and below, λ and λ' are extra indices corresponding to quantum numbers not associated with the group symmetry. The state $|\, \Psi^{j;\lambda'}_m \,\rangle$ transforms as

$$\hat{R}\,\big|\, \Psi^{j,\lambda'}_m \,\big\rangle = \sum_{m'=-j}^{j} \big|\, \Psi^{j,\lambda'}_{m'} \,\big\rangle\, D^{(j)}_{m'm}(R) \quad . \tag{4.147}$$

It follows that

$$\left\langle\, j, m; \lambda \,\middle|\, \hat{Q}^J_M \,\middle|\, j', m'\,; \lambda' \,\right\rangle = \sum_{j'',m''} \left(\begin{array}{cc|c} J & j' & j'' \\ M & m' & m'' \end{array} \right) \left\langle\, j, m\,; \lambda \,\middle|\, \Psi^{j'',\lambda'}_{m''} \,\right\rangle \tag{4.148}$$

where

$$\left\langle\, j, m\,; \lambda \,\middle|\, \Psi^{j'',\lambda'}_{m''} \,\right\rangle = \delta_{jj''}\,\delta_{mm''} \times \frac{1}{2j+1} \sum_{\widetilde{m}=-j}^{j} \left\langle\, j, \widetilde{m}; \lambda \,\middle|\, \Psi^{j,\lambda'}_{\widetilde{m}} \,\right\rangle \tag{4.149}$$

We now define[13]

$$\left\langle\, j\,;\lambda \,\middle\|\, \hat{Q}^J \,\middle\|\, j'\,;\lambda' \,\right\rangle \equiv \frac{1}{\sqrt{2j+1}} \sum_{\widetilde{m}=-j}^{j} \left\langle\, j,\widetilde{m};\lambda \,\middle|\, \Psi_{\widetilde{m}}^{j,\lambda'} \,\right\rangle \quad , \tag{4.150}$$

in which case we have the Wigner-Eckart theorem for $\mathsf{SU}(2)$:[14]

$$\left\langle\, j,m;\lambda \,\middle|\, \hat{Q}^J_M \,\middle|\, j',m'\,;\lambda' \,\right\rangle = \left(\begin{array}{cc|c} J & j' & j \\ M & m' & m \end{array}\right) \frac{\left\langle\, j\,;\lambda \,\middle\|\, \hat{Q}^J \,\middle\|\, j'\,;\lambda' \,\right\rangle}{\sqrt{2j+1}} \quad . \tag{4.151}$$

All the M, m, and m' dependence is in the CGC.

4.4 Joke for Chapter Four

A rabbit one day managed to break free from the laboratory where he had been born and raised. As he scurried away from the fencing of the compound, he felt grass under his little feet and saw the dawn breaking for the first time in his life. 'Wow, this is great,' he thought. It wasn't long before he came to a hedge and, after squeezing under it he saw a wonderful sight: lots of other bunny rabbits, all free and nibbling on the lush green grass.

'Hey,' he called. 'I'm a rabbit from the laboratory and I've just escaped. Are you wild rabbits?'

'Yes. Come and join us!' they cried.

He hopped over to them and started eating the grass. It was delicious. 'What else do you wild rabbits do?' he asked.

'Well,' one of them said. 'You see that field there? It's got carrots growing in it. We dig them up and eat them.'

This, he couldn't resist and he spent the next hour eating the most succulent carrots. They were scrumptious – out of this world.

Later, he asked them again, 'What else do you do?'

'You see that field there? It's got lettuce growing in it. We eat that as well.'

The lettuce was as yummy as the grass and the carrots, and he returned a while later completely full. 'Is there anything else you guys do?' he asked.

One of the other rabbits came a bit closer to him and spoke softly. 'There's one other thing you must try. You see those rabbits there?' he said, pointing to the far corner of the field. 'They're lady rabbits. We shag them. Check it out.'

The rabbit spent the rest of the morning screwing his little heart out until, completely exhausted, he staggered back to the group.

'That was awesome,' he panted.

[13] Where does j' come from in the reduced matrix element on the LHS when it doesn't appear on the RHS? Well, you see, the RHS *does* know about j', as a check of Eqn. 4.146 should make clear. I've suppressed this label in the state $|\,\Psi_{\widetilde{m}}^{j,\lambda'}\,\rangle$ just to keep you on your toes.

[14] Look, I'm very sorry about the awkward $\sqrt{2j+1}$ factors. In my defense, it's a convention which was established long before I was even born.

'So are you going to live with us then?' one of them asked.

'I'm sorry, I had a great time – but I just can't.'

The wild rabbits all stared at him, a bit surprised. 'Why? We thought you liked it here.'

'I do,' he said. 'But I've got to get back to the lab. I'm dying for a cigarette.'

Chapter 5

Crystal Math

5.1 Classification of Crystalline Structures

Crystallography is the classification of spatially periodic structures according to their translational and rotational symmetries. It is a mature field[1], and the possible crystalline symmetries of two and three dimensional structures have been exhaustively classified. We shall not endeavor to prove, *e.g.*, that there are precisely 230 three-dimensional space groups. Rather, our proximate goal is to economically describe the most relevant aspects of the classification scheme, so that we may apply methods of group theory to analyze experimentally relevant physical processes in crystals.

5.1.1 Bravais Lattices

The notion of a *Bravais lattice* was discussed in §4.1.1. To review, a Bravais lattice $\mathcal{L}$ in d space dimensions is defined by a set of linearly independent vectors $\{\boldsymbol{a}_j\}$ with $j \in \{1, \ldots, d\}$ which define a *unit cell*. A general point $\boldsymbol{R}$ in the Bravais lattice is written as $\boldsymbol{R} = \sum_j n_j \boldsymbol{a}_j$, where each $n_j \in \mathbb{Z}$. The unit cell volume is given by

$$\Omega = \epsilon_{\mu_1 \cdots \mu_d} a_1^{\mu_1} \cdots a_d^{\mu_d} \quad , \tag{5.1}$$

and is by definition positive[2]. The choice of the vectors $\{\boldsymbol{a}_j\}$ is not unique, for one can always replace $\boldsymbol{a}_i$ with $\boldsymbol{a}_i + \boldsymbol{a}_j$ for any $j \neq i$, and, due to the antisymmetry of the determinant, Ω is unchanged. It is then conventional to choose the $\{\boldsymbol{a}_j\}$ so that they have the shortest possible length, though even this prescription is not necessarily unique. The lattice of points $\{\boldsymbol{R}\}$ is called the *direct lattice*, and the $\{\boldsymbol{a}_j\}$ are the *elementary* (or *primitive*) *direct lattice vectors*.

[1] Crystallography has enjoyed something of a resurgence in its relevance to recent theories of topological classification of electronic band structures. The interplay between symmetry and topology leads to a new classification for materials known as crystalline topological insulators, for example.

[2] One can always reorder the $\boldsymbol{a}_j$ so that $\Omega > 0$.

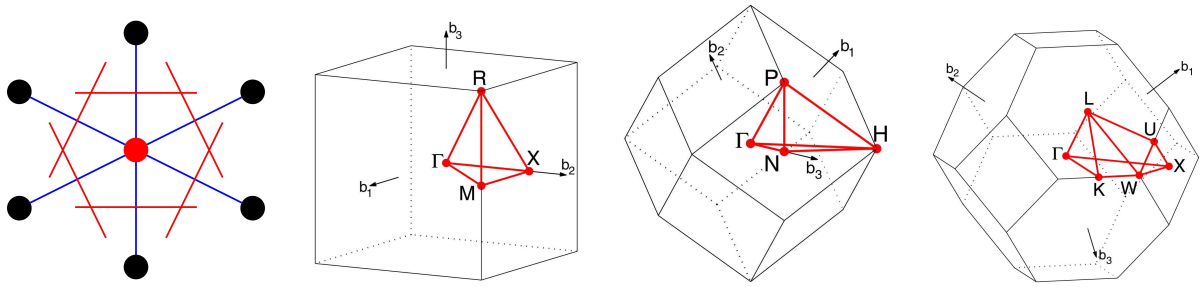


Figure 5.1: First panel shows construction of the first Wigner-Seitz cell or first Brillouin zone for the triangular lattice. Second, third, and fourth panels show first Brillouin zones for the simple cubic, body-centered cubic, and face-centered cubic direct lattices, respectively, with high symmetry points identified. Image credit: *Wikipedia* and Setyawan and Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010.

One can then define the elementary (primitive) *reciprical lattice vectors*,

$$b_k^\nu \equiv \frac{2\pi}{\Omega}\,\epsilon_{\mu_1\cdots\mu_{k-1}\,\nu\,\mu_{k+1}\cdots\mu_d} a_1^{\mu_1}\cdots a_{k-1}^{\mu_{k-1}}\,a_{k+1}^{\mu_{k+1}}\cdots a_d^{\mu_d} \quad , \tag{5.2}$$

which satisfy $\boldsymbol{a}_i\cdot\boldsymbol{b}_j = 2\pi\,\delta_{ij}$. Indeed, we must have

$$\sum_{\mu=1}^{d} a_i^\mu\,b_j^\mu = 2\pi\,\delta_{ij} \qquad , \qquad \sum_{j=1}^{d} a_j^\mu\,b_j^\nu = 2\pi\,\delta_{\mu\nu} \quad , \tag{5.3}$$

because if the square matrices $A_{j,\mu}\equiv a_j^\mu$ and $B^{\mathsf{T}}_{\mu,j}\equiv b_j^\mu$ are inverses, they are each other's right as well as left inverse. For example, with $d=3$ we have $\Omega = \boldsymbol{a}_1\cdot\boldsymbol{a}_2\times\boldsymbol{a}_3$ and

$$\boldsymbol{b}_1 = \frac{2\pi}{\Omega}\,\boldsymbol{a}_2\times\boldsymbol{a}_3 \quad , \quad \boldsymbol{b}_2 = \frac{2\pi}{\Omega}\,\boldsymbol{a}_3\times\boldsymbol{a}_1 \quad , \quad \boldsymbol{b}_3 = \frac{2\pi}{\Omega}\,\boldsymbol{a}_1\times\boldsymbol{a}_2 \quad . \tag{5.4}$$

The set of vectors $\boldsymbol{K} = \sum_{j=1}^d m_j\,\boldsymbol{b}_j$, with each $m_i\in\mathbb{Z}$, is called the *reciprocal lattice*, $\hat{\mathcal{L}}$. The reciprocal lattice is therefore also a Bravais lattice, though not necessarily the same Bravais lattice as the direct lattice. For example, while the reciprocal lattice of a simple cubic lattice is also simple cubic, the reciprocal lattice of a body-centered cubic lattice is face-centered cubic. Constructing the reciprocal lattice of the reciprocal lattice, one arrives back at the original direct lattice. The unit cell volume of the reciprocal lattice is

$$\hat{\Omega} = \epsilon_{\mu_1\cdots\mu_d}\,b_1^{\mu_1}\cdots b_d^{\mu_d} = \frac{(2\pi)^d}{\Omega} \quad . \tag{5.5}$$

The repeating unit cells in the direct and reciprocal lattices may be written as the collection of points $\boldsymbol{r}$ and $\boldsymbol{k}$, respectively, where

$$\boldsymbol{r} = \sum_{j=1}^{d} x_j\,\boldsymbol{a}_j \qquad , \qquad \boldsymbol{k} = \sum_{j=1}^{d} y_j\,\boldsymbol{b}_j \quad , \tag{5.6}$$

where each $x_j, y_j\in[0,1]$. The symmetries of the direct and reciprocal lattices are more fully elicited by shifting each $\boldsymbol{r}$ and $\boldsymbol{k}$ point by a direct or reciprocal lattice vector so that it is as close as possible to the

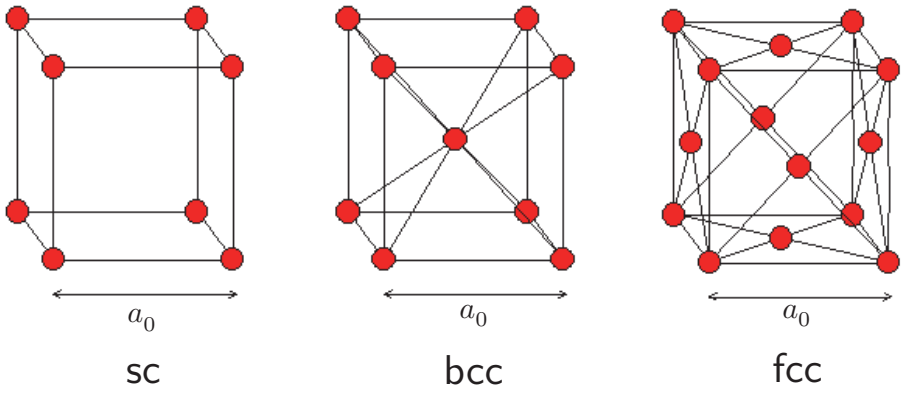


Figure 5.2: Simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices.

origin. Equivalently, sketch all the nonzero shortest direct/reciprocal lattice vectors emanating from the origin[3], and bisect each such vector with a perpendicular plane. The collection of points lying within all the planes will form the first *Wigner-Seitz cell* of the direct lattice, and the first *Brillouin zone* of the reciprocal lattice.

Finally, we cannot resist mentioning the beautiful and extremely important application of the Poisson summation formula to Bravais lattice systems:

$$\sum_{\boldsymbol{K}} e^{i\boldsymbol{K}\cdot\boldsymbol{r}} = \Omega \sum_{\boldsymbol{R}} \delta(\boldsymbol{r}-\boldsymbol{R}) \quad , \quad \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = \hat{\Omega} \sum_{\boldsymbol{K}} \delta(\boldsymbol{k}-\boldsymbol{K}) \quad . \tag{5.7}$$

Example: fcc and bcc lattices

The primitive direct lattice vectors for the fcc structure may be taken as

$$\boldsymbol{a}_1 = \frac{a}{\sqrt{2}}\,(0,1,1) \quad , \quad \boldsymbol{a}_2 = \frac{a}{\sqrt{2}}\,(1,0,1) \quad , \quad \boldsymbol{a}_3 = \frac{a}{\sqrt{2}}\,(1,1,0) \quad . \tag{5.8}$$

The unit cell volume is $\Omega = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3 = 2a^3$. Note that $|\boldsymbol{a}_j| = a$. Each FCC lattice point has twelve nearest neighbors, located at $\pm\boldsymbol{a}_1$, $\pm\boldsymbol{a}_2$, $\pm\boldsymbol{a}_3$, $\pm(\boldsymbol{a}_1-\boldsymbol{a}_2)$, $\pm(\boldsymbol{a}_2-\boldsymbol{a}_3)$, and $\pm(\boldsymbol{a}_3-\boldsymbol{a}_1)$. The corresponding primitive reciprocal lattice vectors are

$$\boldsymbol{b}_1 = \frac{b}{\sqrt{3}}\,(-1,1,1) \quad , \quad \boldsymbol{b}_2 = \frac{b}{\sqrt{3}}\,(1,-1,1) \quad , \quad \boldsymbol{b}_3 = \frac{b}{\sqrt{3}}\,(1,1,-1)\,, \tag{5.9}$$

with $b = \sqrt{6}\,\pi/a$. These primitive vectors form a bcc structure, in which each site has eight nearest neighbors, located at $\pm\boldsymbol{b}_1$, $\pm\boldsymbol{b}_2$, $\pm\boldsymbol{b}_3$, and $\pm(\boldsymbol{b}_1+\boldsymbol{b}_2+\boldsymbol{b}_3)$. The simple, body-centered, and face-centered cubic structures are depicted in Fig. 5.2.

[3]There may be more than d shortest direct/reciprocal lattice vectors. For example, the triangular lattice is two-dimensional, but it has six nonzero shortest direct/reciprocal lattice vectors.

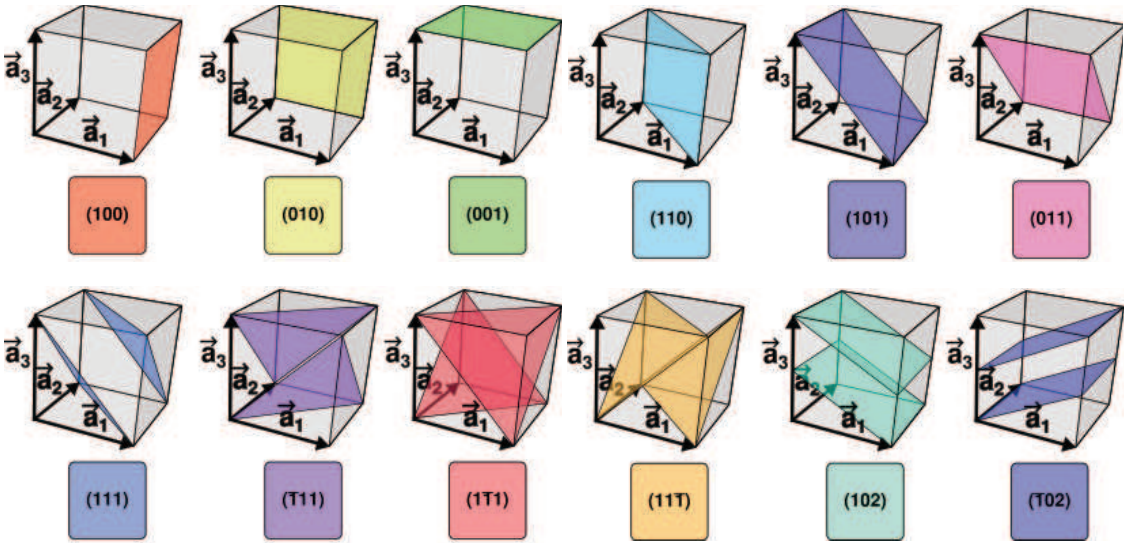


Figure 5.3: Examples of Miller planes. Image credit: Wikipedia.

Be forewarned that in some texts, distances are given in terms of the side length of the cube. In the fcc lattice, if the cube has side length a_0, then the fcc lattice constant, *i.e.* the distance between nearest neighbor sites, is $a = a_0/\sqrt{2}$. Similarly, for the bcc case, if the cube has side length b_0, the corresponding bcc lattice constant is $b = \sqrt{3}\, b_0/2$.

In Fig. 5.1, the two rightmost panels show the first Brillouin zones corresponding to the bcc and fcc direct lattices, respectively. It follows that the same shapes describe the first Wigner-Seitz cells for the fcc and bcc lattices, respectively.

5.1.2 Miller indices

This eponymous notation system, first introduced by the British minerologist William H. Miller in 1839, provides a convenient way of indexing both directions and planes of points in a Bravais lattice. Briefly,

- $[\,h\,k\,l\,]$ represents a direction in the direct lattice given by the vector $h\boldsymbol{a}_1 + k\boldsymbol{a}_2 + l\boldsymbol{a}_3$. For negative numbers, one writes, *e.g.*, $\bar{2}$ instead of -2. Thus, $[\,1\,\bar{2}\,0\,]$ is the direction parallel to $\boldsymbol{a}_1 - 2\boldsymbol{a}_2$. Only integers are used, so the direction parallel to $\frac{1}{4}\boldsymbol{a}_1 + \frac{1}{2}\boldsymbol{a}_2 - \frac{1}{3}\boldsymbol{a}_3$ is written as $[\,3\,6\,\bar{4}\,]$.
- $\langle\,h\,k\,l\,\rangle$ denotes the set of all directions which are related to $[\,h\,k\,l\,]$ by a rotational symmetry.
- $(\,h\,k\,l\,)$ represents a set of *lattice planes* which lie perpendicular to the vector $h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$. Again, only integers are used, and any negative numbers are written with bars rather than minus signs.
- $\{\,h\,k\,l\,\}$ denotes all families of lattice planes related to $(\,h\,k\,l\,)$ by a rotational symmetry.

We can think of the Miller planes in terms of plane waves, *i.e.* as sets of points of constant phase $\phi(\boldsymbol{r}) = \boldsymbol{K}_{hkl} \cdot \boldsymbol{r}$, where $\boldsymbol{K}_{hkl} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$ is a reciprocal lattice vector. If we write $\boldsymbol{R} = r\boldsymbol{a}_1 + s\boldsymbol{a}_2 + t\boldsymbol{a}_3$, we

have $\phi(r,s,t) = 2\pi(hr + ks + lt) \equiv 2\pi N$, and thus the intersection of this plane with the $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$ axes, which in general are not mutually orthogonal, lie at $N\boldsymbol{a}_1/h$, $N\boldsymbol{a}_2/k$, and $N\boldsymbol{a}_3/l$, respectively. In this way, one can identify the Miller indices of any lattice plane by taking the inverses of the respective coefficients and inverting them, then multiplying by the least common denominator if the results turn out to be fractional. From the formula $\exp(i\boldsymbol{K}\cdot\boldsymbol{r}) = 1$, we also see that the distance between consecutive Miller planes is $2\pi/|\boldsymbol{K}|$.

Cubic and hexagonal systems

For cubic systems, it is conventional to index the lattice planes based on the underlying simple cubic Bravais lattice. The bcc lattice is then viewed as a simple cubic lattice with a two element basis (see §5.1.5 below), and the fcc lattice as simple cubic with a four element basis. In hexagonal systems, typically one chooses the primary direct lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ to subtend an angle of 120°, in which case $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ subtend an angle of 60°. Then defining $\boldsymbol{b}_0 \equiv \boldsymbol{b}_2 - \boldsymbol{b}_1$, we have that $\boldsymbol{b}_0$ is rotationally equivalent to $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. Thus, if we define $i \equiv -(h+k)$, then we have the following rotations:

$$\begin{aligned} h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 &= R_{120^\circ}\big(k\,\boldsymbol{b}_1 + i\,\boldsymbol{b}_2\big) = R_{240^\circ}\big(i\,\boldsymbol{b}_1 + h\,\boldsymbol{b}_2\big) \\ &= R_{60^\circ}\big(\bar{i}\,\boldsymbol{b}_1 + \bar{h}\,\boldsymbol{b}_2\big) = R_{180^\circ}\big(\bar{h}\,\boldsymbol{b}_1 + \bar{k}\,\boldsymbol{b}_2\big) = R_{300^\circ}\big(\bar{k}\,\boldsymbol{b}_1 + \bar{i}\,\boldsymbol{b}_2\big) \quad . \end{aligned} \tag{5.10}$$

To reveal this rotational symmetry, the redundant fourth index i is used, and the Miller indices are reported as $(\,h\,k\,i\,l\,)$. The fourth index is always along the c-axis. The virtue of this four index notation is that it makes clear the relations between, *e.g.*, $(\,1\,1\,\bar{2}\,0\,) \equiv (\,1\,1\,0\,)$ and $(\,1\,\bar{2}\,1\,0\,) \equiv (\,1\,\bar{2}\,0\,)$, and in general

$$(\,h\,k\,i\,l\,) \;\to\; (\,\bar{i}\,\bar{h}\,\bar{k}\,l\,) \to\; (\,k\,i\,h\,l\,) \;\to\; (\,\bar{h}\,\bar{k}\,\bar{i}\,l\,) \;\to\; (\,i\,h\,k\,l\,) \;\to\; (\,\bar{k}\,\bar{i}\,\bar{h}\,l\,) \to (\,h\,k\,i\,l\,) \tag{5.11}$$

gives the full sixfold cycle.

5.1.3 Crystallographic restriction theorem

Consider a Bravais lattice and select one point as the origin. Now consider a general rotation $R \in \mathsf{SO}(3)$ and ask how the primary direct lattice vectors transform. If the Bravais lattice is symmetric under the operation R, then each $\boldsymbol{a}_j$ must transform into another Bravais lattice vector, *i.e.*

$$R_{\mu\nu}\,a_i^\nu = K_{ij}\,a_j^\mu \quad , \tag{5.12}$$

where K_{ij} is a matrix composed of integers. Now multiply both sides of the above equation by b_i^ρ and sum on the index i. From Eqn. 5.3, we have $a_i^\nu\,b_i^\rho = 2\pi\delta_{\nu\rho}$, hence $2\pi R_{\mu\rho} = K_{ij}\,a_j^\mu\,b_i^\rho$. Now take the trace over the indices μ and ρ, again invoking Eqn. 5.3, to get $\mathsf{Tr}\,R = \mathsf{Tr}\,K$. Now the trace of any matrix is invariant under similarity transformation, and in $d = 3$ dimensions, and if $R = R(\xi,\hat{\boldsymbol{n}})$ we can always rotate $\hat{\boldsymbol{n}}$ so that it lies along $\hat{\boldsymbol{z}}$, in which case

$$S\,R(\xi,\hat{\boldsymbol{n}})\,S^{-1} = \begin{pmatrix} \cos\xi & -\sin\xi & 0 \\ \sin\xi & \cos\xi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \tag{5.13}$$

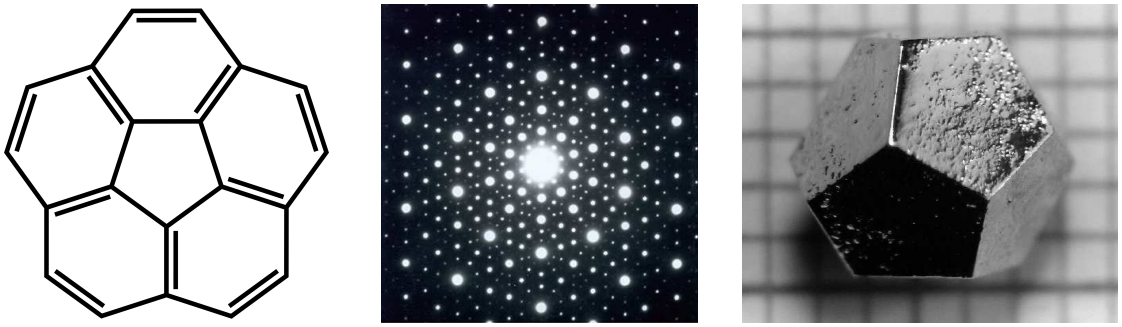


Figure 5.4: Left: Molecular structure of corannulene, $C_{20}H_{10}$. Center: Tenfold-symmetric diffraction pattern from a quasicrystalline alloy of aluminum, copper, and iron. Right: A Ho-Mg-Zn icosahedral quasicrystal forms a beautiful pentagonal dodecahedron (20 sites, 12 pentagonal faces, 30 edges, 3-fold coordinated), a structure dual to the icosahedron (12 sites, 20 triangular faces, 30 edges, 5-fold coordinated). Image credits: Wikipedia.

in which case $\mathrm{Tr}\, R = 2\cos\xi + 1$. In $d = 2$ we have $\mathrm{Tr}\, R = 2\cos\xi$ for proper rotations. Thus, $\mathrm{Tr}\, R \in \mathbb{Z}$ is possible only for $\xi = 2\pi/n$ where $n = 1$, 2, 3, 4, or 6. Fivefold, sevenfold, *etc.* symmetries are forbidden! Note that it is perfectly possible to have a fivefold symmetric molecule, such as $C_{20}H_{10}$, also known as corannulene. But when we insist on having both rotational as well as translational symmetries, the former are strongly restricted. Remarkably, there exists a family of three-dimensional structures, called *quasicrystals*, which exhibit forbidden fivefold or tenfold rotational symmetries. They elude the restriction theorem by virtue of not being true crystals, *i.e.* they are *quasi*periodic structures. See Fig. 5.4.

The result $\mathrm{Tr}\, R = \mathrm{Tr}\, K \in \mathbb{Z}$ is valid in all dimensions and does impose restrictions on the possible rotational symmetries. However, rotations in higher dimensions are in general not planar. Consider that it takes $d-1$ angles to specify an axis in d dimensions, but the dimension of $\mathsf{SO}(d)$ is $\frac{1}{2}d(d-1)$, so an additional $\frac{1}{2}(d-1)(d-2)$ parameters in addition to specifying an axis are required to fix an element of $\mathsf{SO}(d)$. For example, the four-dimensional F_4 lattice is a generalization of the three-dimensional bcc structure, consisting of two interpenetrating four-dimensional hypercubic lattices, and exhibits 12-fold rotational symmetries.

5.1.4 Enumeration of two and three-dimensional Bravais lattices

The complete classification of two and three Bravais lattices is as follows[4]. In two dimensions, there are four *lattice systems*: square, oblique, hexagonal, and rectangular. Of these, the rectangular system supports a subvariety called center rectangular, resulting in a total of five distinct two-dimensional Bravais lattices, shown in Fig. 5.5.

In three dimensions, there are seven lattice systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic[5]. Of these, monoclinic supports two subvarieties or *types* (simple and base-

[4]To reinforce one's memory, there is even a song: https://ww3.haverford.edu/physics/songs/bravais.htm.

[5]The systematic enumeration of three-dimensional lattices based on symmetry was first done by M. L. Frankenheim in 1842. Frankenheim correctly found there were 32 distinct crystal classes, corresponding to the 32 distinct three-dimensional point

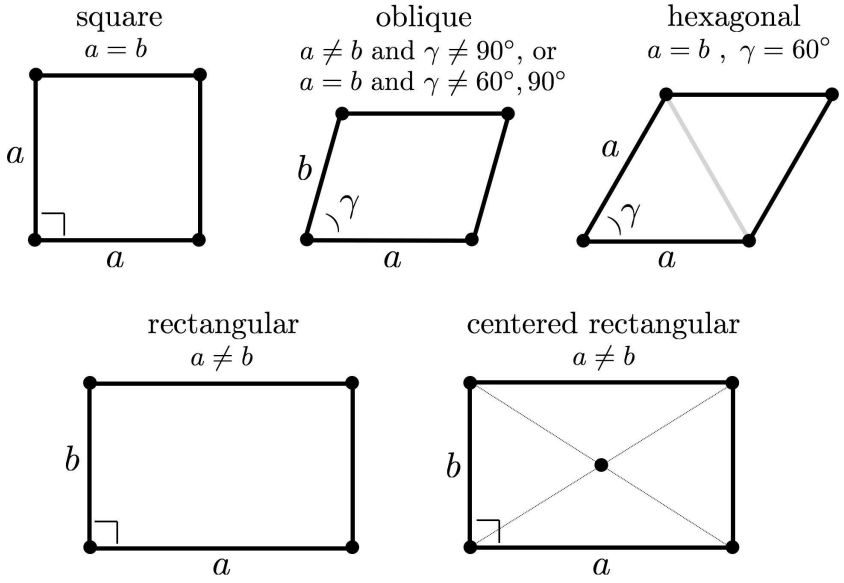


Figure 5.5: The five two-dimensional Bravais lattices.

centered), orthorhombic four subvarieties (simple, base-centered, body-centered, and face-centered), and cubic three subvarieties (simple, face-centered, and body-centered), amounting to a grand total of 14 three-dimensional Bravais lattices:

(i) *Cubic* : this system is the most symmetric, with symmetry group $O_h \cong S_4 \times \mathbb{Z}_2$, which has 48 elements[6]. The $\mathbb{Z}_2$ factor arises from the *inversion* symmetry exhibited by all Bravais lattices. Recall inversion takes (x, y, z) to $(-x, -y, -z)$. The three cubic subvarieties (simple, body-centered, and face-centered) are depicted in the first three panels of 5.6.

(ii) *Tetragonal* : Lowering the cubic symmetry by stretching or compressing along one of the axes, one arrives at the tetragonal system, whose unit cell is a cubic rectangle with side lengths $a = b \neq c$. There are two sub-varieties: simple and body-centered, depicted in the left two panels of Fig. 5.8. Why is there not a face-centered subvariety as well? Because it is equivalent to the body-centered case[7]. The symmetry group is $D_{4h} \cong \mathbb{Z}_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$.

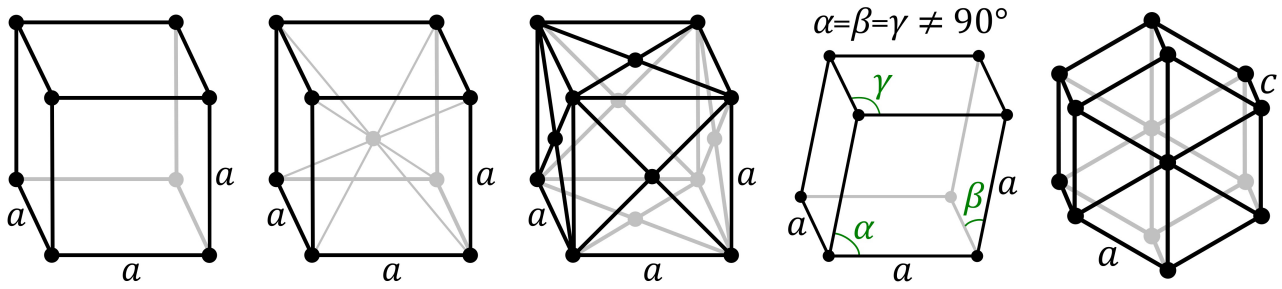
(iii) *Orthorhombic* : Further lowering the symmetry by stretching or compressing in along a second axis, we obtain the orthorhombic system. The only rotational symmetries are the three perpendicular mirror planes bisecting each of the unit cell sides, resulting in a $D_{2h} = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. There are four subvarieties, depicted in Fig. 5.7: simple, base-centered, body-centered, and face-centered.

(iv) *Monoclinic* : Take an orthorhombic lattice and shear it so that the c-axis is no longer along $\hat{\boldsymbol{z}}$, but lies in the (y, z) plane at an angle $\beta \neq 90°$ with respect to the horizontal. There are two distinct

groups, but he erred in counting 15 rather than 14 distinct lattices. A. L. Bravais, in 1845, was the first to get to 14, and for this he was immortalized. The identity of Frankenheim's spurious 15th lattice remains unclear.

[6]Why is the symmetry group of the cube called O (or O_h with inversion)? Because the cube and the octahedron have the same symmetries. Hence O is sometimes called the octahedral group.

[7]See Ashcroft and Mermin, *Solid State Physics*, pp. 116-118.



(a) sc (b) bcc (c) fcc (d) trigonal (e) hex

Figure 5.6: Simple cubic, body-centered cubic, face-centered cubic, trigonal, and hexagonal Bravais lattices. Image credits: Wikipedia.

subvarieties, simple and base-centered, which are shown in the third and fourth panels of Fig. 5.8. The only remaining symmetries are reflection in the (y, z) plane and inversion, hence the symmetry group is $\mathbb{Z}_2 \times \mathbb{Z}_2$.

(v) *Triclinic* : Shearing in a second direction, one obtains the triclinic system, depicted in the right panel of Fig. 5.8. At least two of the angles $\vartheta_{ij} = \cos^{-1}(\hat{\boldsymbol{a}}_i \cdot \hat{\boldsymbol{a}}_j)$ are not $90°$, and all the axes are of unequal lengths. The only remaining symmetry is inversion, so the symmetry group is $\mathbb{Z}_2$.

(vi) *Trigonal* : Starting with the cubic system, rather than squashing it along one of its three orthogonal axes, imagine stretching it along the cube's diagonal. The resulting Bravais lattice is generated by three nonorthogonal primitive vectors which make the same angle with respect to one another, as depicted in the fourth panel of Fig. 5.6. The stretched cube diagonal becomes a threefold axis, and the symmetry group is D_{3d}, which is of order 12.

(vii) *Hexagonal* : Finally, we come to the hexagonal system, which is unrelated to the cube. The simple hexagonal lattice, depicted in the last panel of Fig. 5.6, is its only representative. Two of the primitive direct lattice vectors are of equal length a and subtend a relative angle of $60°$ or $120°$. The third lies perpendicular to the plane defined by the first two, with an independent length c. The symmetry group is D_{6h}, which has 24 elements.

5.1.5 Crystals

A Bravais lattice is a tiling of space with empty unit cells. We are in the position of a painter staring at a beautifully symmetric but otherwise empty canvas. The art with which we fill our canvas is the *crystalline unit cell*, and it consists of a number r of atoms or ions, where ions of species j are located at positions $\boldsymbol{\delta}_j$ relative to any given direct lattice point $\boldsymbol{R}$, with $j \in \{1, \ldots, r\}$. If the direct lattice points $\boldsymbol{R}$ themselves represent the positions of a class of ion, we write $\boldsymbol{\delta}_1 \equiv 0$. The set of vectors $\{\boldsymbol{\delta}_j\}$ is called a *basis*, and without loss of generality, we restrict the basis vectors so they do not lie outside the unit cell.

⋆ *In a crystal, ions of species j are located at positions $\boldsymbol{R} + \boldsymbol{\delta}_j$, where $\boldsymbol{R}$ is a Bravais lattice vector and $\boldsymbol{\delta}_j$ is a basis vector. All basis vectors are taken to lie within a single unit cell of the Bravais lattice.*

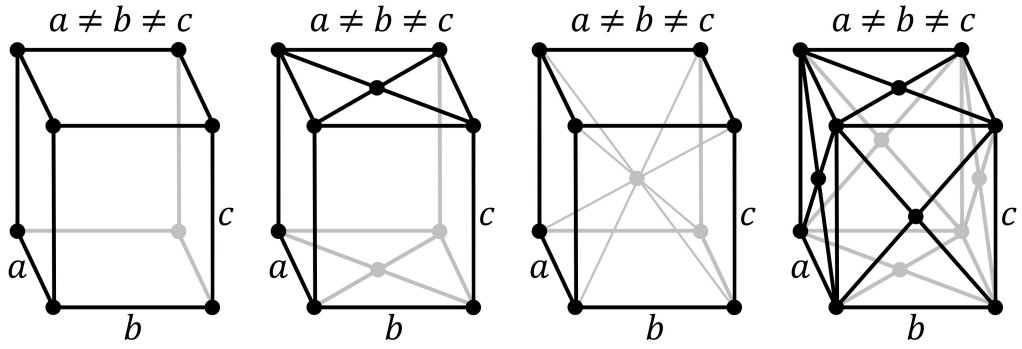


Figure 5.7: (Simple orthorhombic, base-centered orthorhombic, body-centered orthorhombic, and face-centered orthorhombic Bravais lattices. Image credits: Wikipedia.

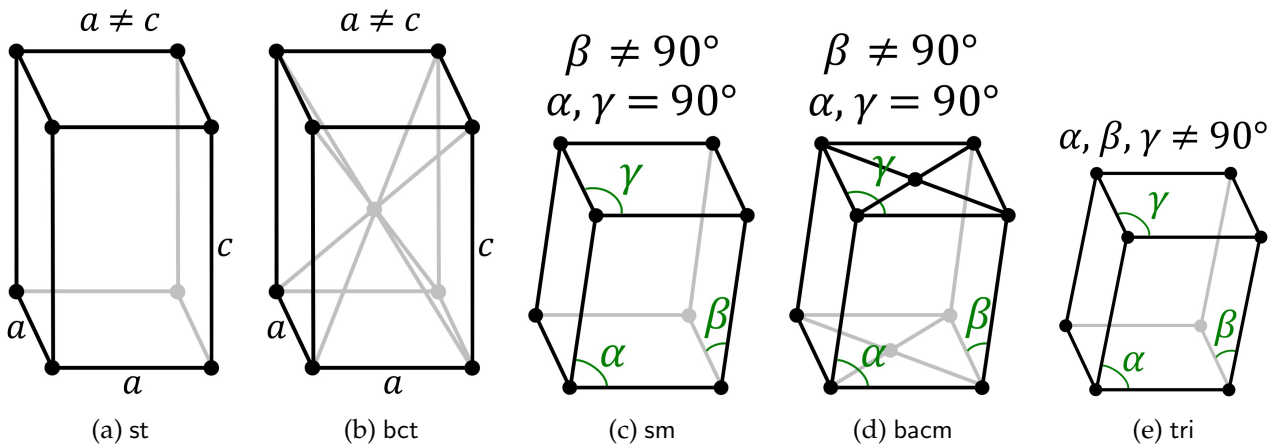


Figure 5.8: Simple tetragonal, body-centered tetragonal, monoclinic, base-centered monoclinic, and triclinic Bravais lattices. Image credits: Wikipedia.

Obviously the existence of a basis, unless it is one of spherical symmetry with respect to each Bravais lattice point, will have consequences for the allowed rotational symmetries of the crystal, in general reducing them to a subgroup of the symmetry group of the Bravais lattice itself. A vivid illustration of this is provided in Fig. 5.9 for the cubic lattice. When our canvas is completely blank, the cube is entirely white, and the symmetry group is O_h, with 48 elements, as shown in the middle bottom panel of the figure. If one of the reflection generators is broken, but all other generators are preserved, the symmetry is reduced from O_h to O, which has 24 elements. By breaking different symmetry operations, O_h can be reduced to the tetrahedral groups T_d and T_h, which also have 24 elements. Finally, each of O, T_d, and T_h may be broken down to the 12 element tetrahedral group T, depicted in the upper left panel. It all depends on how we paint the canvas.

As an example of a filled canvas, consider Fig. 5.10, which shows the unit cells of four high temperature cuprate superconductors. It is a good exercise to verify the stoichiometry in at least one example. Consider the unit cell for LSCO. The blue Cu ions at the top and bottom of the cell are each shared by eight

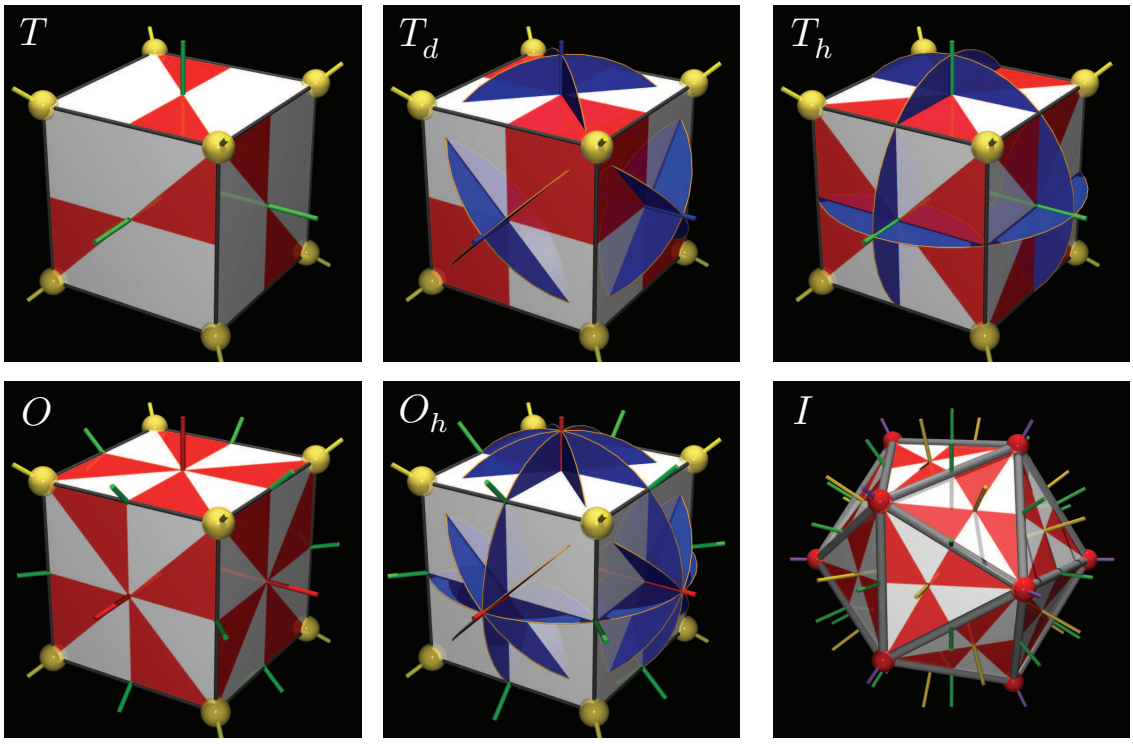


Figure 5.9: Tetrahedral, cubic, and icosahedral group symmetry operations. Twofold, threefold, fourfold, and sixfold axes are shown. The blue fins extend into discs, slicing the cube in two along reflection planes. Image credits: http://azufre.quimica.uniovi.es/d-MolSym/.

of these cubic rectangular cells, so the eight Cu ions at the corners amount to one per cell. The Cu ion in the center belongs completely to this cell, so we have a total of two Cu per cell. Each of the eight green La/Sr ions lying along the vertical columns at the cell edges is shared by four cells, so they amount to a total of two per cell. The two La/Sr ions within the cell toward the top and bottom each count as one, for a total of four La/Sr per cell. Lastly, we come to the oxygen ions, shown in red. Each of the O ions along any of the 12 edges of the cell is shared by four cells. There are 16 such O sites, thus accounting for four O per cell. If you think about the periodic repetition of the cell, you should realize that each Cu ion is surrounded by six O ions arranged in an octahedron. There is also such an octahedron in the center of the cell, on which we now focus. Two of its O ions are displaced vertically with respect to the central Cu ion, and are therefore wholly part of our cell. The other four each lie in the center of a face, and are each shared by two cells. Thus, this central octahedron accounts for an additional four O ions, for a grand total of 8 per cell. Our final tally: two Cu, four La/Sr, and eight O per cell, which is to say $La_{2-x}Sr_xCuO_4$. In the three other compounds, the oxygen stoichiometry is given as $4+\delta$ (Hg1201) or $6+\delta$ (YBCO and Ti2201). The deviation of δ from an integer value (either 0 or 1) accounts for the presence of oxygen vacancies[8].

In an electron diffraction experiment, an incident beam of electrons with wavevector $\boldsymbol{q}$ is scattered from a crystal, and the scattering intensity $I(\boldsymbol{k})$ as a function of the *wavevector transfer* $\boldsymbol{k} = \boldsymbol{q}' - \boldsymbol{q}$ is measured.

[8]It is a good exercise to determine the stoichiometry of these compounds based on the figures.

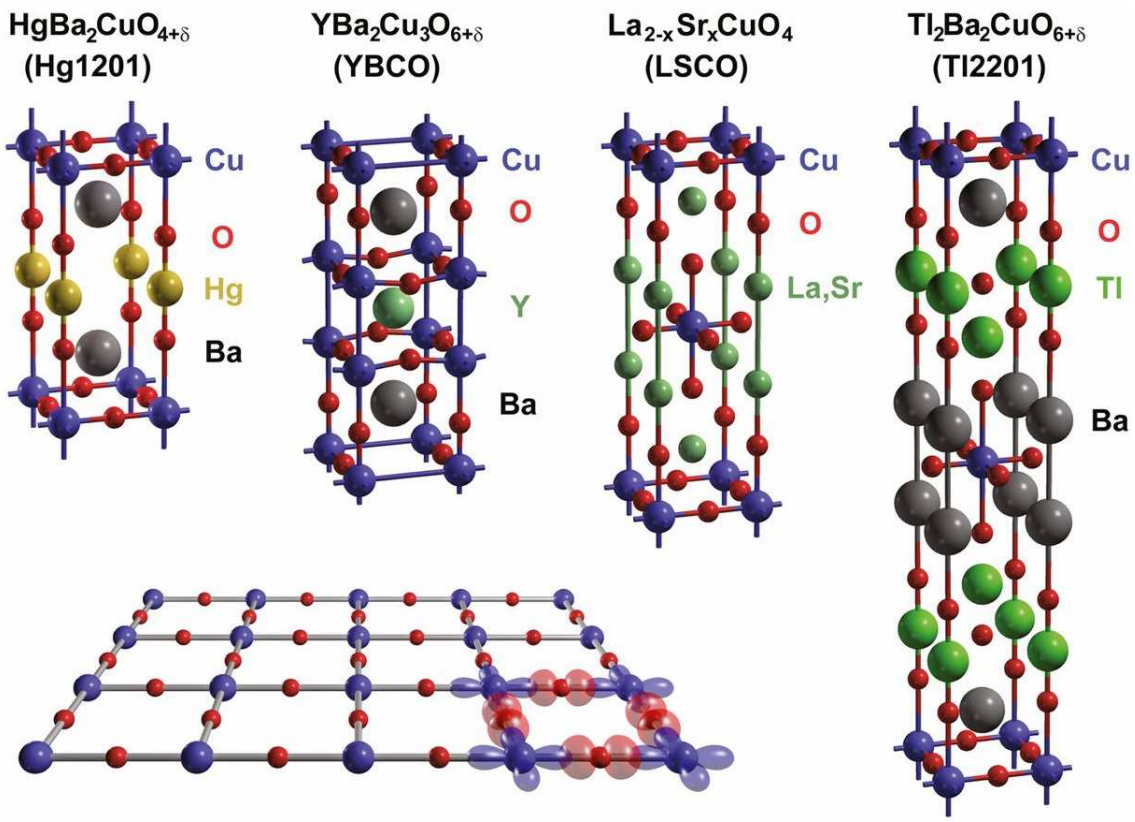


Figure 5.10: Unit cells of four high temperature cuprate superconductors. Lower left shows a sketch of the active electronic orbitals in the Cu-O planes. Image credit: N. Barišić *et al.*, *Proc. Nat. Acad. Sci.* **110**, 12235 (2013).

If the scattering is elastic, $|\boldsymbol{q}'| = |\boldsymbol{q}|$, which means k is related to the scattering angle $\vartheta = \cos^{-1}(\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{q}}')$ by $k = 2q\sin(\frac{1}{2}\vartheta)$. Let us model the $T = 0$ density[9] of the crystal $\rho(\boldsymbol{r})$ as

$$\rho(\boldsymbol{r}) = \sum_{\boldsymbol{R}} \sum_{j} c_j \, \delta(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\delta}_j) \quad , \tag{5.14}$$

where c_j is the weight for ionic species j. The total scattering intensity $I(\boldsymbol{k})$ is proportional to $|\hat{\rho}(\boldsymbol{k})|^2/N$, where $\hat{\rho}(\boldsymbol{k})$ is the Fourier transform of $\rho(\boldsymbol{r})$ and N is the total number of unit cells in the crystal. Choosing units where the prefactor is unity, we have

$$\begin{aligned} I(\boldsymbol{k}) &= \frac{1}{N}\left|\hat{\rho}(\boldsymbol{k})\right|^2 = \frac{1}{N}\sum_{\boldsymbol{R},\boldsymbol{R}'} e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} \sum_{j,j'} c_j \, c_{j'} \, e^{-i\boldsymbol{k}\cdot(\boldsymbol{\delta}_j - \boldsymbol{\delta}_{j'})} \\ &= F(\boldsymbol{k}) \sum_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} = \hat{\Omega} \sum_{\boldsymbol{K}} F(\boldsymbol{K}) \, \delta(\boldsymbol{k} - \boldsymbol{K}) \quad , \end{aligned} \tag{5.15}$$

where we have invoked the Poisson summation formula of Eqn. 5.7, and where we have defined the

[9] What matters for electron diffraction is the electron density.

form factor

$$F(\boldsymbol{K}) = \left| \sum_{j=1}^{r} c_j \, e^{-i\boldsymbol{K}\cdot\boldsymbol{\delta}_j} \right|^2 \quad . \tag{5.16}$$

Thus we expect δ-function *Bragg peaks* in the scattering intensity at values of the wavevector transfer equal to any reciprocal lattice vector $\boldsymbol{K}$. The form factor $F(\boldsymbol{K})$ modifies the intensity and can even lead to systematic *extinctions* of certain reciprocal lattice vectors. Consider, for example, a one-dimensional lattice with lattice spacing a and basis elements $\delta_1 = 0$ and $\delta_2 = \frac{1}{2}a$. If $c_1 = c_2 \equiv c$, the form factor is

$$F(K) = |c|^2 \left|1 + e^{iKa/2}\right|^2 \quad . \tag{5.17}$$

This vanishes for $K = 2\pi j/a$ whenever j is odd. So the lesson here is that the $T = 0$ scattering intensity from a crystal is given by a sum of δ-functions and is singular whenever the wavevector transfer is equal to a reciprocal lattice vector. The presence of a basis modifies each Bragg peak by the form factor $F(\boldsymbol{K})$, which in some cases can even extinguish the peak completely[10].

5.1.6 Trigonal crystal system

While the trigonal point group D_{3d} is a normal subgroup of the hexagonal point group D_{6h}, the trigonal Bravais lattice does not result from an infinitesimal distortion of the simple hexagonal lattice. Contrast this situation with that for, *e.g.*, tetragonal *vis-a-vis* cubic, where a tetragonal lattice is obtained by an infinitesimal stretching along one of the principal axes of the cubic lattice. Any trigonal lattice, however, can be expressed as a hexagonal lattice with a three element basis. To see this, define the vectors

$$\boldsymbol{s}_1 = \tfrac{1}{\sqrt{3}}\, a\big(\tfrac{\sqrt{3}}{2}\,\hat{\boldsymbol{x}} - \tfrac{1}{2}\hat{\boldsymbol{y}}\big) \quad , \quad \boldsymbol{s}_2 = \tfrac{1}{\sqrt{3}}\, a\hat{\boldsymbol{y}} \quad , \quad \boldsymbol{s}_3 = \tfrac{1}{\sqrt{3}}\, a\big(-\tfrac{\sqrt{3}}{2}\,\hat{\boldsymbol{x}} - \tfrac{1}{2}\hat{\boldsymbol{y}}\big) \quad . \tag{5.18}$$

Then $\boldsymbol{a}_1 \equiv \boldsymbol{s}_1 - \boldsymbol{s}_3 = a\hat{\boldsymbol{x}}$ and $\boldsymbol{a}_2 \equiv \boldsymbol{s}_2 - \boldsymbol{s}_3 = a\big(\frac{1}{2}\hat{\boldsymbol{x}} + \frac{\sqrt{3}}{2}\hat{\boldsymbol{y}}\big)$ are primitive DLVs for a two-dimensional hexagonal lattice. The vectors $\boldsymbol{d}_j \equiv \boldsymbol{s}_j + \frac{1}{3}\,c\hat{\boldsymbol{z}}$ for $j = 1, 2, 3$ then constitute three primitive DLVs for the trigonal lattice, each of length $d = \frac{1}{3}\sqrt{3a^2 + c^2}$. They also correspond to a three element basis within the first Wigner-Seitz cell of the simple hexagonal lattice. Conventionally, and equivalently, the three element basis may be taken to be $\boldsymbol{\delta}_1 = 0$, $\frac{1}{3}\boldsymbol{a}_1 + \frac{1}{3}\boldsymbol{a}_2 + \frac{1}{3}c\hat{\boldsymbol{z}}$, and $\frac{2}{3}\boldsymbol{a}_1 + \frac{2}{3}\boldsymbol{a}_3 + \frac{2}{3}c\hat{\boldsymbol{z}}$, all of which are associated with the hexagonal unit cell spanned by vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $c\hat{\boldsymbol{z}}$. Note that this is not a Wigner-Seitz cell, and its projection onto the (x, y) plane is a rhombus rather than a hexagon. Although describing the trigonal Bravais lattice as a hexagonal Bravais lattice with a three element basis might seem an unnecessary complication, in fact it proves to be quite convenient because two pairs of axes in the hexagonal system are orthogonal. Similarly, it is convenient to describe the bcc and fcc cubic lattices as simple cubic with a two and four element basis, respectively, to take advantage of the mutually orthogonal primitive direct lattice vectors of the simple cubic structure.

[10] It is a good exercise to compute $I(\boldsymbol{k})$ for the bcc and fcc structures when they are described in terms of a simple cubic lattice with a two or four element basis. The resulting extinctions limit the Bragg peaks to those wavevectors which are in the bcc or fcc reciprocal lattice.

CRYSTALLOGRAPHY	$d = 2$	$d = 3$
systems	4	7
lattices	5	14
point groups	10	32
space groups	17	230
symmorphic	13	73
non-symmorphic	4	157

Table 5.1: True Facts about two and three-dimensional crystallography.

5.1.7 Point groups, space groups and site groups

A group $\mathcal{P} \subset \mathsf{O}(3)$ of symmetry operations of a structure which leaves one point fixed is known as a *point group*[11]. The point group $\mathcal{P}_{\mathcal{L}}$ of a Bravais lattice is the group of rotational symmetries which fix any of the the Bravais lattice sites. This group is shared by all lattices in the same lattice system, and is known as the *holohedry* of the lattice.

In crystals, not every lattice site is equivalent. This may be due to the fact that different ions occupy different sites, but it is also the case for certain monatomic crystals, such as diamond, which consists of two interpenetrating fcc lattices that are not related by Bravais lattice translation. That is, the diamond structure is an fcc Bravais lattice with a two element basis. The full symmetry group of a crystal consists of both rotations and translations and is called the *space group* $\mathcal{S}$. A space group is a subgroup of the Euclidean group: $\mathcal{S} \subset \mathsf{E}(3)$, and a general space group operation $\{\, g \,|\, \boldsymbol{t} \,\}$ acts as

$$\{\, g \,|\, \boldsymbol{t} \,\}\, \boldsymbol{r} = g\, \boldsymbol{r} + \boldsymbol{t} \quad , \tag{5.19}$$

where $g \in \mathsf{O}(3)$. The identity element in $\mathcal{S}$ is $\{\, E \,|\, 0 \,\}$, where E is the identity in $\mathsf{O}(3)$, and the inverse is given by

$$\{\, g \,|\, \boldsymbol{t} \,\}^{-1} = \{\, g^{-1} \,|\, -g^{-1}\boldsymbol{t} \,\} \quad . \tag{5.20}$$

In order that $\mathcal{S}$ be a group, we must have that

$$\begin{aligned} \{\, g_2 \,|\, \boldsymbol{t}_2 \,\}\{\, g_1 \,|\, \boldsymbol{t}_1 \,\}\, \boldsymbol{r} &= \{\, g_2 \,|\, \boldsymbol{t}_2 \,\}(g_1\, \boldsymbol{r} + \boldsymbol{t}_1) \\ &= g_2\, g_1\, \boldsymbol{r} + g_2\, \boldsymbol{t}_1 + \boldsymbol{t}_2 = \{\, g_2\, g_1 \,|\, g_2\, \boldsymbol{t}_1 + \boldsymbol{t}_2 \,\}\, \boldsymbol{r} \quad , \end{aligned} \tag{5.21}$$

is also in $\mathcal{S}$. This requires that the matrices g themselves form a group, called the *crystallographic point group* $\mathcal{P}$. For a Bravais lattice, $\mathcal{P} = \mathcal{P}_{\mathcal{L}}$, but in general a crystal is of lower symmetry than its underlying Bravais lattice, and the crystallographic point group is a subgroup of the holohedry: $\mathcal{P} \subset \mathcal{P}_{\mathcal{L}}$. Note that $\mathcal{S} \not\equiv \mathcal{P} \times \mathcal{T}$, *i.e.* the space group is not simply a direct product of the point group and the translation group, because multiplication of $(g, \boldsymbol{t}) \in \mathcal{P} \times \mathcal{T}$ satisfies $(g_2, \boldsymbol{t}_2)\,(g_1, \boldsymbol{t}_1) = (g_2\, g_1, \boldsymbol{t}_2 + \boldsymbol{t}_1)$. The abelian group $\mathcal{T} \cong \mathbb{Z}^d$ of Bravais lattice translations $\{\, E \,|\, \boldsymbol{R} \,\}$ forms an invariant subgroup of $\mathcal{S}$. If all the symmetry operations of a particular crystal can be written as $\{\, g \,|\, \boldsymbol{R} \,\}$, the crystal's space group is then said to be

[11] Mathy McMathstein says that a point group is a group of *linear isometries* which have a common fixed point. An isometry is a distance-preserving transformation on a metric space.

symmorphic and we write $\mathcal{S} = \mathcal{P} \rtimes \mathcal{T}$, where the symbol $\rtimes$ indicates a *semi-direct product* of two groups. *In a symmorphic crystal, one may choose an origin about which all point group symmetries are realized.*

However, it turns out that many crystals have space group elements $\{ g \,|\, \boldsymbol{t} \}$ where $g \in \mathcal{P}$ but $\boldsymbol{t} \notin \mathcal{T}$. Rather, for these symmetry operations, $\boldsymbol{t}$ is a fraction of a Bravais lattice translation. In some cases, with a different choice of origin, these operations can be expressed as a rotation followed by Bravais lattice translation[12]. For crystals with *nonsymmorphic* space groups, however, there is no possible choice of origin about which all elements of $\mathcal{S}$ can be decomposed into a point group operation followed by a Bravais lattice translation. Two examples are shown in Fig. 5.11: the three-dimensional hexagonal close packed (hcp) structure, and the two-dimensional Shastry-Sutherland lattice. An hcp crystal is a simple hexagonal lattice with a two element basis. It occurs commonly in nature and describes, for example, the low temperature high pressure phase of ^{4}He just above its melting curve (about 25 atmospheres at $T = 0\,\mathrm{K}$). The primitive direct lattice vectors of the hcp structure are

$$\boldsymbol{a}_1 = \big(\tfrac{1}{2}\hat{\boldsymbol{x}} - \tfrac{\sqrt{3}}{2}\hat{\boldsymbol{y}}\big)a \quad , \quad \boldsymbol{a}_2 = \big(\tfrac{1}{2}\hat{\boldsymbol{x}} + \tfrac{\sqrt{3}}{2}\hat{\boldsymbol{y}}\big)a \quad , \quad \boldsymbol{a}_3 = c\hat{\boldsymbol{z}} \quad , \tag{5.22}$$

with $c = \sqrt{\frac{8}{3}}\,a$. The basis vectors are $\boldsymbol{\delta}_1 = 0$ and $\boldsymbol{\delta}_2 = \frac{1}{3}\boldsymbol{a}_1 + \frac{2}{3}\boldsymbol{a}_2 + \frac{1}{2}\boldsymbol{a}_3$. In the figure, A sublattice sites are depicted in red and B sublattice sites in blue. Note that the B sites lie in the centers of the up-triangles in each A sublattice plane, and displaced by half a unit cell in the $\hat{\boldsymbol{z}}$ diraction. The nonsymmorphic operation in the hcp point group is known as a *screw axis* and it involves a rotation by 60° about the $\hat{\boldsymbol{z}}$ axis through the centers of the A sublattice down triangles, followed by a translation by $\frac{1}{2}\boldsymbol{a}_3$.

The second example is that of the Shastry-Sutherland lattice, which describes the $CuBO_3$ layers in the magnetic compound $SrCu_2(BO_3)_2$. Here we have four sublattices, and the nonsymmorphic operation is known as a *glide mirror*, which involves translation along a plane (or a line in two dimensions) by a half unit cell, followed by a reflection in the plane. See if you can spot the nonsymmorphic symmetry.

A third example is that of diamond, which consists of two interpenetrating fcc lattices, and has a zincblende structure shown in Fig. 5.16. Diamond possesses both a fourfold (4_1) screw axis as well as a glide mirror. While the point group is O_h, there is no point in the diamond lattice about which all operations in O_h are realized. The maximum symmetry at any site is T_d.

In a symmorphic crystal, it is always possible to find some origin within the structural unit cell about which all point group symmetries are realized. In a Bravais lattice, this is true with respect to every lattice point, but obviously it is possible to choose an origin about which the group of rotational symmetries is reduced. For example, the point group of the square lattice is C_{4v}, but by choosing an origin in the center of one of the links the symmetry is reduced to C_{2v}. It is sometimes convenient to speak of the group of rotational symmetries with respect to a specific point $\boldsymbol{r}$ in the crystal structure. We call this the *site group* $\mathcal{P}(\boldsymbol{r})$. When $\boldsymbol{r} = \boldsymbol{R} + \boldsymbol{\delta}_j$ is a site in the crystal, *i.e.* a location of one of the ions, we may denote the site group as $\mathcal{P}(\boldsymbol{R}, j)$.

In a nonsymmorphic crystal, in general *no* sites will realize the symmetry of the point group $\mathcal{P}$. Consider, for example, the Shastry-Sutherland lattice in Fig. 5.11. Choosing the origin as the center of the magenta square unit cell, the site group is $\mathcal{P}(\boldsymbol{0}) = C_{2v}$. But the crystallographic point group for this structure is

[12] In such cases, the putative nonsymmorphic operation is called *removable*. Otherwise, the nonsymmorphic operation is *essential*.

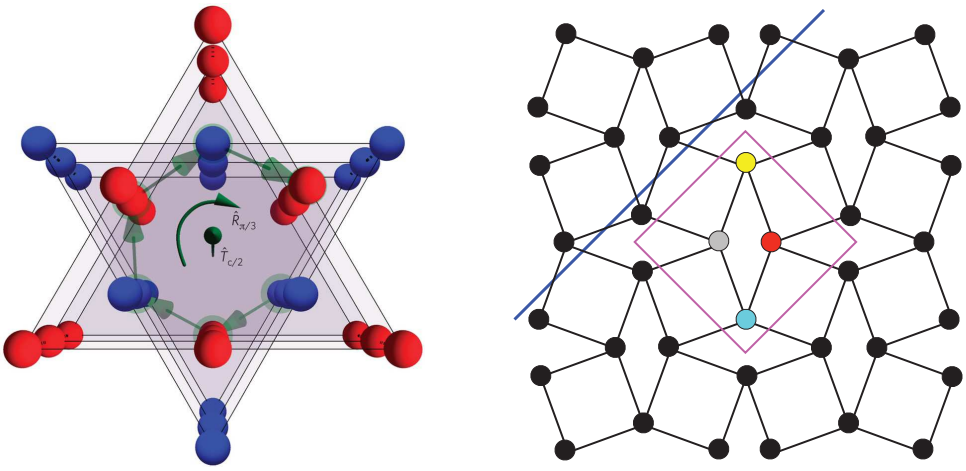


Figure 5.11: Two nonsymmorphic crystal lattices. Left: The hexagonal close packed lattice (space group $P6_3/mmc$) has a two site unit cell (red and blue) and a screw axis symmetry, given by a rotation by 60° followed by a translation of $\frac{1}{2}\boldsymbol{a}_3$ along the c-axis. The underlying Bravais lattice is simple hexagonal. Right: The Shastry-Sutherland lattice (space group $p4g$) has a four site unit cell (shown in center) and a glide mirror (blue line). Translation by half a unit cell along the mirror line followed by a mirror reflection is a lattice symmetry. The underlying Bravais lattice is square.

C_{4v}. Since $\mathcal{P}$ is the group of all rotational symmetries about all possible origins, necessarily $\mathcal{P}(\boldsymbol{r}) \subset \mathcal{P}$ for all sites $\boldsymbol{r}$.

Our crystallographer forbears have precisely tabulated for us all the possible lattices, point groups, and space groups in two and three dimensions (see Tab. 5.1). Proving these results is quite tedious, so we shall be content to take them as received wisdom. Note that a bit more than two thirds (157 out of 230) of the three-dimensional space groups are nonsymmorphic. Of those, all but two involve either a screw axis or a glide plane[13].

5.2 More on Point Groups

5.2.1 Standard notation for point group operations

A list of point group operations is provided in Tab. 5.2. We'll also start to use C_n to denote a group element, *i.e.* a rotation by $2\pi/n$ about a primary axis. If we need to distinguish this element from the cyclic group, which we've thus far also called C_n, we'll instead refer to the group as $\mathcal{C}_n$. Note that inversion can be written as $I = S_2$, and that I commutes with all elements of the point group $\mathcal{P}$, *i.e.* $I \in Z(\mathcal{P})$ is in the center of $\mathcal{P}$.

Any improper operation $g \in \mathsf{O}(3)$ has $\det(g) = -1$. This entails that g must have an eigenvalue $\lambda = -1$,

[13] Space groups no. 24 (also known as $I2_12_12_1$) and no. 199 ($I2_13$) have removable screw axes, but nevertheless there is no single origin about which every symmetry operation can be expressed as $\{\, g \,|\, \boldsymbol{t} \,\}$ with $g \in \mathcal{P}$ and $\boldsymbol{t} \in \mathcal{T}$.

SYMBOL	OPERATION
E	identity
C_n	rotation through $2\pi/n$ about primary axis $\hat{\boldsymbol{n}}$; operator equivalent: $e^{-2\pi i \hat{\boldsymbol{n}}\cdot\boldsymbol{J}/n\hbar}$ where $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$
I	inversion ($\boldsymbol{r} \to -\boldsymbol{r}$) ; leaves spinor coordinates invariant and commutes with all other point group operations
σ	C_2 rotation followed by reflection in plane perpendicular to the axis of rotation ; equivalent to IC_2 or $C_2\, I$
σ_h	reflection in a 'horizontal' plane perpendicular to a primary axis
σ_v	reflection in a 'vertical' plane which contains a primary axis
σ_d	reflection in a 'diagonal' plane containing the primary axis of symmetry and which bisects the angle between neighboring twofold axes perpendicular to the primary axis
S_n	rotoreflection: $S_n = \sigma_h^{-1}\, C_n$, *i.e.* rotation by $2\pi/n$ followed by reflection in the plane perpendicular to that axis (note $I = S_2$)
$\bar{E}$	spinor rotation through 2π ; $\bar{E} = e^{-2\pi i \hat{\boldsymbol{n}}\cdot\boldsymbol{S}}$ ($S = \frac{1}{2}$) ; leaves spatial coordinates (x, y, z) invariant
$\bar{g}$	any point group operation g followed by $\bar{E}$

Table 5.2: Standard notation for point group operations.

and the corresponding eigenvector $\hat{\boldsymbol{m}}$, for which $g\hat{\boldsymbol{m}} = -\hat{\boldsymbol{m}}$, is known as a *reversal axis*. It also follows in all odd dimensions that if g is proper, *i.e.* if $\det(g) = +1$, then g has an eigenvalue $\lambda = +1$, and the corresponding eigenvector $\hat{\boldsymbol{n}}$ which satisfies $g\hat{\boldsymbol{n}} = \hat{\boldsymbol{n}}$ is an *invariant axis*. Improper elements of $\mathsf{O}(n)$ can be written as $Ig(\xi, \hat{\boldsymbol{n}})$, where I is the inversion operator. In even dimensions, the inversion I is equivalent to C_2, but one can form improper rotations via a reflection σ.

The rotoreflection operation is $S_n = \sigma_h^{-1}\, C_n = C_n\, \sigma_h^{-1}$. The reason we write σ_h^{-1} rather than σ_h has to do with what happens when we account for electron spin, in which case $\sigma_h^{-1} = \overline{E}\,\sigma_h$, where $\overline{E}$ is spinor reversal, *i.e.* rotation of the spinor component through 2π. Without spin, we have $\sigma_h^{-1} = \sigma_h$, and for n odd, one then has $(S_n)^n = \sigma_h$ and $(S_n)^{n+1} = C_n$, which says that if $S_n \in \mathcal{P}$ then so are both σ_h and C_n . If, on the other hand, n is even, this may not be the case.

5.2.2 Proper point groups

A proper point group $\mathcal{P}$ is a subgroup of $\mathsf{SO}(3)$[14]. The following are the proper point groups:

[14]Two-dimensional point groups are much simpler to classify as they always involve at most a single rotation axis and/or a planar reflection. They form a subset of the three-dimensional point groups.

(i) *Cyclic groups* : The cyclic group C_n (order n) describes n-fold rotations about a fixed axis. The restriction theorem limits crystallographic cyclic groups to the cases $n = 1, 2, 3, 4$, and 6. Again, molecules, which have no translational symmetries, are not limited by the restriction theorem.

(ii) *Dihedral groups* : The group D_n (order $2n$) has a primary n-fold axis and n twofold axes perpendicular to the primary axis. Note that if one started with only one such perpendicular twofold axis, the C_n operations would generate all the others. For n even, the alternating twofold axes break up into two conjugacy classes, whereas for n odd there is only one such class.

(iii) *Tetrahedral, octahedral, and icosahedral groups* : When there is more than one n-fold axis with $n > 2$, the rotations about either axis will generate new axes. Geometrically, this process run to its conclusion traces out a regular spherical polygon when one traces the intersections of the successively-generated axes on the unit sphere. There are only five possible such regular polyhedra: tetrahedron, cube, octahedron, dodecahedron, and icosahedron. The second two have the same symmetry operations, as do the last two, so there are only three such groups: T, O, and I.

(iiia) *Tetrahedral group* : T is the symmetry group of proper rotations of the tetrahedron. Embedding the tetrahedron in a cube, as in Fig. 5.12, there are three two-fold axes through the cube faces, plus four threefold axes through the cube diagonals, for a total of 12 operations including the identity. Note $T \cong A_4$, the alternating group on four symbols.

(iiib) *Octahedral group* : O consists of all the symmetry operations from T plus 12 more, arising from six new twofold axes running through the centers of each edge, not parallel to any face, and six more operations arising from extending the twofold axes through the faces to fourfold axes (see Fig. 5.9). So, 24 elements in all, shown in Fig. 5.12. Note $O \cong S_4$, the symmetric group on four symbols.

(iiic) *Icosahedral group* : I is the symmetry group of the dodecahedron or icosahedron. There are six fivefold axes, ten threefold axes, and 15 twofold axes, so including the identity there are $1 + 6 \cdot (5 - 1) + 10 \cdot (3 - 1) + 15 \cdot (2 - 1) = 60$ elements. We also have $I \cong A_5$, the alternating group on five symbols.

5.2.3 Commuting operations

The following operations commute:[15]

- Rotations about the same axis.
- Reflections in mutually perpendicular planes. In general the product of reflections in two planes which intersect at an angle α is $\sigma_v \, \sigma_{v'} = C(2\alpha)$, where the rotation is about the axis defined by their intersection line in the direction from the v' plane to the v plane. Thus $\sigma_{v'} = \sigma_v \, C(2\alpha)$.
- Rotations about perpendicular twofold axes: $C_2 \, C_2' = C_2' \, C_2 = C_2''$, where the resulting rotation is about the third perpendicular axis.
- A rotation C_n and a reflection σ_h in a plane perpendicular to the n-fold axis.

[15] See M. Lax, *Symmetry Principles in Solid State and Molecular Physics*, p. 54.

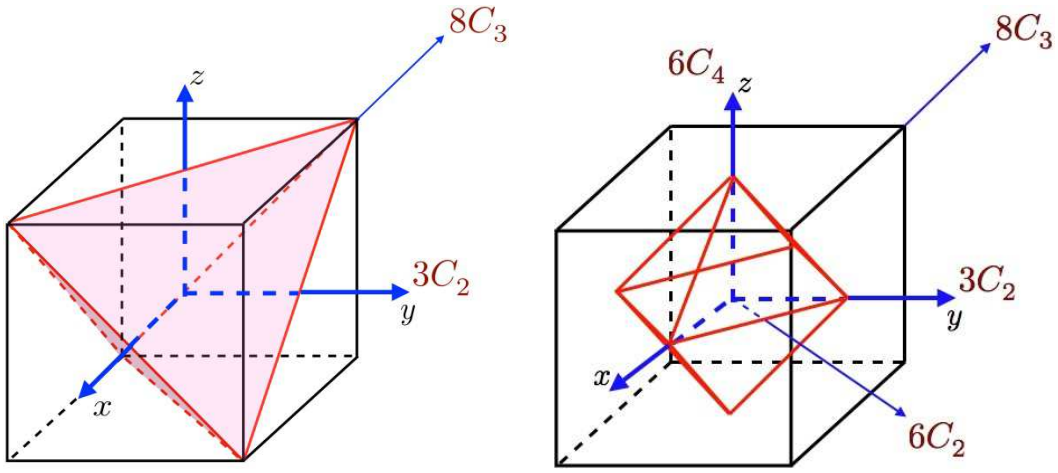


Figure 5.12: Left: Proper rotational symmetries of the tetrahedron, forming the group T. Right: Proper rotational symmetries of the octahedron (or cube), forming the group O.

- Inversion I and any point group operation g (with g a rotation relative to the inversion point)
- A twofold rotation C_2 and a reflection σ_v in a plane containing the rotation axis.

5.2.4 Improper point groups

First, some notation. Since we will start to use C_n to denote the generator of rotations about the primary axis, we'll write $\mathcal{C}_n$ to denote the cyclic group with n elements. Similarly we'll use $\mathcal{S}_{2n}$ to denote the rotoreflection group. In addition to the proper point group $\mathcal{C}_2 = \{E, C_2\} \cong \mathbb{Z}_2$, we will also define two improper $\mathbb{Z}_2$ clones: $\mathcal{C}_i = \{E, I\}$, containing the identity and the inversion operation, and $\mathcal{C}_s \equiv \{E, \sigma_h\}$ containing the identity and the horizontal reflection σ_h. All will play a role in our ensuing discussion.

In §2.10 of Lax, the relations between proper and improper point groups are crisply discussed. Suppose a group G contains both proper and improper elements. We write $G = H \cup M$ where $H \triangleleft G$ is a normal subgroup containing all the proper elements, and M, which is not a group (no identity!) contains all the improper elements. Let $m \in M$ be any of the improper operations. Then $mH = M$ since multiplying any proper element by an improper one yields an improper element, and we conclude that H and M contain the same number of elements. Thus $G \cong H \cup mH$ and only one improper generator is needed. Since the inversion operator commutes with all elements of $\mathsf{O}(3)$, we can always form an improper group which contains I by constructing $G = H \cup IH = H \otimes \mathcal{C}_i$. If $G = H \cup mH$ does not contain the inversion operator I, we can always form a *proper* group $\widetilde{G} = H \cup mIH$ which is isomorphic to G. Consider the case of the improper point group $G = \mathcal{C}_{3v}$, where $H = \mathcal{C}_3 = \left\{E\,,\, C_3\,,\, C_3^{-1}\right\}$ and $m = \sigma_v$ is a vertical reflection plane containing the threefold axis[16]. Then $\tilde{G} = D_3$, which is proper, and which is isomorphic to C_{3v}. Finally, if G is proper, and if it contains an index two subgroup, *i.e.* a subgroup $H \subset G$ such that $N_G = 2N_H$,

[16] Acting with C_3 generates the additional vertical reflections: $C_3\,\sigma_v = \sigma_{v'}$ and $C_3\,\sigma_{v'} = \sigma_{v''}$.

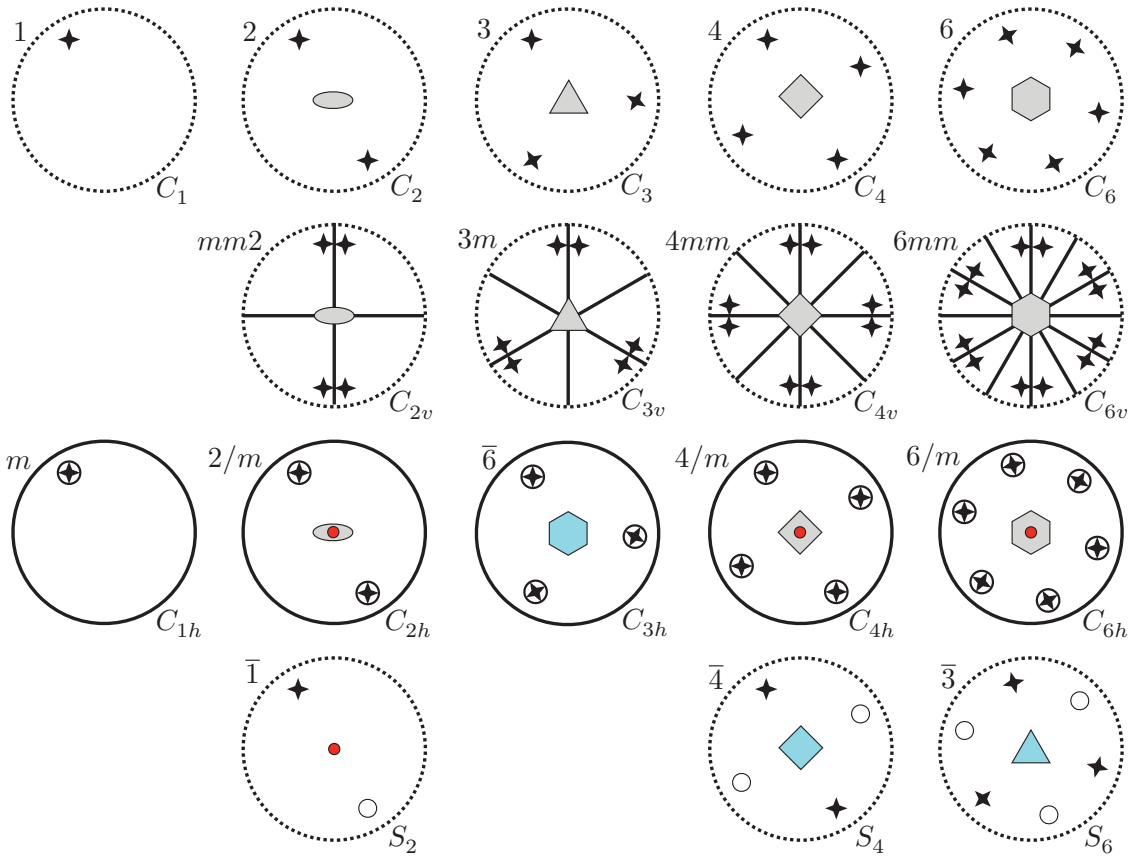


Figure 5.13: Stereographic projections of simple point groups C_n, C_{nv}, C_{nh}, and S_n. Dark lines correspond to reflection planes. C_{6v} looks like what I found the last time I sliced open a kiwi. Note $S_1 \cong C_{1h}$ and $S_3 \cong C_{3h}$. Adapted from Table 4.2 of M. Tinkham, *Group Theory and Quantum Mechanics*.

then we can construct $\tilde{G} = H \cup I\,(G \backslash H)$, where $G \backslash H$ is G with the elements from H removed. Then $\tilde{G}$ is an improper group with no inversion operation.

OK let's finally meet the improper point groups:

$\mathcal{S}_{2n}$: The rotoreflection group $\mathcal{S}_{2n}$ is a cyclic group of order $2n$ generated by $S_{2n} \equiv \sigma_h^{-1} C_{2n}$. In the absence of spin, $\sigma^{-1} = \sigma$ for any reflection. Then for n odd, $(S_{2n})^n = \sigma_h C_2 = I$, hence $\mathcal{S}_n \cong \mathcal{C}_n \otimes \mathcal{C}_i$.

$\mathcal{C}_{nh}$: The $2n$ element group $\mathcal{C}_{nh} \cong \mathcal{C}_n \otimes \mathcal{C}_s$ has two commuting generators, C_n and σ_h. For n odd, $\mathcal{C}_{nh}$ is cyclic and is generated by the single element $\sigma_h C_n$.

$\mathcal{C}_{nv}$: The $2n$ element group $\mathcal{C}_{nv}$ has two noncommuting generators, C_n and σ_v, where σ_v is a reflection in a plane containing the n-fold axis. Repeated application of C_n creates $(n-1)$ additional vertical reflection planes. One has $\mathcal{C}_{nv} \cong D_n$.

D_{nh} : Adding a horizontal reflection plane to D_n, one obtains $D_{nh} \cong D_n \otimes \mathcal{C}_s$. For n even, one also has $D_{nh} \cong D_n \otimes \mathcal{C}_i$. The group has $4n$ elements.

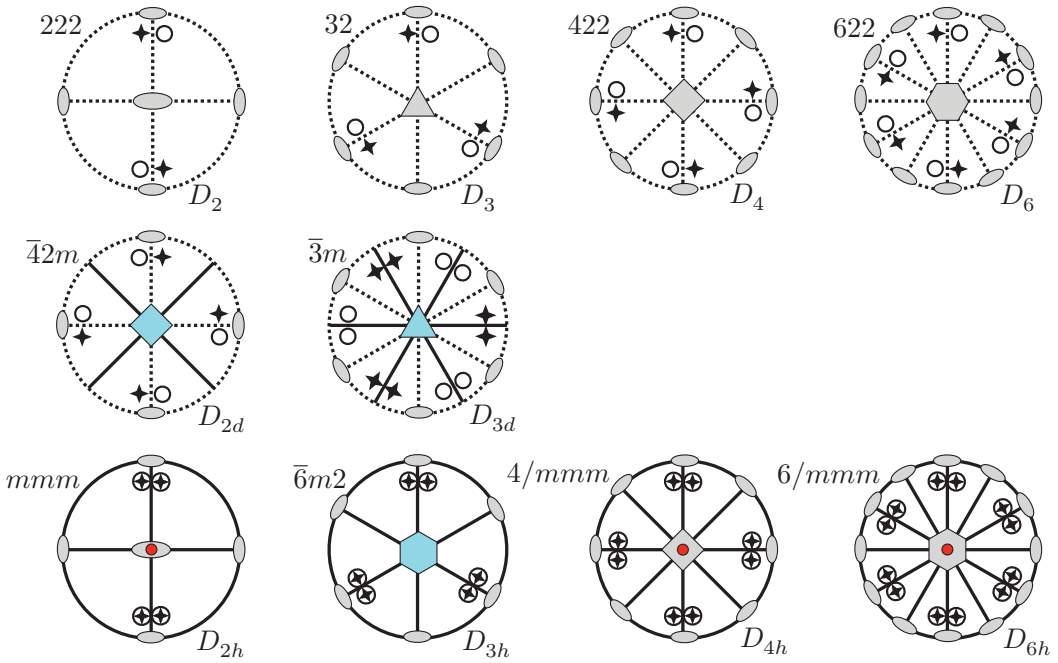


Figure 5.14: Stereograms of simple point groups D_n, D_{nd}, and D_{nh}. Dark lines correspond to reflection planes. Dashed lines correspond to 2-fold rotation axes. Adapted from Table 4.2 of M. Tinkham, *Group Theory and Quantum Mechanics*.

D_{nd} : If instead of adding a horizontal reflection σ_h we add a 'diagonal' reflection σ_d in a plane which bisects the angle between neighboring twofold axes, we arrive at D_{nd}, which also has $4n$ elements.

T_d : Adding a reflection plane passing through one of the edges of the tetrahedron, we double the size of the tetrahedral group from 12 to 24. In Fig. 5.12, such a reflection might permute the vertices 3 and 4. Thus while $T \cong A_4$, we have $T_d \cong S_4$.

T_h : Adding inversion to the proper rotational symmetries of the tetrahedron, we obtain $T_h \cong T \otimes \mathcal{C}_i$, which has 24 elements.

O_h : Adding inversion to the proper rotational symmetries of the cube, we obtain $O_h \cong O \otimes \mathcal{C}_i$, which has 48 elements.

I_h : Adding inversion to the proper rotational symmetries of the icosahedron, we obtain $I_h \cong I \otimes \mathcal{C}_i$, which has 60 elements.

Stereographic projections of the simple point groups are depicted in Figs. 5.13 and 5.14. The subgroup structure of the point groups, which tells us the hierarchy of symmetries, is shown in Fig. 5.17.

Why don't we consider the rotoreflection groups $\mathcal{S}_n$ for n odd? Because for n odd, $\mathcal{S}_n \cong C_{nh}$. For n odd, both S_n and S_{2n} generate cyclic groups of order $2n$. It is perhaps instructive to consider the simplest

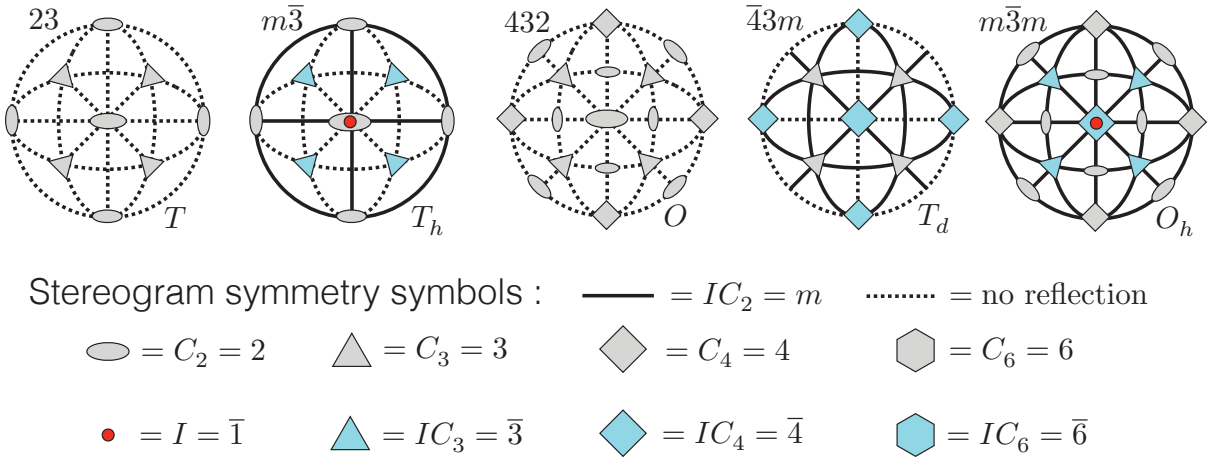


Figure 5.15: Stereograms of tetrahedral and cubic point groups and legend for symbols.

nontrivial case, $n = 3$:

$$\begin{aligned} \mathcal{S}_3 &= \{E\,,\,\sigma_h\,C_3\,,\,C_3^{-1}\,,\,\sigma_h\,,\,C_3\,,\,\sigma_h\,C_3^{-1}\} \\ \mathcal{S}_6 &= \{E\,,\,\sigma_h\,C_6\,,\,C_3\,,\,\sigma_h\,C_2\,,\,C_3^{-1}\,,\,\sigma_h\,C_6^{-1}\} \quad . \end{aligned} \tag{5.23}$$

We see that $\mathcal{C}_{3h}$, which is generated by the pair $(C_3\,,\,\sigma_h)$, contains the same elements as $\mathcal{S}_3$. This result holds for all odd n, because in those cases $\sigma_h \in \mathcal{S}_n$.

5.2.5 The ten two-dimensional point groups

There are ten two-dimensional point groups, listed in Tab. 5.3. As the only allowed elements are 2, 3, 4, and 6-fold rotations about the z-axis, plus vertical (line) mirrors, the only possible groups are C_1, C_2, C_3, C_4, C_6 and their mirrored extensions C_{1v}, C_{2v}, C_{3v}, C_{4v}, and C_{6v}. Note that the group C_{1v} is equivalent to C_{1h}, since in $d = 3$ both have a single reflection plane.

LATTICE SYSTEM	POINT GROUPS			
oblique	C_1	C_2		
rectangular	C_{1h}	C_{2v}		
centered rectangular	C_{1h}	C_{2v}		
square	C_4	C_{4v}		
hexagonal	C_3	C_{3v}	C_6	C_{6v}

Table 5.3: The ten two-dimensional point groups. Note $C_{1h} \cong C_{1v}$.

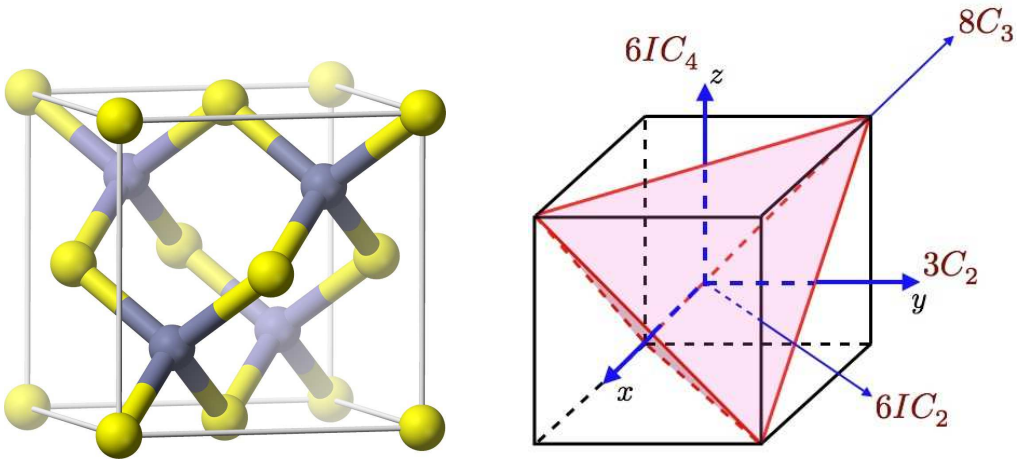


Figure 5.16: Left: The zincblende structure. Right: Proper and improper elements of the group T_d.

5.2.6 The achiral tetrahedral group, T_d

Many materials such as GaAs occur in an AB zincblende structure, which consists of two interpenetrating fcc lattices A and B, separated by $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$, where a is the side length of the cube; see Fig. 5.16. As the figure shows, the B sublattice sites within the cube form a tetrahedron. The crystallographic point group for this structure is T_d, the achiral tetrahedral group. A noteworthy feature is that the zincblende structure has no center of inversion symmetry, hence $I \notin T_d$.

If all the atoms are identical, *i.e.* A = B, then we get the diamond structure, which is the structure of silicon and of course carbon diamond. The diamond lattice is inversion symmetric, with the point of inversion halfway between the A and B sublattice sites. The point group for diamond is the cubic group O_h. This might be surprising upon staring at the structure for a time, because it doesn't possess a cubic symmetry. However, the space group for diamond is non-symmorphic – it has a glide plane.

The group T_d has 24 elements; these are listed in Tab. 5.5. Its character table is provided in Tab. 5.4. These are arranged in five group *classes*. One class is the identity, E. Another class consists of three $180°$

T_d	E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	−1	1
T_2	3	0	−1	1	−1

Table 5.4: Character table for the group T_d.

class	x	y	z	$g \in \mathsf{O}(3)$	class	x	y	z	$g \in \mathsf{O}(3)$
E	x	y	z	1	$6IC_2$	$-y$	$-x$	z	$IR_{[110]}(\pi) = \sigma_{(110)}$
$3C_2$	x	$-y$	$-z$	$R_{[100]}(\pi)$	$(6\sigma_d)$	y	x	z	$IR_{[1\bar{1}0]}(\pi) = \sigma_{(1\bar{1}0)}$
	$-x$	y	$-z$	$R_{[010]}(\pi)$		$-z$	y	$-x$	$IR_{[101]}(\pi) = \sigma_{(101)}$
	$-x$	$-y$	z	$R_{[001]}(\pi)$		z	y	x	$IR_{[10\bar{1}]}(\pi) = \sigma_{(10\bar{1})}$
$8C_3$	z	x	y	$R_{[111]}(+\frac{2\pi}{3})$		x	$-z$	$-y$	$IR_{[011]}(\pi) = \sigma_{(011)}$
	y	z	x	$R_{[111]}(-\frac{2\pi}{3})$		x	z	y	$IR_{[01\bar{1}]}(\pi) = \sigma_{(01\bar{1})}$
	z	$-x$	$-y$	$R_{[1\bar{1}1]}(+\frac{2\pi}{3})$	$6IC_4$	$-x$	z	$-y$	$IR_{[100]}(+\frac{\pi}{2}) = \sigma_{(100)}R_{[100]}(-\frac{\pi}{2})$
	$-y$	$-z$	x	$R_{[1\bar{1}1]}(-\frac{2\pi}{3})$	$(6S_4)$	$-x$	$-z$	y	$IR_{[100]}(-\frac{\pi}{2}) = \sigma_{(100)}R_{[100]}(+\frac{\pi}{2})$
	$-z$	x	$-y$	$R_{[11\bar{1}]}(+\frac{2\pi}{3})$		$-z$	$-y$	x	$IR_{[010]}(+\frac{\pi}{2}) = \sigma_{(010)}R_{[010]}(-\frac{\pi}{2})$
	y	$-z$	$-x$	$R_{[11\bar{1}]}(-\frac{2\pi}{3})$		z	$-y$	$-x$	$IR_{[010]}(-\frac{\pi}{2}) = \sigma_{(010)}R_{[010]}(+\frac{\pi}{2})$
	$-z$	$-x$	y	$R_{[1\bar{1}\bar{1}]}(+\frac{2\pi}{3})$		y	$-x$	$-z$	$IR_{[001]}(+\frac{\pi}{2}) = \sigma_{(001)}R_{[001]}(-\frac{\pi}{2})$
	$-y$	z	$-x$	$R_{[1\bar{1}\bar{1}]}(-\frac{2\pi}{3})$		$-y$	x	$-z$	$IR_{[001]}(-\frac{\pi}{2}) = \sigma_{(001)}R_{[001]}(+\frac{\pi}{2})$

Table 5.5: Table of elements and classes for T_d. Here $I\colon (x,y,z) \to (-x,-y,-z)$ is inversion and $\sigma_{(h,k,l)}$ is a reflection in the plane perpendicular to $h\hat{\boldsymbol{x}} + k\hat{\boldsymbol{y}} + l\hat{\boldsymbol{z}}$. For example $\sigma_{(110)}\colon (x,y,z) \to (-y,-x,z)$. Note that each fourfold rotoinversion can be expressed as a rotoreflection, *i.e.* $6IC_4 \cong 6S_4$, comprising a $\pm\frac{\pi}{2}$ rotation about one of the C_2 axes followed by a reflection in the plane perpendicular to that axis. Similarly, each twofold rotoinversion can be expressed as a reflection $6IC_2 \cong 6\sigma_d$ in one of the six diagonal mirror planes.

rotations about the $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ axes, respectively. A third class, with eight elements, consists of rotations by $\pm 120^\circ$ about each of the four body diagonals. This amounts to 12 group operations, all of which are proper rotations. The remaining 12 elements involve the inversion operator, I, which takes (x,y,z) to $(-x,-y,-z)$, and are therefore improper rotations, with determinant -1.[17] These elements fall into two classes, one of which consists of 180° rotations about diagonals parallel to one of the sides of the cube (*e.g.* the line $y = x$, $z = 0$), followed by inversion. The last class consists of rotations by $\pm\frac{\pi}{2}$ about $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$, also followed by an inversion, or, respectively, rotations by $\mp\frac{\pi}{2}$ about $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{x}}$ followed by a reflection in the plane perpendicular to the rotation axis.

Rotoreflections *versus* **rotoinversions**

In general every rotoinversion $IR(\hat{\boldsymbol{n}},\alpha)$ may be written as a rotoreflection $\sigma_{\hat{\boldsymbol{n}}}\,R(\hat{\boldsymbol{n}},-\alpha)$ where $\sigma_{\hat{\boldsymbol{n}}}$ is a reflection in the plane perpendicular to $\hat{\boldsymbol{n}}$. Both are improper rotations, *i.e.* elements $g \in \mathsf{O}(3)$ with $\det g = -1$. Distinguishing these operations is useful when there is a single preferred rotation axis[18].

[17] Note that I itself is not an element of T_d.

[18] I am grateful to Filipp Rybakov for encouraging me to clarify my thinking regarding rotoreflections *versus* rotoinversions, and for correcting some errors in Tab. 5.5.

Γ	d_Γ	basis functions ψ_μ^Γ for T_d	basis functions ψ_μ^Γ for O
A_1	1	$1 \quad \text{or} \quad xyz$	1
A_2	1	$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$	xyz
E	2	$\left\{\sqrt{3}\,(x^2-y^2)\,,\, 2z^2-x^2-y^2\right\}$	$\left\{\sqrt{3}\,(x^2-y^2)\,,\, 2z^2-x^2-y^2\right\}$
T_1	3	$\left\{x\,(y^2-z^2)\,,\, y\,(z^2-x^2)\,,\, z\,(x^2-y^2)\right\}$	$\left\{x\,,\ y\,,\ z\right\}$
T_2	3	$\left\{x\,,\, y\,,\, z\right\}$	$\left\{yz\,,\, zx\,,\, xy\right\}$

Table 5.6: Irreducible representations and basis functions for T_d and O.

5.2.7 Tetrahedral *vs.* octahedral symmetry

In the case of the octahedral group, O, the inversion operation is not included in the last two classes, and they are written as $6C_2$ and $6C_4$, respectively. The symmetry operations of O are depicted in fig. 5.12. The groups O and T_d are isomorphic. Both are *enantiomorphic* (*i.e.* chiral), and completing either of them by adding in the inversion operator I results in the full cubic group, O_h, which has 48 elements.

While the groups T_d and O are isomorphic, the symmetry of their basis functions in general differs. Consider, for example, the function $\psi = xyz$. It is easy to see from table 5.5 that every element of T_d leaves ψ invariant. Within O, however, the classes $6\sigma_d$ and $6S_4$ are replaced by $6C_2$ and $6C_4$ when the inversion operation is removed. Each element of these classes then takes ψ to $-\psi$. Thus, within T_d, the function $\psi = xyz$ is indistinguishable from unity, and it transforms according to the trivial A_1 representation. Within O, however, ψ is distinguishable from 1 because ψ reverses sign under the operation of all group elements in classes $6C_2$ and $6C_4$.

In O, the triplets of basis functions $\{x, y, z\}$ and $\{yz, zx, xy\}$ belong to different representations (T_1 and T_2, respectively). In T_d, however, they must belong to the same representation, since one set of functions is obtained from the other by dividing into xyz: $x = (xyz)/(yz)$, *et. cyc.* But xyz transforms as the identity, so 'polar' and 'axial' vectors belong to the same representation of T_d.

Finally, let's think about how O differs from O_h. Consider the function

$$\psi = xyz \cdot \left\{x^4\,(y^2-z^2) + y^4\,(z^2-x^2) + z^4\,(x^2-y^2)\right\}. \tag{5.24}$$

One can check that this function is left invariant by every element of O. It therefore transforms according to the A_1 representation of O. But it reverses sign under parity, so within the full cubic group O_h, it transforms according to separate one-dimensional representation. Note that ψ transforms according to the A_2 representation of T_d.

5.2.8 The 32 crystallographic point groups

Tab. 5.7 lists all possible point group symmetries for three-dimensional crystals. The largest possible symmetry group within a given lattice system is the rightmost point group, corresponding to the symmetry of the underlying Bravais lattice. The point groups may be classified as being *centrosymmetric* (*i.e.* including the inversion operation I), *non-centrosymmetric*, or *enantiomorphic*. A centrosymmetric crystal has an inversion center. Enantiomorphic structures are non-centrosymmetric; they have only rotation axes and include no improper operations. They are intrinsically chiral and not superposable on their mirror image. In addition, a point group may be *polar*, meaning every symmetry operation leaves more than one point fixed (*i.e.* those points along the high symmetry *polar axis*). Thus, a group with more than one axis of rotation or with a mirror plane which does not contain the primary axis cannot be polar. A polar axis is only possible in non-centrosymmetric structures. Ferroelectricity and piezoelectricity can only occur in polar crystals.

5.2.9 Hermann-Mauguin (international) notation

The notation with which we have thus far identified point groups and their operations (C_{nv}, T_d, σ_h, *etc.*) is named for the German mathematician A. M. Schoenflies (1853-1928). A more informative system, originally due to German crystallographer C. Hermann and subsequently improved by the French minerologist C.-V. Mauguin, goes by the name *Hermann-Mauguin* (HM) or *international* notation. Since most physics publications today use the international notation, we pause to review it and to explain the method to its madness.

HM notation is defined for both point groups as well as their elements. For the individual symmetry operations, the HM symbols are as follows:

LATTICE SYSTEM	POINT GROUPS						
cubic	T	T_d	T_h	O	O_h		
hexagonal	C_6^*	C_{3h}	C_{6h}	D_6	C_{6v}^*	D_{3h}	D_{6h}
trigonal	C_3^*	S_6	D_3	C_{3v}^*	D_{3d}		
tetragonal	C_4^*	S_4	C_{4h}	D_4	C_{4v}^*	D_{2d}	D_{4h}
orthorhombic	D_2	C_{2v}^*	D_{2h}				
monoclinic	C_2^*	C_s^*	C_{2h}				
triclinic	C_1^*	C_i					

Table 5.7: The 32 three-dimensional crystallographic point groups. Color scheme: centrosymmetric, non-centrosymmetric, enantiomorphic (*i.e.* chiral). Polar point groups are marked with an asterisk *.

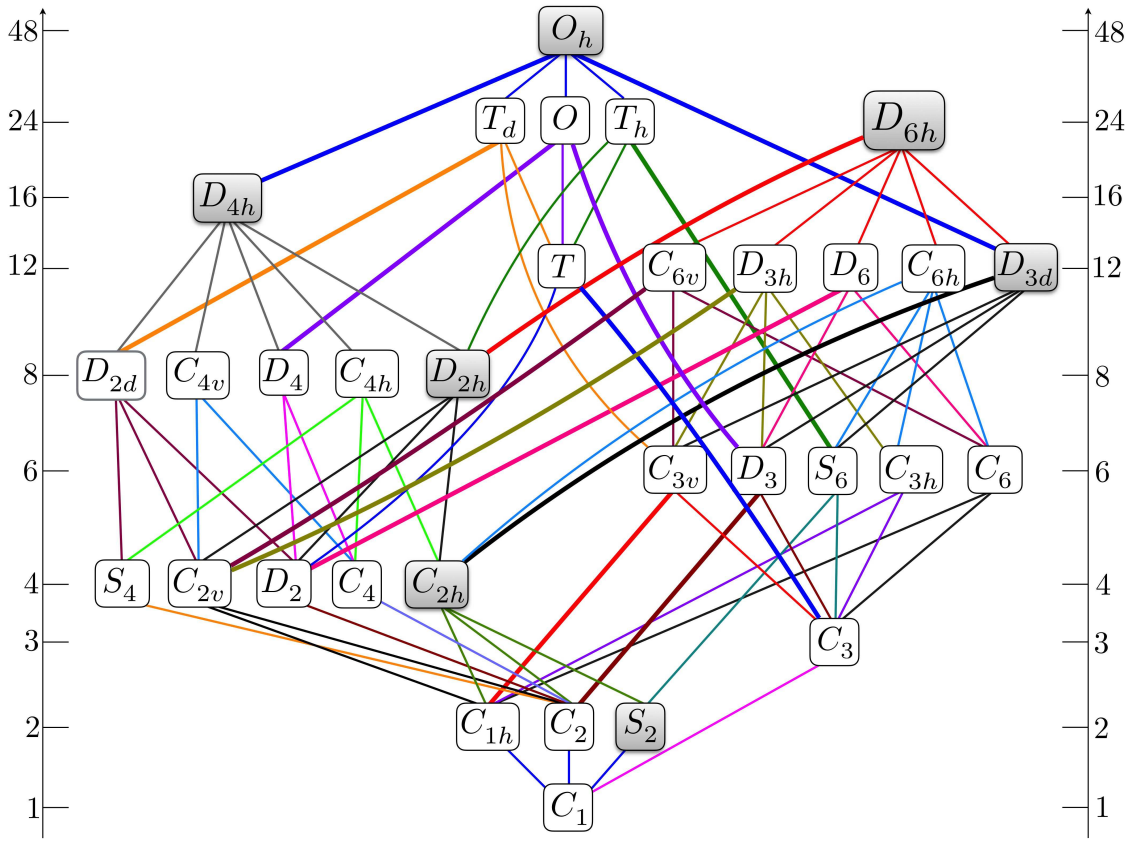


Figure 5.17: The 32 crystallographic point groups, their orders, and their subgroup structure. If the subgroup is not invariant (normal), the line is heavy. Gray boxes indicate holohedral groups, *i.e.* point groups of maximal symmetry within a given lattice system, corresponding to the symmetry of the underlying Bravais lattice itself. (See Tab. 6.1.6 of Lax, or Tab. 5 of Koster *et al.*)

(i) n : rotation by $2\pi/n$ about a primary axis (Schoenflies C_n)

$$\begin{array}{ccccc} 2 = C_2 & 3 = C_3 & 4 = C_4 & 5 = C_5 & 6 = C_6 \\ & 3_2 = C_3^{-1} & 4_3 = C_4^{-1} & 5_4 = C_5^{-1} & 6_5 = C_6^{-1} \end{array} \tag{5.25}$$

(ii) m : reflection in a plane (σ)

$\mathbb{Z}_2$ clones	$\{E, C_2\}$	$\{E, I\}$	$\{E, \sigma_h\}$
Schoenflies	$\mathcal{C}_2$	$\mathcal{C}_i$	$\mathcal{C}_s$
HM	2	$\overline{1}$	m

Table 5.8: Two element point group notation.

- m_h : reflection in a plane perpendicular to the primary axis $\hat{\boldsymbol{n}}$ (σ_h)
- m_v : reflection in a plane containing the primary axis (σ_v)
- m_d : reflection in a plane containing the primary axis and bisecting the angle between two perpendicular 2-fold axes (σ_d)

(iii) $\overline{n}$: rotoinversion IC_n (note $\overline{1}$ is inversion, $\overline{2} = m_h$ is horizontal reflection)

$$\begin{aligned} \overline{3} &= S_6^{-1} & \overline{4} &= S_4^{-1} & \overline{5} &= S_{10}^{-1} & \overline{6} &= S_3^{-1} \\ \overline{3}_2 &= S_6 & \overline{4}_3 &= S_4 & \overline{5}_4 &= S_{10} & \overline{6}_5 &= S_3 \end{aligned} \tag{5.26}$$

(iv) $\widetilde{n}$: rotoreflection $\sigma_h^{-1} C_n = S_n$

The number assignments associated with rotoinversion look strange at first. Pray tell, why do we have $\overline{3} = S_6^{-1}$ but $\overline{4} = S_4^{-1}$ and $\overline{6} = S_3^{-1}$? Well, since you asked so nicely, I will explain, but it will help if you consult Fig. 5.13. The issue here is that the Schoenflies groups $\mathcal{S}_n$ are generated by the *rotoreflection* operation $S_n \equiv \sigma_h^{-1} C_n$ while the HM symbol $\overline{n}$ denotes *rotoinversion* IC_n. The relation between the two is as follows. Let $C(\alpha)$ denote counterclockwise rotation through an angle α. Then $S(\alpha) = I\,C(\alpha - \pi)$. In other words, $S_n = I\,C_2^{-1}\,C_n$. According to this definition,

$$S_2 = I \quad , \quad S_3 = I\,C_6^{-1} \quad , \quad S_4 = I\,C_4^{-1} \quad , \quad S_6 = I\,C_3^{-1} \quad . \tag{5.27}$$

Note that $S_5 = I\,C_5^{-3}$, which produces a ten-fold pattern. In general, for n odd, S_n generates a $2n$-fold pattern.

Now let's talk about the HM symbols for the point groups themselves. The basic idea is to identify symmetry-inequivalent axes and reflection planes. For a single n-fold axis, the Schoenflies group is $\mathcal{C}_n$ and the HM symbol is n. If we add a vertical mirror σ_v to $\mathcal{C}_n$, forming $\mathcal{C}_{nv}$, the HM symbol is nm if n is odd and nmm is n is even. The reason for the difference is that for n even, the alternating vertical reflections break into two classes, whereas for n odd there is only one class (check the character tables!). If we instead we had added a horizontal mirror σ_h to form $\mathcal{C}_{nh}$, the HM symbol would be $\frac{n}{m}$. However, when n is odd, $\mathcal{C}_{nh}$ is generated by the single rotoinversion $\overline{(2n)}$, and the convention is to use that symbol rather than the equivalent $\frac{n}{m}$ because the operation $\overline{(2n)}$ generates a pattern with more points than either n or m_h (though combined of course they generate the same group). For the dihedral groups D_n, the HM symbol is $n22$ if n is even and $n2$ if n is odd, for reasons similar to those for $\mathcal{C}_{nv}$. In general, for groups with a single primary axis, HM symbols can have up to three positions, which are assigned as follows:

- The first position indicates the rotational symmetry n of the primary axis, or $\overline{n}$ if the symmetry is rotoinversion. It can also be $\frac{n}{m}$ in the case of an n-fold axis plus a horizontal reflection plane.
- The second position indicates symmetry of a secondary axis or plane, and can be 2, m, or $\frac{2}{m}$.
- The third position indicates symmetry of a tertiary axis or plane, and can be 2, m, or $\frac{2}{m}$.

Thus, the HM symbol for D_{nd} is $\overline{n}\,\frac{2}{m}$ if n is odd but is $\overline{(2n)}m$ if n is even, while the HM symbol for D_{nh} is $\overline{n}m2$ if n is odd and $\frac{n}{m}\frac{2}{m}\frac{2}{m}$ if n is even. Notation for two element point groups is given in Tab. 5.8

Schoenflies	HM	2	3	4	5	6	$\mathcal{G}$ (HM)	order
$\mathcal{C}_n$	n	2	3	4	5	6	n	n
$\mathcal{S}_n$ (n odd)	$\overline{(2n)}$		$\overline{6}$		$\overline{10}$		$\overline{(2n)}$	$2n$
$\mathcal{S}_n$ ($n = 4k$)	$\overline{n}$			$\overline{4}$			$\overline{n}$	n
$\mathcal{S}_n$ ($n = 4k+2$)	$\overline{(n/2)}$	$\overline{1}$				$\overline{3}$	$\overline{n}$	n
$\mathcal{C}_{nv}$ (n even)	nmm	$2mm$		$4mm$		$6mm$	n, m_v	$2n$
$\mathcal{C}_{nv}$ (n odd)	nm		$3m$		$5m$		n, m_v	$2n$
$\mathcal{C}_{nh}$ (n even)	$\frac{n}{m}$	$\frac{2}{m}$		$\frac{4}{m}$		$\frac{6}{m}$	n, m_h	$2n$
$\mathcal{C}_{nh}$ (n odd)	$\overline{(2n)}$		$\overline{6}$		$\overline{10}$		n, m_h	$2n$
D_n (n even)	$n22$	222		422		622	$n, 2$	$2n$
D_n (n odd)	$n2$		32		52		$n, 2$	$2n$
D_{nd} (n even)	$\overline{(2n)}\,2m$	$\overline{4}2m$		$\overline{8}2m$		$\overline{12}\,2m$	$n, 2, m_d$	$4n$
D_{nd} (n odd)	$\overline{n}\,\frac{2}{m}$		$\overline{3}\,\frac{2}{m}$		$\overline{5}\,\frac{2}{m}$		$n, 2, m_d$	$4n$
D_{nh} (n even)	$\frac{n}{m}\frac{2}{m}\frac{2}{m}$	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$		$\frac{4}{m}\frac{2}{m}\frac{2}{m}$		$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	$n, 2, m_h$	$4n$
D_{nh} (n odd)	$\overline{(2n)}\,m2$		$\overline{6}m2$		$\overline{10}\,m2$		$n, 2, m_h$	$4n$

Table 5.9: Schoenflies and Hermann-Mauguin (international) notation for simple crystallographic point groups. The last columns list the generators $\mathcal{G}$ and the number of elements. Note $\mathcal{S}_n = \mathcal{C}_{nh}$ for n odd, and that $\overline{(2n)}\,2m = \overline{(2n)}\,m2$.

Schoenflies	T	T_h	T_d	O	O_h	I	I_h
HM	23	$\frac{2}{m}\,\overline{3}$	$\overline{4}3m$	432	$\frac{4}{m}\,\overline{3}\,\frac{2}{m}$	532	$\frac{2}{m}\,\overline{3}\,\overline{5}$
generators	$3, 2$	$3, 2, m_h$	$3, 2, m_d$	$4, 3, 2$	$4, 3, 2, m_h$	$5, 3, 2$	$5, 3, 2, m_h$
order	12	24	24	24	48	60	120

Table 5.10: Schoenflies and Hermann-Mauguin notation for multi-axis point groups. Indices for generators refer to distinct (though not necessarily orthogonal) axes.

Finally we come to the tetrahedral, octahedral, and icosahedral groups, all of which have more than one high order ($n > 2$) axis. For the tetrahedral group T, the HM symbol is 23 because the 2-fold

No.	HM short	HM full	Schoenflies	No.	HM short	HM full	Schoenflies
1	1	1	C_1	17	$\overline{3}$	$\overline{3}$	$C_{3i}\ (S_6)$
2	$\overline{1}$	$\overline{1}$	$C_i\ (S_2)$	18	32	32	D_3
3	2	2	C_2	19	$3m$	$3m$	C_{3v}
4	m	m	$C_s\ (C_{1h})$	20	$\overline{3}m$	$\overline{3}\frac{2}{m}$	D_{3d}
5	$2/m$	$\frac{2}{m}$	C_{2h}	21	6	6	C_6
6	222	222	$D_2\ (V)$	22	$\overline{6}$	$\overline{6}$	C_{3h}
7	$mm2$	$mm2$	C_{2v}	23	$6/m$	$\frac{6}{m}$	C_{6h}
8	mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}\ (V_h)$	24	622	622	D_6
9	4	4	C_4	25	$6mm$	$6mm$	C_{6v}
10	$\overline{4}$	$\overline{4}$	S_4	26	$\overline{6}m2$	$\overline{6}m2$	D_{3h}
11	$4/m$	$\frac{4}{m}$	C_{4h}	27	$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}
12	422	422	D_4	28	23	23	T
13	$4mm$	$4mm$	C_{4v}	29	$m\overline{3}$	$\frac{2}{m}\overline{3}$	T_h
14	$\overline{4}2m$	$\overline{4}2m$	$D_{2d}\ (V_d)$	30	432	432	O
15	$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	D_{4h}	31	$\overline{4}3m$	$\overline{4}3m$	T_d
16	3	3	C_3	32	$m\overline{3}m$	$\frac{4}{m}\overline{3}\frac{2}{m}$	O_h

Table 5.11: HM and Schoenflies notation for the 32 crystallographic point groups.

axes are oriented parallel to the axes of the cube containing the tetrahedron, as shown in Figs. 5.9 and 5.12. The octahedral group O is written 432 in HM notation, because the fourfold axes are parallel to the cube axes, there are secondary threefold axes along the cube diagonals, and tertiary twofold axes running through the centers of the cube edges. The HM symbol for the icosahedral group I is 532. There are primary fivefold axes, through the vertices, secondary threefold axes through the face centers, and tertiary twofold axes through the edge centers (once again, see Fig. 5.9). Now add an improper element: inversion or a mirror plane. For the pyritohedral group T_h, we start with T and then add mirror planes perpendicular to the twofold axes, turning the threefold axes into inversion axes[19]. Consequently the HM symbol is $\frac{2}{m}\,\overline{3}$. For the achiral tetrahedral group T_d, we add mirrors perpendicular to the diagonal threefold axes, resulting in fourfold inversion axes and the symbol $\overline{4}3m$. When it comes to the cubic group O, we may add either a mirror or inversion. Since they are equivalent, consider the mirror, which bisects the fourfold axes, turning the threefold axes into inversion axes, and generating new mirrors perpendicular to the teriary twofold axes. The HM symbol is then $\frac{4}{m}\,\overline{3}\,\frac{2}{m}$. Finally, adding a mirror to the icosahedron turns I into I_h, with HM symbol $\overline{5}\,\overline{3}\,\frac{2}{m}$.

[19] The seams of a volleyball have pyritohedral symmetry.

5.2.10 Double groups

The group operations act on electron wavefunctions, which are spinor functions of the spatial coordinates $\boldsymbol{r} = (x, y, z)$:

$$\vec{\psi}(\boldsymbol{r}) = \begin{pmatrix} \psi_\uparrow(\boldsymbol{r}) \\ \psi_\downarrow(\boldsymbol{r}) \end{pmatrix} \ . \tag{5.28}$$

Rotations by an angle θ about an axis $\hat{\boldsymbol{n}}$ are represented by the unitary operator $U(\theta;\hat{\boldsymbol{n}}) = e^{-i\theta\hat{\boldsymbol{n}}\cdot\boldsymbol{J}/\hbar}$, where $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is the sum of orbital ($\boldsymbol{L}$) and intrinsic spin ($\boldsymbol{S}$) angular momenta. For crystallographic point groups, $\theta = 2\pi/n$ where $n = 1$, 2, 3, 4, or 6.

When spin is neglected, we have the point groups we have studied. With spin, we must deal with the fact that $\mathsf{SU}(2)$ gives us a *projective representation* of $\mathsf{SO}(3)$. Recall that $\hat{D}(G)$ is a projective representation of G if

$$\hat{D}(g)\,\hat{D}(h) = \omega(g,h)\,\hat{D}(gh) \tag{5.29}$$

where associativity imposes the following condition on the cocycle $\omega(g,h)$:

$$\frac{\omega(g,h)}{\omega(h,k)} = \frac{\omega(g,hk)}{\omega(gh,k)} \quad . \tag{5.30}$$

In our case, $G = \mathsf{SO}(3)$ and $\hat{D}\big(R(\xi,\hat{\boldsymbol{n}})\big) = \exp(-i\xi\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{J}})$ where $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$ and $S = \frac{1}{2}$. For example, any C_2 operation has $\xi = \pi$, hence $(C_2)^2 = C_1 = \exp(-2\pi i\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{S}}) = -1$, which is to say spinor inversion, *i.e.* $\begin{pmatrix} u \\ v \end{pmatrix} \to -\begin{pmatrix} u \\ v \end{pmatrix}$. *For any point group $\mathcal{P}$, the multiplication table for the projective representation $\hat{D}(\mathcal{P})$ looks exactly like that for $\mathcal{P}$, except some entries get multiplied by -1. I.e.* all the cocycles $\omega(g,h)$ are ± 1. We can *lift* this projective representation to an enlarged point group, called the *double group*, $\mathcal{P}'$, by introducing a generator $\overline{E}$, representing spinor inversion, with $\overline{E}^2 = E$. To each element $g \in \mathcal{P}$, there corresponds a counterpart $\bar{g} \equiv g\overline{E}$. Thus, $N_{\mathcal{P}'} = 2N_{\mathcal{P}}$. Note that $\overline{E}$ leaves $\boldsymbol{r}$ unchanged, and that the bar of g^{-1} is the inverse of $\bar{g}$. A schematic illustration of proper rotations within a double group is shown in Fig. 5.18. *Do not confuse the barring operation in double groups with the HM symbol for rotoinversion!*

Remarks about double group multiplication

Some noteworthy aspects regarding multiplication of double group elements:

- ◇ The element $\overline{E}$ is given by $\overline{E} = C_1 = C(\pm 2\pi)$. Note $C(4\pi) = E$.
- ◇ For any group element g, whether barred or unbarred, $gg^{-1} = E$.
- ◇ For the inversion operator I, $I^2 = \bar{I}^2 = E$ and $I\bar{I} = \bar{I}I = \overline{E}$.
- ◇ Any reflection σ obeys $\sigma^2 = \overline{E}$. This is because we can always write $\sigma = IC_2$ where C_2 is a twofold rotation about an axis normal to the reflection plane, whence $\sigma^2 = I^2\,C_2^2 = C_1 = \overline{E}$.

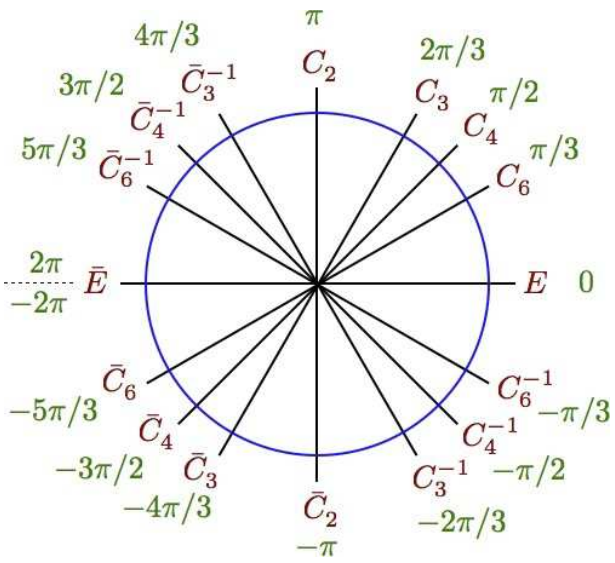


Figure 5.18: Schematic diagram of (common axis) double group rotation generators. Based on Fig. 1 of Koster *et al.* (1963). Note that $C_1 = \overline{E}$, *i.e.* a rotation by 2π.

◇ For $n > 2$, we define $C_n \equiv \hat{R}(2\pi/n)$ to be a counterclockwise rotation by $2\pi/n$ and $C_n^{-1} \equiv \hat{R}(-2\pi/n)$ to be the inverse operation, *i.e.* clockwise rotation by $2\pi/n$. Then $C_2^2 = C_1 = \overline{E}$, hence $C_2^{-1} = \overline{C}_2$. More fully, according to Fig. 5.18, we have

$$
\begin{aligned}
&C_2\,C_3^{-1} = C_6 \qquad &&C_2\,C_4^{-1} = C_4 \qquad &&C_2\,C_6^{-1} = C_3 \\
&C_2\,C_6 = \overline{C}_3^{-1} \qquad &&C_2\,C_4 = \overline{C}_4^{-1} \qquad &&C_2\,C_3 = \overline{C}_6^{-1} \\
&C_2\,\overline{C}_3^{-1} = \overline{C}_6 \qquad &&C_2\,\overline{C}_4^{-1} = \overline{C}_4 \qquad &&C_2\,\overline{C}_6^{-1} = \overline{C}_3 \\
&C_2\,\overline{C}_6 = C_3^{-1} \qquad &&C_2\,\overline{C}_4 = C_4^{-1} \qquad &&C_2\,\overline{C}_3 = C_6^{-1} \quad ,
\end{aligned}
\tag{5.31}
$$

where all rotations are about the same axis.

◇ To compute the product of σ_h with a rotation, recall the definition of the rotoreflection operation $S_n \equiv \sigma_h^{-1}\,C_n = I\,C_2^{-1}\,C_n$, which entails $S_n^{-1} = \sigma_h\,C_n^{-1} = I\,C_2\,C_n^{-1}$. One then has

$$
\sigma_h\,C_n = \overline{S}_n \quad , \quad \sigma_h\,\overline{C}_n^{-1} = \overline{S}_n^{-1} \quad , \quad \sigma_h\,\overline{C}_n = S_n \quad , \quad \sigma_h\,C_n^{-1} = S_n^{-1} \quad . \tag{5.32}
$$

◇ We may then apply σ_h to Eqns. 5.31 and 5.32 to obtain results such as

$$
C_2\,S_3^{-1} = \overline{S}_6 \quad , \quad C_2\,S_6 = S_3^{-1} \quad , \quad \sigma_h\,S_n = C_n \quad , \quad \sigma_h\,S_n^{-1} = \overline{C}_n^{-1} \quad . \tag{5.33}
$$

◇ What about σ_v ? If $\{\sigma_v\,,\,\sigma_{v'}\,,\,\sigma_{v''}\}$ denote vertical reflection planes oriented at angles 0, $2\pi/3$, and $4\pi/3$, respectively, then we should have either $C_3\,\sigma_v = \sigma_{v'}$ or $C_3\,\sigma_v = \overline{\sigma}_{v'}$. Which is it? If we apply

C_3 twice, for either initial case we obtain $C_3^2\,\sigma_v = \sigma_{v''}$. Applying C_3 yet again yields $C_3\,\sigma_{v''} = \overline{\sigma}_v$. Thus we have

$$C_3\,\sigma_v = \overline{\sigma}_{v'} \quad , \quad C_3\,\sigma_{v'} = \overline{\sigma}_{v''} \quad , \quad C_3\,\sigma_{v''} = \overline{\sigma}_v \quad . \tag{5.34}$$

Note then that $\sigma_{v'}\,\sigma_v = C_3$ and $\sigma_v\,\sigma_{v'} = C_3^{-1}$, *et. cyc.*

To summarize, let $C(\alpha)$ denote counterclockwise rotation through an angle α, and let $C_n = C(\alpha_n)$ *etc.* with $\alpha_n = 2\pi/n$. Then

$$\overline{C}(\alpha) = C(\alpha - 2\pi) \quad , \quad S(\alpha) = I\,C(\alpha - \pi) \quad , \quad \overline{S}(\alpha) = I\,C(\alpha + \pi) \tag{5.35}$$

and

$$\sigma = I\,C(\pi) \quad , \quad \overline{\sigma} = I\,C(-\pi) \quad . \tag{5.36}$$

Character tables for double groups

One might at first suspect that any conjugacy class $\mathcal{C}$ of the point group $\mathcal{P}$ spawns two classes within the double group $\mathcal{P}'$, *i.e.* $\mathcal{C}$ and $\overline{\mathcal{C}} \equiv \overline{E}\,\mathcal{C}$. This is always true provided the elements of C don't square to the identity. But for twofold axes C_2 and reflections σ, a theorem due to Opechowski (1940) guarantees:

- For proper twofold operations, C_2 and $\bar{C}_2$ adjoin to the same class if either
  - there exists a second twofold axis perpendicular to the initial axis, or
  - there exists a reflection plane containing the initial axis.
- For improper twofold operations, σ and $\bar{\sigma}$ adjoin to the same class if either
  - there exists a second reflection plane perpendicular to the initial one, or
  - there exists a twofold axis lying within the initial plane.

In these cases, the resulting total number of classes in $\mathcal{P}'$ is less than twice that for $\mathcal{P}$. As an example, consider the tetrahedral group T_d. There are three twofold axis: $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$. All are bilateral because a rotation by π about $\hat{\boldsymbol{x}}$ reverses the direction of both $\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{z}}$, *etc.* Accordingly, in the character table Tab. 5.12 for the double group of T_d, the classes C_2 and $\bar{C}_2$ are adjoined, as are σ_d and $\bar{\sigma}_d$.

With the exception of those twofold operations satisfying the conditions in Opechowski's theorem, the classes $\mathcal{C}$ and $\overline{\mathcal{C}}$ are distinct in the double group. Any IRREP of $\mathcal{P}$ will be an IRREP of $\mathcal{P}'$ with $\chi(\overline{\mathcal{C}}) = \chi(\mathcal{C})$. But since the number of elements is doubled in $\mathcal{P}'$, there must be new IRREPs specific to the double group. For these additional IRREPs, one has $\chi(\overline{\mathcal{C}}) = -\chi(\mathcal{C})$, hence if $\mathcal{C}$ and $\overline{\mathcal{C}}$ adjoin to $\mathcal{C} \cup \overline{\mathcal{C}}$ by Opechowski, one must have $\chi(\mathcal{C} \cup \overline{\mathcal{C}}) = 0$. Checking Tab. 5.12, we see that in the extra IRREPs $\Gamma_{6,7,8}$, $\chi(\overline{\mathcal{C}}) = -\chi(\mathcal{C})$ except in the case of the adjoined classes, for which $\chi(\mathcal{C} \cup \overline{\mathcal{C}}) = 0$.

We can understand that twofold rotations and reflections are special in this regard from the result we obtained for $\mathsf{SU}(2)$ characters,

$$\chi^{(j)}(\xi) = \frac{\sin\,(j + \frac{1}{2})\xi}{\sin\,\frac{1}{2}\xi} \tag{5.37}$$

T_d'	E	$\overline{E}$	$8C_3$	$8\overline{C}_3$	$\begin{matrix}3C_2\\3\overline{C}_2\end{matrix}$	$\begin{matrix}6\sigma_d\\6\overline{\sigma}_d\end{matrix}$	$6S_4$	$6\overline{S}_4$
$\Gamma_1\ (A_1)$	1	1	1	1	1	1	1	1
$\Gamma_2\ (A_2)$	1	1	1	1	1	−1	−1	−1
$\Gamma_3\ (E)$	2	2	−1	−1	2	0	0	0
$\Gamma_4\ (T_1)$	3	3	0	0	−1	−1	1	1
$\Gamma_5\ (T_2)$	3	3	0	0	−1	1	−1	−1
Γ_6	2	−2	1	−1	0	0	$\sqrt{2}$	$-\sqrt{2}$
Γ_7	2	−2	1	−1	0	0	$-\sqrt{2}$	$\sqrt{2}$
Γ_8	4	−4	−1	1	0	0	0	0

Table 5.12: Character table for the double group of T_d.

for rotation by an angle ξ about any axis. Thus $\chi^{(j)}(\alpha + 2\pi) = (-1)^{2j}\chi^{(j)}(\alpha)$. For $j = \frac{1}{2}$, or indeed for any half odd integer j, we have $\chi(\pi) = \chi(3\pi) = 0$. Thus C_2 and $\overline{C}_2$ have the same character. A similar result holds for reflections, because $\sigma = IC_2$ and $\overline{\sigma} = I\overline{C}_2$. Therefore the classes C_2 and $\overline{C}_2$ are not distinguished by character, nor are σ and $\overline{\sigma}$. This is true in any IRREP in which $\chi(\overline{E}) = -\chi(E)$.

5.2.11 The three amigos : D_4 , C_{4v} , D_{2d}

Let's try to apply some of what we've just learned to the groups D_4, C_{4v}, and D_{2d}. All these eight-element groups are isomorphic to each other. The character table for all three is given in Tab. 5.13. Although they are all isomorphic, they include different sets of symmetry operations, and therefore they will have different basis representations.

Let's now discuss all the classes of these three groups. Recall that

$$R(\xi, \hat{\boldsymbol{n}})_{ab} = n^a n^b + \left(\delta^{ab} - n^a n^b\right)\cos\xi - \epsilon_{abc}\, n^c \sin\xi \quad . \tag{5.38}$$

- C_2 : This class is present in all three groups. It consists of a single element which is rotation by π about the $\hat{\boldsymbol{z}}$ axis, and represented by the 3×3 matrix

$$R_z^\pi \equiv R(\pi, \hat{\boldsymbol{z}}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{5.39}$$

- $2C_4$: Present in D_4 and C_{4v}. Contains the elements

$$R_z^{\pi/2} \equiv R(\tfrac{\pi}{2}, \hat{\boldsymbol{z}}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad R_z^{-\pi/2} \equiv R(-\tfrac{\pi}{2}, \hat{\boldsymbol{z}}) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{5.40}$$

  These elements are inverses of each other.

D_4	E	$2C_4$	C_2	$2C_2'$	$2C_2''$			
C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$			
D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$	D_4 basis	C_{4v} basis	D_{2d} basis
A_1	1	1	1	1	1	x^2+y^2	x^2+y^2 or z	x^2+y^2
A_2	1	1	1	-1	-1	L_z or z	L_z	L_z
B_1	1	-1	1	1	-1	x^2-y^2	x^2-y^2	x^2-y^2
B_2	1	-1	1	-1	1	xy	xy	xy or z
E	2	0	-2	0	0	$\{x\,,\,y\}$	$\{x\,,\,y\}$	$\{x\,,\,y\}$

Table 5.13: Character table for the point groups D_4, C_{4v}, and D_{2d}.

- $2S_4$: Present only in D_{2d} . These are rotoreflections, *i.e.* $2C_4$ followed by $z \to -z$:

$$S_z^{\pi/2} \equiv S(\tfrac{\pi}{2},\hat{\boldsymbol{z}}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad , \quad S_z^{-\pi/2} \equiv S(-\tfrac{\pi}{2},\hat{\boldsymbol{z}}) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad . \tag{5.41}$$

  These two are also inverses within $\mathsf{O}(3)$. In general we have $S(\alpha) = IC(\alpha-\pi)$, in which case $S_z^{\pi/2} = IR_z^{-\pi}R_z^{\pi/2}$ and $S_z^{-\pi/2} = IR_z^{-\pi}R_z^{-\pi/2}$. Why do we distinguish R_z^{π} and $R_z^{-\pi}$ when they are represented by the same matrix? This will be important when we construct the corresponding matrix representation for the double groups[20].

- $2C_2'$: Present in D_4 and D_{2d} , this class consists of twofold rotations about $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$:

$$R_x^{\pi} \equiv R(\pi,\hat{\boldsymbol{x}}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad , \quad R_y^{\pi} \equiv R(\pi,\hat{\boldsymbol{y}}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad . \tag{5.42}$$

- $2\sigma_v$: This occurs only in C_{4v} and corresponds to reflections $x \to -x$ and $y \to -y$:

$$\Sigma_x \equiv IR_x^{\pi} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \Sigma_y \equiv IR_y^{\pi} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{5.43}$$

- $2C_2''$: Occurring only in D_4 , these operations are twofold rotations about the diagonal axes $y = x$ and $y = -x$:

$$R_{xy}^{\pi} \equiv R(\pi,\tfrac{\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}}{\sqrt{2}}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad , \quad R_{x\overline{y}}^{\pi} \equiv R(\pi,\tfrac{\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}}{\sqrt{2}}) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad . \tag{5.44}$$

[20] See the explanation of Eqn. 5.32.

- $2\sigma_d$: Occurring in C_{4v} and D_{2d}, this class of reflections is equivalent to IC_2'', hence

$$\Sigma_{xy} \equiv IR^\pi_{xy} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \qquad \Sigma_{x\overline{y}} \equiv IR^\pi_{x\overline{y}} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{5.45}$$

I apologize for the loose notation where we are using the same symbols to refer to group elements as well as their 3×3 matrix representations. Notice that all the matrices representing elements of C_{4v} have a block-diagonal structure with an upper left 2×2 block and a lower right 1×1 block, where the latter is always 1. This is because we never need to speak of the z-direction when we talk about C_{4v} as all its operations involve x and y alone.

Now let's talk about the basis functions. The projectors onto the various representations are given by

$$\Pi^\Gamma = \frac{d_\Gamma}{N_G} \sum_{g \in G} \chi^{\Gamma^*}(g)\, D(g) \quad , \tag{5.46}$$

where $N_G = 8$ for the three amigos. It should be clear how the basis functions in Tab. 5.13 are eigenfunctions of these projectors, but let's note the following to obviate any confusion. First of all, what do we mean by L_z as a basis function of the A_2 IRREP in the case of C_{4v} and D_{2d}? We mean the angular momentum operator, $L_z = xp_y - yp_x$. We know that $L_\alpha = \varepsilon_{\alpha\beta\gamma} r^\beta p^\gamma$ transforms as a vector under proper rotations, however it is known as an *axial vector* because it transforms differently under improper rotations. That is, under the operation σ_h (which, *nota bene* is present in none of our three groups), z is odd but L_z is even. Similarly, under either of the σ_v operations, z is even but L_z is odd. For D_4, the basis function $f(z) = z$ corresponds to the A_2 IRREP because it is even under E, $2C_4$, and C_2 and odd under $2C_2'$ and $2C_2''$. But in C_{4v}, whose operations all leave z invariant, $f(z) = z$ transforms as the A_1 IRREP. And for D_{2d}, where $2S_4$ and $2C_2'$ reverse z but $2\sigma_d$ does not, $f(z) = z$ transforms as the B_2 IRREP! Note that other valid choices of basis functions are possible. For example, rather than the pair $\{x\,,\,y\}$, we could have chosen $\{L_x\,,\,L_y\}$ as basis functions for the E IRREP.

Double group matrices and projectors

Now let's tackle the corresponding double groups. We will need the 2×2 matrices representing the various point group operations. Recall for a rotation by ξ about $\hat{\boldsymbol{n}}$,

$$\exp(-i\xi\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}/2) = \cos(\tfrac{1}{2}\xi) - i \sin(\tfrac{1}{2}\xi)\, \hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma} \quad . \tag{5.47}$$

We'll write the elements of $D^{(1/2)}(G)$ as $U(g)$. We then have

$$U(R^\pi_z) = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \quad , \quad U(R^{\pi/2}_z) = \begin{pmatrix} e^{-i\pi/4} & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \quad , \quad U(R^{-\pi/2}_z) = \begin{pmatrix} e^{i\pi/4} & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix} \quad . \tag{5.48}$$

For the rotoreflections,

$$U(S^{\pi/2}_z) = \begin{pmatrix} e^{i\pi/4} & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix} \quad , \quad U(S^{\pi/2}_z) = \begin{pmatrix} -e^{-i\pi/4} & 0 \\ 0 & -e^{i\pi/4} \end{pmatrix} \quad . \tag{5.49}$$

D_4'	E	$\overline{E}$	$2C_4$	$2\overline{C}_4$	$C_2 \cup \overline{C}_2$	$2C_2' \cup 2\overline{C}_2'$	$2C_2'' \cup 2\overline{C}_2''$	
C_{4v}'	E	$\overline{E}$	$2C_4$	$2\overline{C}_4$	$C_2 \cup \overline{C}_2$	$2\sigma_v \cup 2\overline{\sigma}_v$	$2\sigma_d \cup 2\overline{\sigma}_d$	
D_{2d}'	E	$\overline{E}$	$2S_4$	$2\overline{S}_4$	$C_2 \cup \overline{C}_2$	$2C_2' \cup 2\overline{C}_2'$	$2\sigma_d \cup 2\overline{\sigma}_d$	basis
Γ_1	1	1	1	1	1	1	1	x^2+y^2
Γ_2	1	1	1	1	1	-1	-1	L_z
Γ_3	1	1	-1	-1	1	1	-1	x^2-y^2
Γ_4	1	1	-1	-1	1	-1	1	xy
Γ_5	2	2	0	0	-2	0	0	$\{x\,,\,y\}$ or $\{L_x\,,\,L_y\}$
Γ_6	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	$\{\vert\uparrow\rangle\,,\,\vert\downarrow\rangle\}$
Γ_7	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	$\Gamma_3 \times \Gamma_6$ or $\Gamma_4 \times \Gamma_6$

Table 5.14: Character table for the double groups of D_4, C_{4v}, and D_{2d}.

Note that $U(S_z^{\pm\pi/2}) = I\,U(R_z^{-\pi})\,U(R_z^{\pm\pi/2})$, where $R_z^{-\pi} = -R_z^{\pi}$ and that I acts as the identity matrix on spinors. Note that $U(S_z^{\pi/2}) = U(R_z^{-\pi/2})$. Next, we need

$$U(\Sigma_x) = U(R_x^{\pi}) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \quad , \quad U(\Sigma_y) = U(R_y^{\pi}) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad . \tag{5.50}$$

Since the only difference between the twofold rotations and the corresponding reflections in the planes perpendicular to their axes is the inversion I, their representations in $D^{1/2}(G)$ are identical. The remaining matrices are

$$U(\Sigma_{xy}) = U(R_{xy}^{\pi}) = \begin{pmatrix} 0 & -e^{i\pi/4} \\ e^{-i\pi/4} & 0 \end{pmatrix} \quad , \quad U(\Sigma_{x\overline{y}}) = U(R_{x\overline{y}}^{\pi}) = \begin{pmatrix} 0 & e^{-i\pi/4} \\ -e^{i\pi/4} & 0 \end{pmatrix} \quad . \tag{5.51}$$

Note that their product is $U(\Sigma_{x\overline{y}})\,U(\Sigma_{xy}) = U(R_z^{\pi})$. Note also that $\det U(g) = 1$ since each $U(g) \in \mathsf{SU}(2)$.

Appealing to the character table in Tab. 5.14, we can now construct the double group projectors. We write the projectors as

$$\Pi^{\Gamma} = \frac{d_{\Gamma}}{N_G} \sum_{g \in G} \chi^{\Gamma^*}(g)\, D(g) \otimes U(g) \quad . \tag{5.52}$$

where G is any of D_4', C_{4v}', and D_{2d}', and $N_G = 16$, since each of the double groups of the three amigos has 16 elements. For the IRREPs $\{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4, \Gamma_5\}$ we may use the basis functions $\psi_\mu^{\Gamma}(\boldsymbol{r})$ from the proper point groups. *I.e.* we can simply ignore all the U-matrices and pretend there is no spin component. More correctly, we can consider the spin component of each basis function to be a *singlet*,

$$\big|\,\mathrm{S}\,\big\rangle = \frac{1}{\sqrt{2}}\Big(\big|\uparrow\big\rangle \otimes \big|\downarrow\big\rangle - \big|\downarrow\big\rangle \otimes \big|\uparrow\big\rangle\Big) \quad . \tag{5.53}$$

One can check that $U(g)\,|\,\mathrm{S}\,\rangle = |\,\mathrm{S}\,\rangle$ for all g, which follows from $\det U(g) = 1$. For Γ_6 and Γ_7, though, the projectors annihilate any basis function of the form $f(\boldsymbol{r})\,|\,\mathrm{S}\,\rangle$. However, a basis function of the form $|\uparrow\rangle$ or $|\downarrow\rangle$ (*i.e.* with no spatial dependence) does the trick. In spinor notation, we have

$$\begin{aligned} \frac{2}{16}\left[\chi^{\Gamma_6}(E)\,U(E) + \chi^{\Gamma_6}(\overline{E})\,U(\overline{E})\right]\begin{pmatrix} u \\ v \end{pmatrix} &= \frac{1}{2}\begin{pmatrix} u \\ v \end{pmatrix} \\ \frac{2}{16}\left[\chi^{\Gamma_6}(2C_4) + \chi^{\Gamma_6}(2\overline{C}_4)\,\overline{E}\right]\left[U(R_z^{\pi/2}) + U(R_z^{-\pi/2})\right]\begin{pmatrix} u \\ v \end{pmatrix} &= \frac{1}{2}\begin{pmatrix} u \\ v \end{pmatrix} \quad . \end{aligned} \tag{5.54}$$

Thus, $\begin{pmatrix} u \\ v \end{pmatrix}$ is an eigenfunction of the projector Π^{Γ_6}. In order to keep this spinor from being annihilated by Π^{Γ_7}, we need to multiply it by a scalar function $\psi(\boldsymbol{r})$ which reverses the sign from the characters of the classes $2C_4$ and $2\overline{C}_4$. According to Tab. 5.13, the basis function from either the B_1 or the B_2 IRREPs will work. This explains the basis functions in Tab. 5.14[21]. Other valid choices of basis functions are of course possible.

Do we always need the double group?

Although electrons carry spin $S = \frac{1}{2}$, we usually don't need to invoke the double group formalism if the spin-orbit coupling is sufficiently weak. That is, we may use $\boldsymbol{L}$ rather than $\boldsymbol{J}$ as the generator of rotations, since $\left[\hat{H}, L^\alpha\right] = 0$. Each electronic energy level is of course doubly degenerate due to the spin, which just "comes along for the ride". In the presence of significant spin-orbit coupling, $\left[\hat{H}, L^\alpha\right] \neq 0$ but $\left[\hat{H}, J^\alpha\right] = 0$. Thus we must use the total angular momentum $\boldsymbol{J}$ as the generator of rotations, which entails the double point group symmetries.

5.3 Space Groups

The full group of symmetry operations of an n-dimensional crystal is called its *space group*, $\mathcal{S}$. Any crystallographic space group is a subgroup of the Euclidean group: $\mathcal{S} \subset \mathsf{E}(n)$. Space groups are infinite discrete groups. Two-dimensional space groups are called *wallpaper groups*. An accounting of the total number of lattices, point groups, and space groups for two and three dimensional crystals is provided in Tab. 5.1.

5.3.1 Space group elements and their properties

Each element $\left\{\, g \,\middle|\, \boldsymbol{t} \,\right\} \in \mathcal{S}$ represents a compounded operation of rotation by a rotation g (either proper or improper) and a translation $\boldsymbol{t}$. When $g = E$, the space group operations are pure translations, and are all of the form $\left\{\, E \,\middle|\, \boldsymbol{R} \,\right\}$, where $\boldsymbol{R} \in \mathcal{L}$ is a vector in the underlying Bravais lattice. As discussed in

[21] The spin component of the basis functions for the Γ_1 through Γ_5 IRREPs should be considered to be the singlet $|\,\mathrm{S}\,\rangle$.

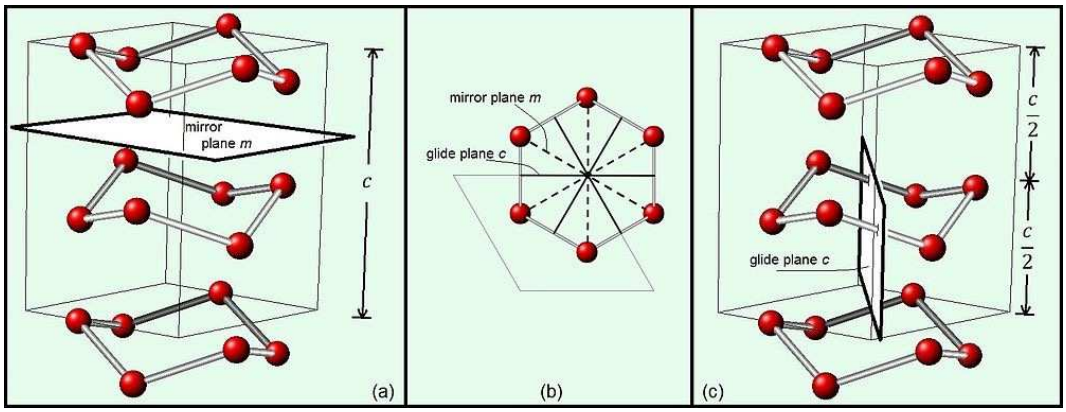


Figure 5.19: Structure of hexagonal H_2O ice, with red spheres showing location of oxygen atoms. The space group is $P6_3/mmc$. The 6_3 symbol indicates a sixfold screw axis. The first two m symbols indicate mirror planes perpendicular and parallel to the c-axis. The c symbol indicates a glide plane where the translation is along the c-axis. (Image credit: *Wikipedia*).

§5.1.7, the operations $\{\, g \,|\, \boldsymbol{t} \,\}$ form a group, with

$$\begin{aligned} \{\, g \,|\, \boldsymbol{t} \,\}\{\, g' \,|\, \boldsymbol{t}' \,\} &= \{\, gg' \,|\, g\boldsymbol{t}' + \boldsymbol{t} \,\} \\ \{\, g \,|\, \boldsymbol{t} \,\}^{-1} &= \{\, g^{-1} \,|\, -g^{-1}\boldsymbol{t} \,\} \quad . \end{aligned} \tag{5.55}$$

We see that the rotations g must themselves form a group, which is the *point group* $\mathcal{P}$ of the crystal. Pure translations $\{\, E \,|\, \boldsymbol{R} \,\}$ by a direct lattice vector are part of the space group, and indeed form a normal subgroup thereof: $\{\, g \,|\, \boldsymbol{t} \,\}^{-1}\{\, E \,|\, \boldsymbol{R} \,\}\{\, g \,|\, \boldsymbol{t} \,\} = \{\, E \,|\, g^{-1}\boldsymbol{R} \,\}$. Thus, $g^{-1}\boldsymbol{R} \in \mathcal{L}$ for any $g \in \mathcal{P}$, which means, as noted above in §5.1.7, that the point group $\mathcal{P}$ of any crystal is a subgroup of the point group $\mathcal{P}_{\mathcal{L}}$ of its underlying Bravais lattice (*i.e.* the holohedry).

Fom Eqn. 5.55, we have the group conjugation property

$$\{\, h \,|\, \boldsymbol{s} \,\}^{-1}\{\, g \,|\, \boldsymbol{t} \,\}\{\, h \,|\, \boldsymbol{s} \,\} = \{\, h^{-1}gh \,|\, h^{-1}g\boldsymbol{s} - h^{-1}\boldsymbol{s} + h^{-1}\boldsymbol{t} \,\} \equiv \{\, g' \,|\, \boldsymbol{t}' \,\} \quad , \tag{5.56}$$

for which the rotation is $g' = h^{-1}gh$ and the translation is $\boldsymbol{t}' = h^{-1}g\boldsymbol{s} - h^{-1}\boldsymbol{s} + h^{-1}\boldsymbol{t}$. When $h = E$, we have $g' = g$ and

$$\boldsymbol{t} - \boldsymbol{t}' = (E - g)\,\boldsymbol{s} \quad . \tag{5.57}$$

Suppose we further demand $\boldsymbol{t}' = 0$, *i.e.* that the conjugated operation is equivalent to a pure rotation, with no translation, about a different choice of origin. We see that this is possible if we choose $\boldsymbol{s}$ such that $\boldsymbol{t} = (E - g)\,\boldsymbol{s}$.

Now it was noted in §5.2.1 that when the dimension n of space is odd, $g \in \mathsf{O}(n)$ always preserves some axis, meaning it has an eigenvalue $\lambda = 1$. The other two eigenvalues may be written as $e^{\pm i\alpha}$ where $\alpha = 2\pi/n$ with $n = 2$, 3, 4, or 6. (The case $n = 1$ corresponds to the identity E.) A mirror reflection, which is an improper operation, has an inversion axis corresponding to an eigenvalue $\lambda = -1$, with all remaining eigenvalues $\lambda = +1$. Proper rotations therefore have an *invariant axis*, while mirror reflections

have an *invariant plane*. Thus we can write

$$\begin{aligned} \text{proper rotation}: \quad & r = |\,\hat{\boldsymbol{e}}_1\,\rangle\langle\,\hat{\boldsymbol{e}}_1\,| + e^{i\alpha}\,|\,\hat{\boldsymbol{e}}_2\,\rangle\langle\,\hat{\boldsymbol{e}}_2\,| + e^{-i\alpha}\,|\,\hat{\boldsymbol{e}}_3\,\rangle\langle\,\hat{\boldsymbol{e}}_3\,| \\ \text{mirror reflection}: \quad & m = -|\,\hat{\boldsymbol{e}}_1\,\rangle\langle\,\hat{\boldsymbol{e}}_1\,| + |\,\hat{\boldsymbol{e}}_2\,\rangle\langle\,\hat{\boldsymbol{e}}_2\,| + |\,\hat{\boldsymbol{e}}_3\,\rangle\langle\,\hat{\boldsymbol{e}}_3\,| \quad . \end{aligned} \tag{5.58}$$

We now see that if $g = r$ is a proper rotation, $\boldsymbol{t} = (E - r)\,\boldsymbol{s}$ cannot be solved for $\boldsymbol{s}$ if $\boldsymbol{t}$ has any component along the invariant axis $\hat{\boldsymbol{e}}_1$. Similarly, if $g = m$ is a mirror, $\boldsymbol{t} = (E - m)\,\boldsymbol{s}$ cannot be solved for $\boldsymbol{s}$ if $\boldsymbol{t}$ has any component in the invariant plane spanned by $\{\hat{\boldsymbol{e}}_2, \hat{\boldsymbol{e}}_3\}$. Space group operations $\{\, r \,|\, \boldsymbol{t} \,\}$ for which $\boldsymbol{t}$ is parallel to the invariant axis of r are called *screws*, while those for which $\boldsymbol{t}$ is parallel to an invariant plane of m are called *glides*. As we shall see, the possible values of $\boldsymbol{t}$ are strongly constrained in either case. Screws and glides may be considered *intrinsic translations* because they cannot be removed simply by a new choice of origin.

Next we note that if $\{\, g \,|\, \boldsymbol{t} \,\} \in \mathcal{S}$, we can always choose the translation component $\boldsymbol{t}$ to either be in the direct lattice or to lie within the first Wigner-Seitz (WS) cell[22]. If $\boldsymbol{t} \equiv \boldsymbol{\tau} \notin \mathcal{T}$, then it must be unique for a given g, because if both $\{\, g \,|\, \boldsymbol{\tau} \,\}$ and $\{\, g \,|\, \boldsymbol{\tau}' \,\}$ are in $\mathcal{S}$, then so is $\{\, g \,|\, \boldsymbol{\tau}' \,\}^{-1}\{\, g \,|\, \boldsymbol{\tau} \,\} = \{\, E \,|\, g^{-1}(\boldsymbol{\tau} - \boldsymbol{\tau}') \,\}$, which means that $g^{-1}(\boldsymbol{\tau} - \boldsymbol{\tau}') \in \mathcal{T}$ and therefore $\boldsymbol{\tau} - \boldsymbol{\tau}' \in \mathcal{T}$. Since by assumption both $\boldsymbol{\tau}$ and $\boldsymbol{\tau}'$ lie within the first WS cell, we must have $\boldsymbol{\tau}' = \boldsymbol{\tau}$. Thus, all space group elements are of the form $\{\, g \,|\, \boldsymbol{R} + \boldsymbol{\tau}_g \,\}$, where $\boldsymbol{\tau}_g$ may either be zero or a unique nonzero vector within the first WS cell. Now the point group $\mathcal{P}$ is of finite order, so each element $g \in \mathcal{P}$ satisfies $g^n = E$ where n is finite and taken to be the smallest positive integer which satisfies this relation. Therefore

$$\{\, g \,|\, \boldsymbol{\tau}_g \,\}^n = \{\, g^n \,|\, \boldsymbol{\tau}_g + g\boldsymbol{\tau}_g + \ldots + g^{n-1}\boldsymbol{\tau}_g \,\} \quad , \tag{5.59}$$

and since $g^n = E$, we must have that $\boldsymbol{\tau}_g + g\boldsymbol{\tau}_g + \ldots + g^{n-1}\boldsymbol{\tau}_g = \boldsymbol{R}$ is a direct lattice vector. Note that for $g = r$ we can have $n = 2$, 3, 4, or 6, while for $g = m$ we necessarily have $n = 2$.

According to Eqn. 5.58, we have

$$E + g + g^2 + \ldots + g^{n-1} = n\,P_{\parallel}(g) \quad , \tag{5.60}$$

where $P_{\parallel}(r) \equiv |\,\hat{\boldsymbol{e}}_1\,\rangle\langle\,\hat{\boldsymbol{e}}_1\,|$ is the projector onto the invariant axis of r, and $P_{\parallel}(m) \equiv |\,\hat{\boldsymbol{e}}_2\,\rangle\langle\,\hat{\boldsymbol{e}}_2\,| + |\,\hat{\boldsymbol{e}}_3\,\rangle\langle\,\hat{\boldsymbol{e}}_3\,|$ the projector onto the invariant plane of m. Thus we conclude $n\,P_{\parallel}(g)\,\boldsymbol{\tau}_g = \boldsymbol{R}$, which is to say that the nonremovable part of the translation $\boldsymbol{\tau}_g$, *i.e.* its projection onto the rotation axis or mirror plane, is equal to $\boldsymbol{R}/n$. Note also that in $d = 2$, there is no preserved rotation axis, since it would be orthogonal to the (x, y) plane. Therefore two dimensional point groups can at most have glides and no screws.

We may now identify all possible screws with the symbols 2_1, 3_1, 4_1, 4_2, 6_1, 6_2, and 6_3, as well as their enantiomorphous counterparts 3_2, 4_3, 6_4, and 6_5. Glide planes are denoted by the symbols a, b, c, n, and d, depending on the direction of the translation component. Let the symmetry axes of the crystal be $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$. Then

- For a glides, $\boldsymbol{\tau} = \frac{1}{2}\boldsymbol{a}$.
- For b glides, $\boldsymbol{\tau} = \frac{1}{2}\boldsymbol{b}$.
- For c glides, $\boldsymbol{\tau} = \frac{1}{2}\boldsymbol{c}$.

[22] A translation $\boldsymbol{t}$ which is not a direct lattice vector can always be brought into the first WS cell by a direct lattice translation.

Nos.	lattice	$\mathcal{P}^{(\mathrm{Sch})}$	$\mathcal{P}^{(\mathrm{HM})}$	order	$\mathcal{S}$ (sym)	$\mathcal{S}$ (n-sym)
1	oblique	C_1	1	1	$p1$	
2	oblique	C_2	2	2	$p2$	
3 - 4	rectangular	C_{1v}	m	2	pm	pg
5 - 6	rectangular	C_{2v}	$2mm$	4	pmm	pmg
7	centered rectangular	C_{1v}	m	2	cm	
8 - 9	centered rectangular	C_{2v}	$2mm$	2	cmm	pgg
10	square	C_4	4	4	$p4$	
11 - 12	square	C_{4v}	$4mm$	8	$p4m$	$p4g$
13	hexagonal	C_3	3	3	$p3$	
14 - 15	hexagonal	C_{3v}	$3m$	6	$p3m1$, $p31m$	
16	hexagonal	C_6	6	6	$p6$	
17	hexagonal	C_{6v}	$6mm$	12	$p6m$	

Table 5.15: The 17 wallpaper groups and their short notation.

- For n glides, $\boldsymbol{\tau} = \frac{1}{2}(\boldsymbol{a}+\boldsymbol{b})$, $\frac{1}{2}(\boldsymbol{b}+\boldsymbol{c})$, $\frac{1}{2}(\boldsymbol{a}+\boldsymbol{c})$, or $\frac{1}{2}(\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})$.
- For d glides, $\boldsymbol{\tau} = \frac{1}{4}(\boldsymbol{a}+\boldsymbol{b})$, $\frac{1}{4}(\boldsymbol{b}+\boldsymbol{c})$, $\frac{1}{4}(\boldsymbol{a}+\boldsymbol{c})$, or $\frac{1}{4}(\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})$.

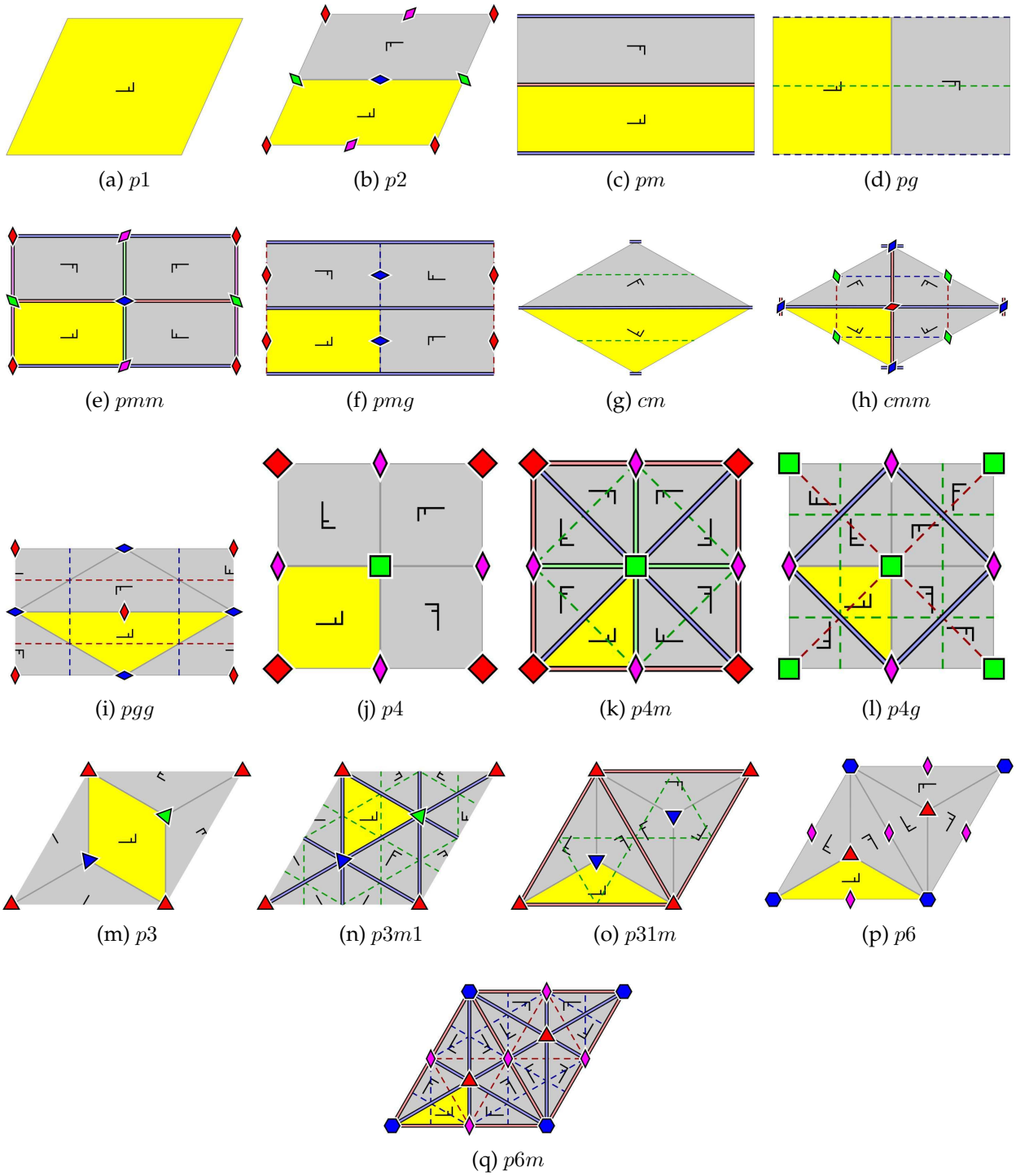
The d-glide is called the *diamond glide* and is present in the diamond lattice.

Be forewarned that it is possible for a *symmorphic* space group to include screw and glide operations provided they are *removable* by choosing a different origin. Such nonsymmorphic operations are called *inessential*. In other words, if $\mathcal{S}$ contains nonsymmorphic operations (screws or glides), but there exists some $\rho \equiv \{\, h \,|\, \boldsymbol{s} \,\}$ such that all elements of $\rho^{-1}\mathcal{S}\rho$ are of the form $\{\, g \,|\, \boldsymbol{R} \,\}$, then $\mathcal{S}$ is symmorphic. A nonsymmorphic space group contains *essential* (*i.e.* unremovable) screws or glides[23].

5.3.2 Factor groups

In the dim and distant past – specifically, in §1.3.1 – we discussed the concept of a *factor group*. Recall that if $H \subset G$ is a subgroup, there is a unique *left coset decomposition* of G as $G = \bigcup_i r_i\, H$ where $i \in \{1, \ldots, N_G/N_H\}$. If $H \triangleleft G$ is a normal subgroup, meaning $gHg^{-1} \in H$ for all $g \in G$, the cosets $r_i\, H$ form a group under multiplication, called the *factor group* G/H.

[23] As noted above, there are two nonsymmorphic space groups which contain neither screws nor glides, but for which one can nevertheless not write $\mathcal{S} = \mathcal{P} \rtimes \mathcal{T}$.



(a) $p1$ (b) $p2$ (c) pm (d) pg

(e) pmm (f) pmg (g) cm (h) cmm

(i) pgg (j) $p4$ (k) $p4m$ (l) $p4g$

(m) $p3$ (n) $p3m1$ (o) $p31m$ (p) $p6$

(q) $p6m$

Figure 5.20: Unit cells for the 17 two-dimensional space groups (wallpaper groups). (Image credit: *Wikipedia*.)

crystal system	type	symmorphic space groups
triclinic	P	$P1$, $P\overline{1}$
monoclinic	P	$P2$, Pm , $P2/m$
	A/C	$C2$, Cm , $C2/m$
orthorhombic	P	$P222$, $Pmm2$, $Pmmm$
	A/C	$C222$, $Cmm2$, $Cmmm$, $Amm2$
	I	$I222$, $Imm2$, $Immm$
	F	$F222$, $Fmm2$, $Fmmm$
tetragonal	P	$P4$, $P\overline{4}$, $P4/m$, $P422$, $P4mm$
		$P\overline{4}2m$, $P\overline{4}m2$, $P4/mmm$
	I	$I4$, $I\overline{4}$, $I4/m$, $I422$, $I4mm$
		$I\overline{4}2m$, $I\overline{4}m2$, $I4/mmm$
trigonal	P	$P3$, $P\overline{3}$, $P321$, $P3m1$, $P\overline{3}m1$
		$P312$, $P31m$, $P\overline{3}1m$
(rhombohedral)	R	$R3$, $R\overline{3}$, $R32$, $R3m$, $R\overline{3}m$
hexagonal	P	$P6$, $P\overline{6}$, $P6/m$, $P622$, $P6mm$
		$P\overline{6}m2$, $P\overline{6}2m$, $P6/mmm$
cubic	P	$P23$, $Pm3$, $P432$, $P\overline{4}3m$, $Pm\overline{3}m$
	I	$I23$, $Im3$, $I432$, $I\overline{4}3m$, $Im\overline{3}m$
	F	$F23$, $Fm3$, $F432$, $F\overline{4}3m$, $Fm\overline{3}m$

Table 5.16: The 73 symmorphic three-dimensional space groups and their short notation. Bravais lattice types are primitive (P), base-centered (A/C), body-centered (I), and face-centered (F). Space groups printed in red indicate cases where there are two inequivalent $\mathcal{P}$-invariant space lattice orientations.

Since the abelian group $\mathcal{T}$ of Bravais lattice translations is a normal subgroup of the space group, we can decompose $\mathcal{S}$ as

$$\mathcal{S} = \bigcup_g \left\{ g \,\middle|\, \boldsymbol{\tau}_g \right\} \mathcal{T} = \mathcal{T} + \left\{ g_2 \,\middle|\, \boldsymbol{\tau}_{g_2} \right\} \mathcal{T} + \ldots + \left\{ g_{N_{\mathcal{P}}} \,\middle|\, \boldsymbol{\tau}_{g_{N_{\mathcal{P}}}} \right\} \mathcal{T} \quad . \tag{5.61}$$

This says that the space group $\mathcal{S}$ is generated by all Bravais lattice translations $\left\{ E \,\middle|\, \boldsymbol{R} \right\}$ and all operations $\left\{ g \,\middle|\, \boldsymbol{\tau}_g \right\}$. If, as in §5.3.5 below, we impose periodic boundary conditions, so that space is compactified into a three-dimensional torus of $N_1 \times N_2 \times N_3$ unit cells, then the translation group $\mathcal{T}$ is of finite order $|\mathcal{T}| = N_1 N_2 N_3$, and the order of the space group is $|\mathcal{S}| = |\mathcal{P}| \cdot |\mathcal{T}|$.

The set of operations $\left\{ g \,\middle|\, \boldsymbol{\tau}_g \right\}$ is thus the factor group $\mathcal{F} \equiv \mathcal{S}/\mathcal{T}$. While there exists a bijective map $\left\{ g \,\middle|\, \boldsymbol{\tau}_g \right\} \longleftrightarrow \left\{ g \,\middle|\, \boldsymbol{0} \right\}$ between the factor group $\mathcal{F}$ and the point group $\mathcal{P}$, multiplication within the factor group is always modulo $\mathcal{T}$. Group multiplication of the factor group elements results in a projective

representation of the point group,

$$\left\{\, g \,\middle|\, \boldsymbol{\tau}_g \,\right\} \left\{\, h \,\middle|\, \boldsymbol{\tau}_h \,\right\} = \left\{\, E \,\middle|\, \boldsymbol{R}_{g,h} \,\right\} \left\{\, gh \,\middle|\, \boldsymbol{\tau}_{gh} \,\right\} \quad , \tag{5.62}$$

and one can *lift* the projective representation of $\mathcal{P}$ to its *central extension*, which is to say $\mathcal{S}$. Here

$$\boldsymbol{R}_{g,h} = \boldsymbol{\tau}_g + g\boldsymbol{\tau}_h - \boldsymbol{\tau}_{gh} \tag{5.63}$$

must be in the Bravais lattice. Note that the cocycles here are actually translation operators rather than actual phases. Below we shall see how by diagonalizing the translation part of the space group, the cocycles become phases.

The case of diamond

Diamond is a rather typical nonsymmorphic space group. Recall the primitive direct lattice vectors for the fcc Bravais lattice,

$$\boldsymbol{a}_1 = \tfrac{1}{2}a_0\,(0,1,1) \quad , \quad \boldsymbol{a}_2 = \tfrac{1}{2}a_0\,(1,0,1) \quad , \quad \boldsymbol{a}_3 = \tfrac{1}{2}a_0\,(1,1,0) \quad , \tag{5.64}$$

where a_0 is the side length of the simple cubic lattice whose four element basis describes the fcc structure. The space group of diamond is $\mathcal{S} = Fd\overline{3}m$, this the point group is $m\overline{3}m$, which is O_h. Thus there are 48 cosets in the factor group $\mathcal{F}$, which is the order of O_h. These cosets break up into two collections. One consists of operations of the form $\left\{\, h \,\middle|\, \mathbf{0} \,\right\} \mathcal{T}$ where $h \in T_d$. The other consists of operations of the form $\left\{\, I \,\middle|\, \boldsymbol{\tau} \,\right\} \left\{\, h \,\middle|\, \mathbf{0} \,\right\} \mathcal{T}$ where I is the inversion operator and $\boldsymbol{\tau} = \frac{1}{4}\boldsymbol{a}_1 + \frac{1}{4}\boldsymbol{a}_2 + \frac{1}{4}\boldsymbol{a}_3 = \frac{1}{4}a_0\,(1,1,1)$. The elements from the first collection thus constitute a group in their own right, which is the zincblende space group $\widetilde{\mathcal{S}} = F\overline{4}3m$. This is a normal subgroup of $\mathcal{S}$ of index two, *i.e.* $\mathcal{S}/\widetilde{\mathcal{S}} \cong \mathbb{Z}_2$. Explicitly, we then have $\mathcal{S} = \widetilde{\mathcal{S}} \cup \left\{\, I \,\middle|\, \boldsymbol{\tau} \,\right\} \widetilde{\mathcal{S}}$.

5.3.3 How to make a symmorphic space group

The simplest recipe:

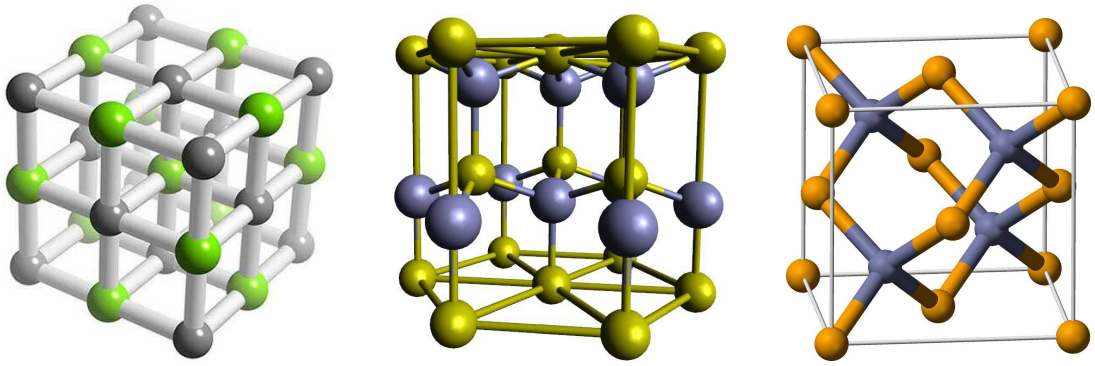
(i) Start with a lattice system.

(ii) Choose a point group consistent with the lattice system.

(iii) Choose an allowed lattice type (*i.e.* centering).

(iv) Congratulations, you've just specified a symmorphic point group.

To see this method in practice, let's try it out in two dimensions, where there 13 of the 17 space (wallpaper) groups are symmorphic. There are four crystal systems (oblique, rectangular, square, hexagonal), and the rectangular system can either have a primitive or a centered unit cell. For oblique lattices the allowed point groups are C_1 and C_2, so two possibilities. For rectangular lattices, the allowed point groups are C_{1v} and C_{2v}. There are two possible centerings, for a total of four possibilities. For square



(a) Rocksalt, $Fm\overline{3}m$ (b) Wurzite, $P6_3mc$ (c) Zincblende, $F\overline{4}3m$

Figure 5.21: Some common AB crystal structures and their space groups.

lattices, $\mathcal{P}$ can be either C_4 or C_{4v} – another two. For hexagonal, either C_3, C_{3v}, C_6, or C_{6v}, so four total. We arrive at 12 so we are missing a space group. The reason is there can be two inequivalent orientations of the space lattice which the point group leaves invariant, thereby leading to another space group. This happens in the case of the hexagonal lattice with C_{3v} ($3m$) point group symmetry. There are two space groups, called $p3m1$ and $p31m$.

A table of the 17 wallpaper groups is provided in Tab. 5.15, and sketches of the unit cells of each of them are depicted in Fig. 5.20. Study the nonsymmorphic cases pg, pmg, pgg, and $p4g$ to see if you can identify the glide mirrors. Note also how the naming convention works: the leading p or c character stands for primitive or centered. Information about the point group is contained in the space group label. Finally, the symbol g is used to indicate the presence of a glide mirror.

The naming convention for three-dimensional space groups is somewhat more complex, but the procedure is as described in the above recipe. There are seven distinct crystal systems, and Bravais lattice types are either primitive (P), base-centered (A/C), body-centered (I), or face-centered (F). Consider an fcc lattice with point group O_h ($m\overline{3}m$ in HM short notation). The corresponding symmorphic space group is $Fm\overline{3}m$, the full symbol for which is $F\frac{4}{m}\overline{3}\frac{2}{m}$. Proceeding in this way, accounting for all the crystal systems, their allowed point groups, and possible centerings, one obtains 66 symmorphic space groups. As in the two-dimensional case, when inequivalent orientations of the space lattice are both preserved by the point group, we get an extra space group. Such cases are indicated in red in Tab. 5.16. For example, for the case $C_{2v} = mm2$, the A and C centering types lead to different space groups, $Amm2$ and $Cmm2$, respectively. They are distinct space groups because in the latter case the centering is along a twofold axis, while in the former it is not.

5.3.4 Nonsymmorphic space groups

Returning to our example space group $F\frac{4}{m}\overline{3}\frac{2}{m}$, a check of the tables[24] reveals that there are a total of four space groups generated from the fcc lattice and point group $O_h = \frac{4}{m}\overline{3}\frac{2}{m}$. The other three are $F\frac{4}{m}\overline{3}\frac{2}{c}$, $F\frac{4_1}{d}\overline{3}\frac{2}{m}$, and $F\frac{4_1}{d}\overline{3}\frac{2}{c}$; their short names are $Fm\overline{3}c$, $Fd\overline{3}m$, and $Fd\overline{3}c$, respectively. These three space

[24] See http://www.wikiwand.com/en/List_of_space_groups.

groups are all nonsymmorphic and involve either screws (4_1), glides (c, d), or both. The second of these three corresponds to carbon diamond. Schoenflies' names for the four point groups generated from fcc and O_h were O_h^5, O_h^6, O_h^7, and O_h^8, respectively, which convey little information other than the order in which he derived them from the point group O_h.[25]

Of the 230 three-dimensional space groups, 157 are nonsymmorphic and contain operations $\{ g \,|\, \boldsymbol{\tau}_g \}$ where $\boldsymbol{\tau}_g \notin \mathcal{T}$ is not in the direct lattice, and no single change of origin can reduce all the $\boldsymbol{\tau}_g$ to zero or to a direct lattice vector.

Some of the nonsymmorphic space groups with screw axes have mirror images, and together are known as *enantiomorphic pairs*. For example, space groups $(P4_1\,,\, P4_3)$ form such a pair, as do $(P4_12_12\,,\, P4_32_12)$, $(P3_112\,,\, P3_212)$, $(P6_222\,,\, P6_422)$, *etc.*

5.3.5 Translations and their representations

The set of translations $\mathcal{T}$ is a subgroup of $\mathcal{S}$, consisting of the elements $\{ E \,|\, \boldsymbol{R} \}$, where $\boldsymbol{R} = \sum_{j=1}^d m_j \, \boldsymbol{a}_j$ is a sum over the primitive direct lattice vectors with integer coefficients. It is convenient to work with discrete groups of finite order, so to this end we invoke periodic boundary conditions, which places our system on a d-dimensional torus extending for N_j unit cells in the $\boldsymbol{a}_j$ direction for each $j \in \{1, \ldots, d\}$. This means that $\boldsymbol{R}$ is equivalent to $\boldsymbol{R} + \sum_{j=1}^d l_j \, \boldsymbol{L}_j$ with $L_j = N_j \, \boldsymbol{a}_j$ and each $l_j \in \mathbb{Z}$. Our Bravais lattice translation group $\mathcal{T}$ now has $N = \prod_{j=1}^d N_j$ elements, which is the total number of unit cells in the real space torus.

Next we ask about irreducible representations of $\mathcal{T}$. Since $\mathcal{T}$ is an abelian group, all its IRREPs are one-dimensional. If $\psi(\boldsymbol{r})$ is a basis function for a unitary one-dimensional IRREP of $\mathcal{T}$, then

$$\{ E \,|\, \boldsymbol{R} \}\, \psi(\boldsymbol{r}) = \psi\big(\{ E \,|\, \boldsymbol{R} \}^{-1} \boldsymbol{r}\big) = \psi(\boldsymbol{r} - \boldsymbol{R}) = e^{-i\omega(\boldsymbol{R})}\, \psi(\boldsymbol{r}) \quad . \tag{5.65}$$

In order that the group multiplication law be satisfied, we must have $e^{-i\omega(\boldsymbol{R})}\, e^{-i\omega(\boldsymbol{R}')} = e^{-i\omega(\boldsymbol{R}+\boldsymbol{R}')}$, which tells us that $\omega(\boldsymbol{R})$ is linear in $\boldsymbol{R}$, *i.e.*

$$\omega(m_1 \, \boldsymbol{a}_1 + \ldots + m_d \, \boldsymbol{a}_d) = m_1 \, \omega(\boldsymbol{a}_1) + \ldots + m_d \, \omega(\boldsymbol{a}_d) \tag{5.66}$$

to within an additive multiple of 2π. We may define $\omega(\boldsymbol{a}_j) \equiv \theta_j$, in which case the IRREP is labeled by the set of angles $\boldsymbol{\theta}$. Furthermore, we must have $\omega(\boldsymbol{R}) = \omega(\boldsymbol{R} + \boldsymbol{L}_j)$ for all $j \in \{1, \ldots, d\}$, which says that $N_j \, \theta_j$ is congruent to zero modulo 2π, *i.e.* $\theta_j = 2\pi l_j / N_j$, where $l_j \in \{1, \ldots, N_j\}$. So the θ_j values are quantized and there are $N = \prod_j N_j$ distinct values of the vector $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_d)$.

Recall the definition of the reciprocal lattice vectors $\boldsymbol{b}_j$ which satisfy $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi \, \delta_{ij}$. Then if we define the wavevector $\boldsymbol{k} \equiv \sum_{j=1}^d \theta_j \, \boldsymbol{b}_j / 2\pi$, we then have $\omega(\boldsymbol{R}) = \boldsymbol{k} \cdot \boldsymbol{R}$, and our basis functions may be written as $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = u(\boldsymbol{r})\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ where $u(\boldsymbol{r} - \boldsymbol{R}) = u(\boldsymbol{r})$ for all $\boldsymbol{R} \in \mathcal{L}$ is a periodic *cell function*. Any cell function may be expanded as a discrete Fourier series, *viz.*

$$u(\boldsymbol{r}) = \sum_{\boldsymbol{K}} C_{\boldsymbol{K}}\, e^{i\boldsymbol{K}\cdot\boldsymbol{r}} \quad , \tag{5.67}$$

[25] Schoenflies' O_h^1 through O_h^4 correspond to primitive cubic lattices, and O_h^9 and O_h^{10} to bcc lattices.

system	$\mathcal{P}^{(\mathrm{Sch})}$	$\mathcal{P}^{\mathrm{HM}}$	$N_{\mathcal{P}}$	nonsymmorphic space groups
triclinic	C_1	1	1	none
	C_i	$\overline{1}$	2	none
monoclinic	C_2	2	2	$P2_1$
	C_s	m	2	Pc, Cc
	C_{2h}	$2/m$	4	$P2_1m$, $P2/c$, $P2_1/c$, $C2/c$
orthorhombic	D_2	222	4	$P222_1$, $P2_12_12$, $P2_12_12_1$, $C222_1$, $I2_12_12_1$
	C_{2v}	$mm2$	4	$Pmc2_1$, $Pcc2$, $Pma2$, $Pca2_1$, $Pnc2$, $Pmn2_1$, $Pba2$,
				$Pna2_1$, $Pnn2$
				$Cmc2_1$, $Ccc2$, $Abm2$, $Ama2$, $Aba2$, $Fdd2$, $Iba2$, $Ima2$
	D_{2h}	mmm	8	$Pnnn$, $Pccm$, $Pban$, $Pmma$, $Pnna$, $Pmna$, $Pcca$, $Pbam$,
				$Pccm$, $Pbcm$, $Pnnm$, $Pmmn$, $Pbcn$, $Pbca$, $Pnma$
				$Cmcm$, $Cmca$, $Cccm$, $Cmma$, $Ccca$, $Fddd$, $Ibam$, $Ibcm$, $Imma$
tetragonal	C_4	4	4	$P4_1$, $P4_2$, $P4_3$, $I4_1$
	S_4	$\overline{4}$	4	none
	C_{4h}	$4/m$	8	$P4_2/m$, $P4/n$, $P4_2/n$, $I4_1/a$
	D_4	422	8	$P42_12_1$, $P4_122$, $P4_12_12$, $P4_222$, $P4_22_12$, $P4_322$, $P4_32_12$, $I4_122$
	C_{4v}	$4mm$	8	$P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$, $P4_2bc$
				$I4cm$, $I4_1md$, $I\overline{4}2d$
	D_{2d}	$\overline{4}2m$	8	$P\overline{4}2c$, $P\overline{4}2_1m$, $P\overline{4}2_1c$, $P\overline{4}c2$, $P\overline{4}c2$, $P\overline{4}n2$, $I\overline{4}c2$, $I\overline{4}2d$
	D_{4h}	$4/mmm$	16	$P4/mcc$, $P4/nbm$, $P4/nnc$, $P4/mbm$, $P4/mnc$, $P4/nmm$,
				$P4/ncc$, $P4_2/mmc$, $P4_2/mcm$, $P4_2/nbc$, $P4_2/nnm$, $P4_2/mbc$,
				$P4_2/mnm$, $P4_2/nmc$, $P4_2/ncm$
				$I4/mcm$, $I4_1/amd$, $I4_1/acd$
trigonal	C_3	3	3	$P3_1$, $P3_2$
	S_6	$\overline{3}$	3	none
	D_3	32	6	$P3_112$, $P3_121$, $P3_212$, $P3_221$
	C_{3v}	$3m$	6	$P31c$, $P3c1$, $R3c$
	D_{3d}	$\overline{3}m$	12	$P\overline{3}1c$, $P\overline{3}c1$, $R\overline{3}c$
hexagonal	C_6	6	6	$P6_1$, $P6_2$, $P6_3$, $P6_4$, $P6_5$
	C_{3h}	$\overline{6}$	6	none
	C_{6h}	$6/m$	12	$P6_3/m$
	D_6	622	12	$P6_122$, $P6_222$, $P6_322$, $P6_422$, $P6_522$
	C_{6v}	$6mm$	12	$P6cc$, $P6_3cm$, $P6_3mc$
	D_{3h}	$\overline{6}m2$	12	$P\overline{6}c2$, $P\overline{6}2c$
	D_{6h}	$6/mmm$	24	$P6/mcc$, $P6_3/mcm$, $P6_3/mmc$
cubic	T	23	12	$P2_13$, $I2_13$
	T_h	$m\overline{3}$	24	$Pn\overline{3}$, $Pa\overline{3}$, $Fd\overline{3}$, $Ia\overline{3}$
	O	432	24	$P4_132$, $P4_232$, $P4_332$, $I4_132$, $F4_132$
	T_d	$\overline{4}3m$	24	$P\overline{4}3n$, $F\overline{4}3c$, $I\overline{4}3d$
	O_h	$m\overline{3}m$	48	$Pn\overline{3}n$, $Pm\overline{3}n$, $Pn\overline{3}n$, $Fm\overline{3}c$, $Fd\overline{3}m$, $Fd\overline{3}c$, $Ia\overline{3}d$

Table 5.17: The 157 nonsymmorphic three-dimensional space groups.

where $\boldsymbol{K} = \sum_{j=1}^{d} n_j \, \boldsymbol{b}_j$ is a reciprocal lattice vector, which satisfies $\exp(i\boldsymbol{K}\cdot\boldsymbol{R}) = 1$ for all direct lattice vectors $\boldsymbol{R}$, and the $\{C_{\boldsymbol{K}}\}$ are a set of coefficients. What we have just shown is known as *Bloch's theorem*, which says that the eigenfunctions of any Hamiltonian $\hat{H}$ which commutes with all Bravais lattice translations may be written in the form $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, u(\boldsymbol{r})$, where $u(\boldsymbol{r})$ is a cell function and $\boldsymbol{k}$ lies within the first Brillouin zone of the reciprocal lattice. The reason that $\boldsymbol{k}$ is confined to this region is that $\boldsymbol{k} \to \boldsymbol{k} + \boldsymbol{K}$ amounts to a change of the cell function $u(\boldsymbol{r}) \to u(\boldsymbol{r})\, e^{i\boldsymbol{K}\cdot\boldsymbol{r}}$. Note that quantization of $\boldsymbol{\theta}$ entails quantization of $\boldsymbol{k}$ to one of N possible values.

The character of the space group element $\{\, E \,|\, \boldsymbol{R} \,\}$ in the $\boldsymbol{k}$ IRREP is thus $\chi^{(\boldsymbol{k})}(\boldsymbol{R}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$, in suitably abbreviated notation. The great orthogonality and completeness theorems then tell us

$$\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}} = N\,\delta_{\boldsymbol{k},\boldsymbol{k}'} \qquad , \qquad \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} = N\,\delta_{\boldsymbol{R},\boldsymbol{R}'} \quad . \tag{5.68}$$

In the limit $N \to \infty$, these equations become

$$\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}} = \hat{\Omega}\sum_{\boldsymbol{K}} \delta(\boldsymbol{k}' - \boldsymbol{k} - \boldsymbol{K}) \qquad , \qquad \Omega\int\limits_{\hat{\Omega}} \frac{d^d k}{(2\pi)^d}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} = \delta_{\boldsymbol{R},\boldsymbol{R}'} \quad . \tag{5.69}$$

The first of these is the generalized Poisson summation formula from Eqn. 5.7. In the second, the integral is over the first Brillouin zone, $\hat{\Omega}$. Recall $\mathrm{vol}(\Omega) = \Omega$ and $\mathrm{vol}(\hat{\Omega}) = \hat{\Omega} = (2\pi)^d/\Omega$.

5.3.6 Space group representations

We follow Lax §8.6 and §8.7. When solving for electronic or vibrational states of a crystal, the first order of business is to classify eigenstates by wavevector, *i.e.* to diagonalize the operations $\{\, E \,|\, \boldsymbol{R} \,\}$ in the space group $\mathcal{S}$. For states of crystal momentum $\boldsymbol{k}$, we have $\{\, E \,|\, \boldsymbol{R} \,\}\,|\,\boldsymbol{k},\lambda\,\rangle = e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\,|\,\boldsymbol{k},\lambda\,\rangle$, where λ denotes other quantum numbers not related to crystal momentum.

Acting on Bloch states, a general space group operation has the following action:

$$\begin{aligned} \{\, g \,|\, \boldsymbol{t} \,\}\, \overbrace{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, u(\boldsymbol{r})}^{\psi_{\boldsymbol{k}}(\boldsymbol{r})} &= \exp\Big[i\boldsymbol{k}\cdot \{\, g \,|\, \boldsymbol{t} \,\}^{-1}\boldsymbol{r} \Big]\, u\big(\{\, g \,|\, \boldsymbol{t} \,\}^{-1}\boldsymbol{r}\big) \\ &= e^{ig\boldsymbol{k}\boldsymbol{r}}\, u\big(g^{-1}(\boldsymbol{r}-\boldsymbol{t})\big) \equiv e^{ig\boldsymbol{k}\cdot\boldsymbol{r}}\, e^{-ig\boldsymbol{k}\cdot\boldsymbol{t}}\, \widetilde{u}(\boldsymbol{r}) = \widetilde{\psi}_{g\boldsymbol{k}}(\boldsymbol{r}) \quad , \end{aligned} \tag{5.70}$$

where if $u(\boldsymbol{r}) = \sum_{\boldsymbol{K}} C_{\boldsymbol{K}}\, e^{i\boldsymbol{K}\cdot\boldsymbol{r}}$ is the original cell function, then

$$\widetilde{u}(\boldsymbol{r}) = \sum_{\boldsymbol{K}} C_{g^{-1}\boldsymbol{K}}\, e^{-i\boldsymbol{K}\cdot\boldsymbol{t}}\, e^{i\boldsymbol{K}\cdot\boldsymbol{r}} \equiv \sum_{\boldsymbol{K}} \widetilde{C}_{\boldsymbol{K}}\, e^{i\boldsymbol{K}\cdot\boldsymbol{r}} \tag{5.71}$$

is a new cell function, *i.e.* it satisfies $\widetilde{u}(\boldsymbol{r}+\boldsymbol{R}) = \widetilde{u}(\boldsymbol{r})$ for all direct lattice vectors $\boldsymbol{R}$. Thus, application of $\{\, g \,|\, \boldsymbol{t} \,\} \in \mathcal{S}$ to a Bloch function $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ generates a new Bloch function $\widetilde{\psi}_{g\boldsymbol{k}}(\boldsymbol{r})$ at wavevector $g\boldsymbol{k}$.[26]

[26] The phase $e^{-ig\boldsymbol{k}\cdot\boldsymbol{t}}$ amounts to a gauge transformation.

Group and star of the wavevector $\boldsymbol{k}$

If $g\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{K}$, then $\{\, g \,|\, \boldsymbol{t} \,\}$ does not change the wavevector of the Bloch function. We define the *point group* $\mathcal{P}_{\boldsymbol{k}}$ *of the wavevector* $\boldsymbol{k}$ to be those point group operations $g \in \mathcal{P}$ which leave $\boldsymbol{k}$ unchanged up to a reciprocal lattice vector[27]. The space group of the wavevector $\mathcal{S}_{\boldsymbol{k}}$ is then all $\{\, g \,|\, \boldsymbol{t} \,\} \in \mathcal{S}$ for which $g \in \mathcal{P}_{\boldsymbol{k}}$. The *star of the wavevector* $\boldsymbol{k}$ is defined to be the set of points including $\boldsymbol{k}$ and all its images $g\boldsymbol{k}$, where $g \in \mathcal{P} \setminus \mathcal{P}_{\boldsymbol{k}}$.[28]

Algebra and representation of the space group

Recall the results of Eqns. 5.62 and 5.63. From

$$\{\, g \,|\, \boldsymbol{\tau}_g \,\}\, \{\, h \,|\, \boldsymbol{\tau}_h \,\} = \{\, E \,|\, \boldsymbol{R}_{g,h} \,\}\, \{\, gh \,|\, \boldsymbol{\tau}_{gh} \,\} = \{\, gh \,|\, \boldsymbol{\tau}_{gh} \,\}\, \{\, E \,|\, (gh)^{-1}\boldsymbol{R}_{g,h} \,\} \quad , \tag{5.72}$$

we see that, acting on a Bloch state,

$$\{\, g \,|\, \boldsymbol{\tau}_g \,\}\, \{\, h \,|\, \boldsymbol{\tau}_h \,\}\, \psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{-igh\boldsymbol{k}\cdot\boldsymbol{R}_{g,h}}\, \{\, gh \,|\, \boldsymbol{\tau}_{gh} \,\}\, \psi_{\boldsymbol{k}}(\boldsymbol{r}) \quad , \tag{5.73}$$

and so if g and h are both elements of $\mathcal{P}_{\boldsymbol{k}}$, then

$$\{\, g \,|\, \boldsymbol{\tau}_g \,\}\, \{\, h \,|\, \boldsymbol{\tau}_h \,\} = e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_{g,h}}\, \{\, gh \,|\, \boldsymbol{\tau}_{gh} \,\} \tag{5.74}$$

when acting on Bloch states of crystal momentum $\boldsymbol{k}$, where $\boldsymbol{R}_{g,h} = \boldsymbol{\tau}_g + g\boldsymbol{\tau}_h - \boldsymbol{\tau}_{gh}$ is a direct lattice vector. The above equation establishes a projective representation for $\mathcal{S}_{\boldsymbol{k}}$. Alternatively, one may define the operators

$$\Lambda_{\boldsymbol{k}}(g) \equiv \{\, g \,|\, \boldsymbol{\tau}_g \,\}\, e^{i\boldsymbol{k}\cdot\boldsymbol{\tau}_g} = \{\, g \,|\, \boldsymbol{R} + \boldsymbol{\tau}_g \,\}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\tau}_g)} \quad , \tag{5.75}$$

which act on states of crystal momentum $\boldsymbol{k}$, and which satisfy the projective algebra

$$\begin{aligned} \Lambda_{\boldsymbol{k}}(g)\,\Lambda_{\boldsymbol{k}}(h) &= \omega_{\boldsymbol{k}}(g,h)\,\Lambda(gh) \\ \omega_{\boldsymbol{k}}(g,h) &= e^{i\boldsymbol{k}\cdot(\boldsymbol{\tau}_h - g\boldsymbol{\tau}_h)} = e^{i\boldsymbol{K}_g\cdot\boldsymbol{\tau}_h} \end{aligned} \tag{5.76}$$

because $\boldsymbol{k}\cdot g\boldsymbol{\tau}_h = g^{-1}\boldsymbol{k}\cdot\boldsymbol{\tau}_h \equiv (\boldsymbol{k} - \boldsymbol{K}_g)\cdot\boldsymbol{\tau}_h$, with $\boldsymbol{K}_g = \boldsymbol{k} - g^{-1}\boldsymbol{k} = \boldsymbol{k} - \boldsymbol{k}g$.

Representations of symmorphic space groups

When $\mathcal{S}$ is symmorphic, $\boldsymbol{\tau}_g = 0$ for all $g \in \mathcal{P}$, hence $\omega_{\boldsymbol{k}}(g,h) = 1$ for all $\boldsymbol{k}$. We don't have to worry about projective representations of the little groups, and therefore

$$\begin{aligned} D^{\Gamma;\mathcal{S}_{\boldsymbol{k}}}\big(\{\, g \,|\, \boldsymbol{0} \,\}\big) &= D^{\Gamma;\mathcal{P}_{\boldsymbol{k}}}(g) \\ \chi^{\Gamma;\mathcal{S}_{\boldsymbol{k}}}\big(\{\, g \,|\, \boldsymbol{0} \,\}\big) &= \chi^{\Gamma;\mathcal{P}_{\boldsymbol{k}}}(g) \quad , \end{aligned} \tag{5.77}$$

i.e. we can use the ordinary point group representation matrices.

[27] $\mathcal{P}_{\boldsymbol{k}}$ is also known as the *little group* of $\boldsymbol{k}$.

[28] We use the notation $A \setminus B$ to denote set subtraction, with $B \subseteq A$. *I.e.* $A \setminus B = A - B$, which is to say the set of elements in A that are not in B.

Representations of nonsymmorphic space groups

If $\boldsymbol{k} \notin \partial\hat{\Omega}$ lies in the interior of the Brillouin zone and not on its boundary, then both $\boldsymbol{k}$ and $g^{-1}\boldsymbol{k}$ lie inside $\hat{\Omega}$, which means $\boldsymbol{k}_g = 0$ and the cocycle is unity: $\omega_{\boldsymbol{k}}(g,h) = 1$. Thus we have

$$\begin{aligned} D^{\Gamma\,;\mathcal{S}_{\boldsymbol{k}}}\big(\{\, g \,|\, \boldsymbol{\tau}_g \,\}\big) &= e^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_g}\, D^{\Gamma\,;\mathcal{P}_{\boldsymbol{k}}}(g) \\ \chi^{\Gamma\,;\mathcal{S}_{\boldsymbol{k}}}\big(\{\, g \,|\, \boldsymbol{\tau}_g \,\}\big) &= e^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_g}\, \chi^{\Gamma\,;\mathcal{P}_{\boldsymbol{k}}}(g) \quad , \end{aligned} \tag{5.78}$$

where Γ can only be the trivial representation if $\boldsymbol{k} \neq \mathbf{0}$. Again, we only need the ordinary point group representation matrices.

If $\boldsymbol{k} \in \partial\hat{\Omega}$, then $\mathcal{P}_{\boldsymbol{k}}$ may be nontrivial. In this case there are two possibilities:

(i) If there is a one-dimensional IRREP of $\mathcal{S}_{\boldsymbol{k}}$, $d_{\boldsymbol{k}}(g)$, with $d_{\boldsymbol{k}}(g)\, d_{\boldsymbol{k}}(h) = \omega_{\boldsymbol{k}}(g,h)\, d_{\boldsymbol{k}}(gh)$, define the ratio $\widetilde{\Lambda}_{\boldsymbol{k}}(g) \equiv \Lambda_{\boldsymbol{k}}(g)/d_{\boldsymbol{k}}(g)$. The operators $\widetilde{\Lambda}_{\boldsymbol{k}}(g)$ then satisfy $\widetilde{\Lambda}_{\boldsymbol{k}}(g)\,\widetilde{\Lambda}_{\boldsymbol{k}}(h) = \widetilde{\Lambda}_{\boldsymbol{k}}(gh)$, *i.e.* the point group multiplication table. Thus,

$$\begin{aligned} D^{\Gamma\,;\mathcal{S}_{\boldsymbol{k}}}\big(\{\, g \,|\, \boldsymbol{\tau}_g \,\}\big) &= e^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_g}\, d_{\boldsymbol{k}}(g)\, D^{\Gamma\,;\mathcal{P}_{\boldsymbol{k}}}(g) \\ \chi^{\Gamma\,;\mathcal{S}_{\boldsymbol{k}}}\big(\{\, g \,|\, \boldsymbol{\tau}_g \,\}\big) &= e^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_g}\, d_{\boldsymbol{k}}(g)\, \chi^{\Gamma\,;\mathcal{P}_{\boldsymbol{k}}}(g) \quad . \end{aligned} \tag{5.79}$$

and again we can use the ordinary point group representations.

(ii) If there is no one-dimensional IRREP of $\mathcal{S}_{\boldsymbol{k}}$, if one wishes to avoid needless work, one can consult tables, *e.g.* in appendix F of Lax, or appendix C of Dresselhaus, Dresselhaus, and Jorio.

5.4 Fourier Space Crystallography

Thus far our understanding of crystallography has been based on real space structures and their transformation properties under point and space group operations. An equivalent approach, originally due to Bienenstock and Ewald (1962), and formalized and further developed by Mermin and collaborators in the 1990s, focuses on the Fourier modes $\hat{\rho}(\boldsymbol{K})$ of the density $\rho(\boldsymbol{r})$. This is known in the literature as *Fourier space crystallography*[29]. Writing $\rho(\boldsymbol{r})$ as a Fourier sum,

$$\rho(\boldsymbol{r}) = \sum_{\boldsymbol{K}} \hat{\rho}(\boldsymbol{K})\, e^{i\boldsymbol{K}\cdot\boldsymbol{r}} \quad , \tag{5.80}$$

where each $\boldsymbol{K} \in \hat{\mathcal{L}}$. Since $\rho(\boldsymbol{r}) \in \mathbb{R}$ is real, we have $\hat{\rho}(-\boldsymbol{K}) = \hat{\rho}^*(\boldsymbol{K})$ for all $\boldsymbol{K} \in \hat{\mathcal{L}}$. The inverse of the above relation is

$$\hat{\rho}(\boldsymbol{K}) = \int d^d r\; \rho(\boldsymbol{r})\, e^{-i\boldsymbol{K}\cdot\boldsymbol{r}} \quad . \tag{5.81}$$

Note that if $\rho'(\boldsymbol{r}) = \rho(\boldsymbol{r} + \boldsymbol{d})$ then $\hat{\rho}'(\boldsymbol{K}) = \hat{\rho}(\boldsymbol{K})\, e^{i\chi(\boldsymbol{K})}$ where $\chi(\boldsymbol{K}) = \boldsymbol{K}\cdot\boldsymbol{d}$ is a linear function on $\hat{\mathcal{L}}$.

[29] Here we follow the pedagogical treatment in A. König and N. D. Mermin, *Am. J. Phys.* **68**, 525 (2000), with some minor notational differences.

5.4.1 Space group symmetries

We now ask how the $\hat{\rho}(\boldsymbol{K})$ transform under space group operations of the crystal. The general space group operation may be written as $\{\, g \,|\, \boldsymbol{R} + \boldsymbol{\tau}_g \,\}$. We have already accounted for the symmetries under Bravais lattice translations, which says that $\rho(\boldsymbol{r})$ is given as the above Fourier sum. So now restrict our attention to operations of the form $\{\, g \,|\, \boldsymbol{\tau}_g \,\}$. If $\rho(\boldsymbol{r})$ is invariant under all space group operations, we must have

$$\rho(\boldsymbol{r}) = \{\, g \,|\, \boldsymbol{\tau}_g \,\}\, \rho(\boldsymbol{r}) = \rho\big(\{\, g \,|\, \boldsymbol{\tau}_g \,\}^{-1} \boldsymbol{r}\big) = \rho\big(g^{-1}(\boldsymbol{r} - \boldsymbol{\tau}_g)\big) \quad . \tag{5.82}$$

Taking the Fourier transform, we have

$$\hat{\rho}(\boldsymbol{K}) = \int d^d r\, \rho\big(g^{-1}(\boldsymbol{r} - \boldsymbol{\tau}_g)\big)\, e^{-i\boldsymbol{K}\cdot\boldsymbol{r}} = \hat{\rho}(\boldsymbol{K}g)\, e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_g} \quad , \tag{5.83}$$

which is easily established by changing the integration variables[30] from $\boldsymbol{r}$ to $\boldsymbol{r}' = g^{-1}(\boldsymbol{r} - \boldsymbol{\tau}_g)$. Note that g denotes both an abstract element of the point group $\mathcal{P}$ as well as its 3×3 matrix representation, and that by $\boldsymbol{K}g$ we treat $\boldsymbol{K}$ as a row vector and multiply by the matrix of g on the right. We therefore have

$$\hat{\rho}(\boldsymbol{K}g) = \hat{\rho}(\boldsymbol{K})\, e^{i\phi_g(\boldsymbol{K})} \quad , \tag{5.84}$$

where $\phi_g(\boldsymbol{K}) = \boldsymbol{K} \cdot \boldsymbol{\tau}_g$ acts linearly on $\hat{\mathcal{L}}$, with $\phi_g(\boldsymbol{0}) \cong 0$ for all $g \in \mathcal{P}$ and $\phi_E(\boldsymbol{K}) \cong 0$ for all $\boldsymbol{K} \in \hat{\mathcal{L}}$. Here the symbol $\cong$ denotes equality modulo 2π. We call $\phi_g(\boldsymbol{K})$ a *phase function* on the reciprocal lattice.

We then have

$$\begin{aligned} \hat{\rho}(\boldsymbol{K}gh) &= \hat{\rho}(\boldsymbol{K}g)\, e^{i\phi_h(\boldsymbol{K}g)} = \hat{\rho}(\boldsymbol{K})\, e^{i\phi_g(\boldsymbol{K})}\, e^{i\phi_h(\boldsymbol{K}g)} \\ &= \hat{\rho}(\boldsymbol{K})\, e^{i\phi_{gh}(\boldsymbol{K})} \quad , \end{aligned} \tag{5.85}$$

and therefore the *group compatibility condition* for the phase functions is

$$\phi_{gh}(\boldsymbol{K}) \cong \phi_h(\boldsymbol{K}g) + \phi_g(\boldsymbol{K}) \quad , \tag{5.86}$$

which is the same condition as that in eqn. 5.63.

Suppose $\rho'(\boldsymbol{r})$ and $\rho(\boldsymbol{r})$ differ by a translation. Then $\hat{\rho}'(\boldsymbol{K}) = \hat{\rho}(\boldsymbol{K})\, e^{i\chi(\boldsymbol{K})}$, hence

$$\begin{aligned} \hat{\rho}'(\boldsymbol{K}g) &= \hat{\rho}'(\boldsymbol{K})\, e^{i\phi'_g(\boldsymbol{K})} = \hat{\rho}(\boldsymbol{K})\, e^{i\chi(\boldsymbol{K})}\, e^{i\phi'_g(\boldsymbol{K})} \\ &= \hat{\rho}(\boldsymbol{K}g)\, e^{i\chi(\boldsymbol{K}g)} = \hat{\rho}(\boldsymbol{K})\, e^{i\phi_g(\boldsymbol{K})}\, e^{i\chi(\boldsymbol{K}g)} \quad , \end{aligned} \tag{5.87}$$

and therefore

$$\phi'_{\boldsymbol{g}}(\boldsymbol{K}) \cong \phi_g(\boldsymbol{K}) + \overbrace{\chi(\boldsymbol{K}g) - \chi(\boldsymbol{K})}^{\chi(\boldsymbol{K}g - \boldsymbol{K})} \quad . \tag{5.88}$$

We say that the the above equation constitutes a *gauge transformation* and thus that the functions $\phi'_g(\boldsymbol{K})$ and $\phi_g(\boldsymbol{K})$ are *gauge equivalent*. We then have the following:

- ⋄ *A space group $\mathcal{S}$ is symmorphic iff there exists a gauge in which $\phi_g(\boldsymbol{K}) \cong 0$ for all $g \in \mathcal{P}$ and all $\boldsymbol{K} \in \hat{\mathcal{L}}$.*

[30] Since $g \in \mathsf{O}(n)$, we have that the Jacobian of the transformation is $|\det g| = 1$.

5.4.2 Extinctions

In §5.1.5 we noted how in certain crystals, the amplitude of Bravais lattice Bragg peaks observed in a diffraction experiment can be reduced or even extinguished due to the crystal structure. Bragg peak extinction is thus a physical manifestation of the crystallographic point group symmetry, and as such must be encoded in the gauge-invariant content of the phase functions. Suppose that $\boldsymbol{K}g = \boldsymbol{K}$. Then

$$\hat{\rho}(\boldsymbol{K}) = \hat{\rho}(\boldsymbol{K}g) = \hat{\rho}(\boldsymbol{K})\, e^{i\phi_g(\boldsymbol{K})} \quad , \tag{5.89}$$

and thus if $\phi_g(\boldsymbol{K}) \not\cong 0$, we necessarily have $\hat{\rho}(\boldsymbol{K}) = 0$, *i.e.* the Bragg peak at $\boldsymbol{K}$ is extinguished. $\boldsymbol{K}g = g^{\mathsf{T}}\boldsymbol{K} = \boldsymbol{K}$ means that $\boldsymbol{K}$ lies within the invariant subspace of g (and that of $g^{\mathsf{T}} = g^{-1}$ as well, of course). Now the only nontrivial ($g \neq E$) point group operations (in three dimensions) with invariant subspaces are (i) proper rotations r, and (ii) mirror reflections m. Every proper rotation has an invariant axis, and every mirror reflection has an invariant plane. We now consider the consequences of each for extinctions.

- *Mirrors* : If m is a mirror, then $m^2 = E$. Consider a reciprocal lattice vector $\boldsymbol{K} = \boldsymbol{K}m$ lying in the invariant plane of m. Then

$$0 \cong \phi_E(\boldsymbol{K}) \cong \phi_{m^2}(\boldsymbol{K}) \cong \phi_m(\boldsymbol{K}m) + \phi_m(\boldsymbol{K}) \cong 2\phi_m(\boldsymbol{K}) \quad . \tag{5.90}$$

  Thus, $2\phi_m(\boldsymbol{K}) \cong 0$ which means either $\phi_m(\boldsymbol{K}) \cong 0$ or $\phi_m(\boldsymbol{K}) \cong \pi$. *Unless $\phi_m(\boldsymbol{K}) = 0$ for all $\boldsymbol{K} = \boldsymbol{K}m$ in the mirror plane, we say that m is a glide mirror.* Let $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ be basis vectors for the two-dimensional sublattice of $\hat{\mathcal{L}}$ in the invariant plane of m. Linearity of the phase functions says

$$\phi_m(n_1\,\boldsymbol{\beta}_1 + n_2\,\boldsymbol{\beta}_2) = n_1\,\phi_m(\boldsymbol{\beta}_1) + n_2\,\phi_m(\boldsymbol{\beta}_2) \quad . \tag{5.91}$$

  Suppose now that $\phi_m(\boldsymbol{\beta}_1) \cong \phi_m(\boldsymbol{\beta}_2) \cong 0$. In this case, the mirror is ordinary and we have not a glide, *i.e.* there are no extinctions due to m. Next suppose $\phi_m(\boldsymbol{\beta}_1) \cong \pi$ and $\phi_m(\boldsymbol{\beta}_2) \cong 0$. In this case, we have extinctions for all $\boldsymbol{K} = n_1\,\boldsymbol{\beta}_1 + n_2\,\boldsymbol{\beta}_2$ with n_1 odd, for all n_2. A corresponding result holds for the case $\phi_m(\boldsymbol{\beta}_1) \cong 0$ and $\phi_m(\boldsymbol{\beta}_2) \cong \pi$. Finally, suppose $\phi_m(\boldsymbol{\beta}_1) \cong \phi_m(\boldsymbol{\beta}_2) \cong \pi$. Then $\boldsymbol{K}$ is extinguished whenever $n_1 + n_2$ is odd.

- *Proper rotations* : In this case, $r^n = E$ with $n = 2$, 3, 4, or 6. Suppose $\boldsymbol{K} = \boldsymbol{K}r$ lies along the invariant axis of r. Then

$$0 \cong \phi_E(\boldsymbol{K}) \cong \phi_{r^n}(\boldsymbol{K}) \cong n\,\phi_r(\boldsymbol{K}) \quad , \tag{5.92}$$

  which says $\phi_r(\boldsymbol{K}) = 2\pi j/n$. If $\phi_r(\boldsymbol{K}) = 0$ for all $\boldsymbol{K} = \boldsymbol{K}r$, the rotation is ordinary. *If $\phi_r(\boldsymbol{K}) \not\cong 0$ for any $\boldsymbol{K} = \boldsymbol{K}r$ along the invariant axis, we say that r is a screw.* Let $\boldsymbol{\beta}_1$ be the basis vector for $\boldsymbol{K}$ points along the invariant axis. Then $\phi_r(\boldsymbol{\beta}_1) \cong 2\pi j/n$, with $j \in \{0, \ldots, n-1\}$. The case $j = 0$ corresponds to an ordinary rotation. For $\boldsymbol{K} = l\,\boldsymbol{\beta}_1$, we have $\phi_r(\boldsymbol{K}) \cong 2\pi jl/n$, and Bragg vectors with $jl \neq 0$ modulo n are extinguished.

- *Special circumstances* : Suppose an n-fold proper rotation r lies within the invariant plane of a mirror m. Then $rmr = m$, *i.e.* $mrm = r^{-1}$. This is the case, for example, for the groups C_{nv}, D_{nd}, and D_{nh}. Let $\boldsymbol{K} = \boldsymbol{K}r = \boldsymbol{K}m$. Then

$$\begin{aligned} \phi_m(\boldsymbol{K}) &= \phi_{rmr}(\boldsymbol{K}) \cong \phi_{mr}(\boldsymbol{K}r) + \phi_r(\boldsymbol{K}) \\ &\cong \phi_r(\boldsymbol{K}rm) + \phi_m(\boldsymbol{K}r) + \phi_r(\boldsymbol{K}) \cong 2\phi_r(\boldsymbol{K}) + \phi_m(\boldsymbol{K}) \quad . \end{aligned} \tag{5.93}$$

We then have $2\phi_r(\boldsymbol{K}) \cong 0$, and so the screw symmetry is restricted to two possible cases: either $\phi_r(\boldsymbol{K}) \cong 0$ or $\phi_r(\boldsymbol{K}) \cong \pi$. Such a screw requires n even and $j = \frac{1}{2}n$.

Suppose next that the n-fold rotation axis is perpendicular to a mirror plane, as in the groups C_{nh} and D_{nh}. In this case $mr = rm$, and we have

$$\begin{aligned} \phi_{mr}(\boldsymbol{K}) &= \phi_r(\boldsymbol{K}m) + \phi_m(\boldsymbol{K}) \\ \phi_{rm}(\boldsymbol{K}) &= \phi_m(\boldsymbol{K}r) + \phi_r(\boldsymbol{K}) \quad . \end{aligned} \tag{5.94}$$

There are two interesting possibilities. First, if $\boldsymbol{K} = \boldsymbol{K}r$ is along the invariant axis of r, then $\boldsymbol{K}m = -\boldsymbol{K}$, and we have $\phi_r(\boldsymbol{K}) \cong \phi_r(-\boldsymbol{K}) \cong -\phi_r(\boldsymbol{K})$, hence $2\phi_r(\boldsymbol{K}) \cong 0$, which entails the same restrictions as in the case where $rmr = m$ analyzed above. Second, if $\boldsymbol{K}m = \boldsymbol{K}$, then we obtain $\phi_m(\boldsymbol{K}r) = \phi_m(\boldsymbol{K})$, which says that the diffraction pattern in the invariant plane, including any extinctions, is symmetric under the r operation.

5.4.3 Sticky bands

Consider now the Schrödinger equation $\hat{H}\psi = E\psi$, where[31]

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) \quad , \tag{5.95}$$

where $V(\boldsymbol{r})$ is invariant under space group operations. Typically $V(\boldsymbol{r})$ is purely due to (screened) Coulomb interactions between a given electron and the combined electron-ion charge density $\rho(\boldsymbol{r})$, in which case

$$V(\boldsymbol{r}) = \int d^d r' \, v(\boldsymbol{r} - \boldsymbol{r}') \, \rho(\boldsymbol{r}') \quad , \tag{5.96}$$

where $v(\boldsymbol{r}) = v(r)$ is the screened potential at separation $\boldsymbol{r}$. According to Bloch's theorem, eigenfunctions $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$ of H are labeled by crystal momentum $\boldsymbol{k} \in \hat{\Omega}$ as well as by a *band index* n, and may be written as

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{K}} C_{n\boldsymbol{k}}(\boldsymbol{K}) \, e^{i(\boldsymbol{K}+\boldsymbol{k})\cdot\boldsymbol{r}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r}) \quad , \tag{5.97}$$

where $u_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{R})$ is the cell function for band n, which is periodic in the direct lattice. The Schrödinger equation for band n can then be written as

$$E\, C_{n\boldsymbol{k}}(\boldsymbol{K}) = \sum_{\boldsymbol{K}'} \overbrace{\left[\frac{\hbar^2(\boldsymbol{K}+\boldsymbol{k})^2}{2m} \, \delta_{\boldsymbol{K},\boldsymbol{K}'} + \hat{V}(\boldsymbol{K} - \boldsymbol{K}') \right]}^{\langle\, \boldsymbol{K} \,|\, \hat{H}(\boldsymbol{k}) \,|\, \boldsymbol{K}' \,\rangle} C_{n\boldsymbol{k}}(\boldsymbol{K}') \quad , \tag{5.98}$$

where $\hat{V}(\boldsymbol{K}) = \hat{v}(\boldsymbol{K})\,\hat{\rho}(\boldsymbol{K})$, since the Fourier transform of a convolution is the product of the Fourier transforms. Since $v(\boldsymbol{r})$ is isotropic, we have $\hat{v}(\boldsymbol{q}\,g) = \hat{v}(\boldsymbol{q})$ for all $\boldsymbol{q}$, and therefore $\hat{V}(\boldsymbol{K}g) = \hat{V}(\boldsymbol{K})\, e^{i\phi_g(\boldsymbol{K})}$. Let us define $\hat{\omega}(\boldsymbol{q}) \equiv \hbar^2\boldsymbol{q}^2/2m$, which is the isotropic free particle dispersion. Note that

$$\hat{\omega}(\boldsymbol{K}g + \boldsymbol{k}) = \hat{\omega}\big((\boldsymbol{K} + \boldsymbol{k})\,g + (\boldsymbol{k} - \boldsymbol{k}\,g)\big) \quad . \tag{5.99}$$

We now (re-)introduce the notion of the *little group* of a wavevector:

[31] In this section, we will use hats to denote operators as well as Fourier transformed quantities, so keep on your toes to recognize the meaning of the hat symbol in context.

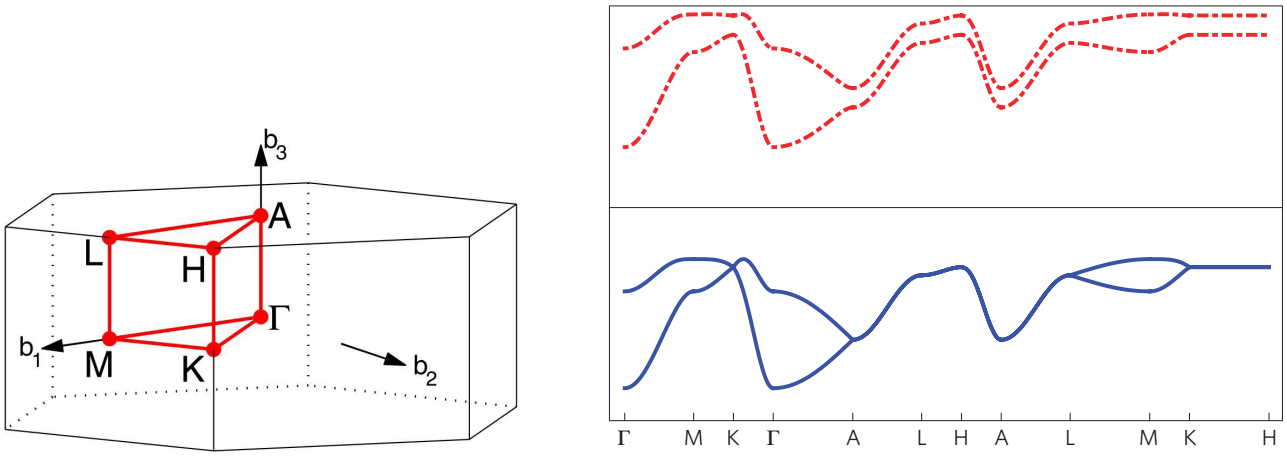


Figure 5.22: Stickiness of tight binding energy bands $\varepsilon_n(\boldsymbol{q})$ in an hcp crystal. Left: First Brillouin zone of the hexagonal Bravais lattice, with high symmetry points identified. Right: Tight binding energy levels for the hcp structure are shown in blue. Note the degeneracies at $\boldsymbol{q} = \mathrm{K}$, $\boldsymbol{q} = \mathrm{H}$, and all along the $\mathrm{A} - \mathrm{H} - \mathrm{L} - \mathrm{A}$ triangle on the top face and along the $\mathrm{K} - \mathrm{H}$ edge. When an alternating site energy on the two sublattices is present (dashed red curves), the screw symmetry is broken, and the space group is reduced from $P6_3/mmc$ to $P\overline{6}m2$.

DEFINITION : Given a wavevector $\boldsymbol{k} \in \hat{\Omega}$, the set of all $g \in \mathcal{P}$ for which $\boldsymbol{K}_g \equiv \boldsymbol{k} - \boldsymbol{k}g$ is in $\hat{\mathcal{L}}$ is called the *little group* of $\boldsymbol{k}$, and notated $\mathcal{P}_{\boldsymbol{k}}$.

Since $\boldsymbol{k}g$ must also lie within $\hat{\Omega}$, we have that $\mathcal{P}_{\boldsymbol{k}} = \{E\}$ if $\boldsymbol{k}$ lies at a generic point in the interior of the first Brillouin zone, *i.e.* not along an axis of rotational symmetry or along a mirror plane. However, if $\boldsymbol{k}$ lies in an invariant (one-dimensional) subspace of a proper rotation $r \in \mathcal{P}$ or within an invariant (two-dimensional) subspace of a mirror $m \in \mathcal{P}$, then $\boldsymbol{K}_r = \boldsymbol{k}r - \boldsymbol{k}$ and $\boldsymbol{K}_m = \boldsymbol{k}m - \boldsymbol{k}$ vanish, respectively, and the operations r and/or m are thus included in $\mathcal{P}_{\boldsymbol{k}}$.

For wavevectors $\boldsymbol{k} \in \partial\hat{\Omega}$ lying on the boundary of $\hat{\Omega}$, the little group $\mathcal{P}_{\boldsymbol{k}}$ can contain other elements. Consider for example the case of a square lattice, for which $\hat{\Omega}$ is itself a square, and let $\boldsymbol{k} = \frac{1}{2}\boldsymbol{b}_1$, which lies at the center of one of the edges. Let $\mathcal{P} = C_{4v}$, which is generated by r (90° rotation) and σ (x-axis reflection). Then E and σ are in $P_{\boldsymbol{k}}$ because they leave $\boldsymbol{k}$ fixed and hence $\boldsymbol{K}_g = \boldsymbol{0}$, but so are r^2 and σr^2, which send $\boldsymbol{k} \to -\boldsymbol{k}$, in which case $\boldsymbol{K}_g = \boldsymbol{b}_1 \in \hat{\mathcal{L}}$. It should be clear that $\mathcal{P}_{\boldsymbol{k}} \subset \mathcal{P}$ is a subgroup of the crystallographic point group, containing those operations $g \in \mathcal{P}$ which leave $\boldsymbol{k}$ invariant or changed by a reciprocal lattice vector. Note that if $g, h \in \mathcal{P}_{\boldsymbol{k}}$, then

$$\boldsymbol{K}_{gh} = \boldsymbol{k} - \boldsymbol{k}gh = (\boldsymbol{k} - \boldsymbol{k}h) + (\boldsymbol{k}h - \boldsymbol{k}gh) = \boldsymbol{K}_h + \boldsymbol{K}_g\, h \quad . \tag{5.100}$$

For each element g of the little group $\mathcal{P}_{\boldsymbol{k}}$, define the unitary operator $\hat{U}(g)$ such that

$$\hat{U}^\dagger(g) \,\big|\, \boldsymbol{K} \,\big\rangle = e^{i\phi_g(\boldsymbol{K})} \big|\, \boldsymbol{K}g - \boldsymbol{K}_g \,\big\rangle \quad . \tag{5.101}$$

We then have

$$\begin{aligned}\big\langle\, \boldsymbol{K} \,\big|\, \hat{U}(g)\,\hat{H}(\boldsymbol{k})\,\hat{U}^\dagger(g) \,\big|\, \boldsymbol{K}' \,\big\rangle &= \big\langle\, \boldsymbol{K}g - \boldsymbol{K}_g \,\big|\, \hat{H}(\boldsymbol{k}) \,\big|\, \boldsymbol{K}'g - \boldsymbol{K}_g \,\big\rangle\, e^{i\phi_g(\boldsymbol{K}'-\boldsymbol{K})} \\ &= \hat{\omega}\big(\boldsymbol{K}g - \boldsymbol{K}_g + \boldsymbol{K}\big)\,\delta_{\boldsymbol{K},\boldsymbol{K}'} + \hat{V}(\boldsymbol{K}-\boldsymbol{K}') \\ &= \hat{\omega}\big((\boldsymbol{K}+\boldsymbol{k})\,g\big)\,\delta_{\boldsymbol{K},\boldsymbol{K}'} + \hat{V}(\boldsymbol{K}-\boldsymbol{K}') = \big\langle\, \boldsymbol{K} \,\big|\, \hat{H}(\boldsymbol{k}) \,\big|\, \boldsymbol{K}' \,\big\rangle\end{aligned} \tag{5.102}$$

for all $\boldsymbol{k}$, $\boldsymbol{K}$, and $\boldsymbol{K}'$. This tells us that $\big[\hat{H}(\boldsymbol{k}), \hat{U}(g)\big] = 0$ for all $\boldsymbol{k} \in \hat{\Omega}$ and $g \in \mathcal{P}_{\boldsymbol{k}}$. Next, we have

$$\begin{aligned}\hat{U}^\dagger(h)\,\hat{U}^\dagger(g) \,\big|\, \boldsymbol{K} \,\big\rangle &= e^{i\phi_g(\boldsymbol{K})}\, e^{i\phi_h(\boldsymbol{K}g-\boldsymbol{K}_g)} \,\big|\, \boldsymbol{K}gh - \boldsymbol{K}_g\, h - \boldsymbol{K}_h \,\big\rangle \\ \hat{U}^\dagger(gh) \,\big|\, \boldsymbol{K} \,\big\rangle &= e^{i\phi_{gh}(\boldsymbol{K})} \,\big|\, \boldsymbol{K}gh - \boldsymbol{K}_{gh} \,\big\rangle \quad .\end{aligned} \tag{5.103}$$

Invoking Eqn. 5.100, we see that the ket vectors on the RHS of the above two equations are identical. Appealing to the compatibility condition Eqn. 5.86, we conclude $\hat{U}^\dagger(h)\,\hat{U}^\dagger(g) = \hat{U}^\dagger(gh)\,e^{-i\phi_h(\boldsymbol{K}_g)}$, *i.e.*

$$\hat{U}(g)\,\hat{U}(h) = \hat{U}(gh)\,e^{i\phi_h(\boldsymbol{K}_g)} \quad , \tag{5.104}$$

which is to say a projective representation of the little group.

Suppose $\hat{H}(\boldsymbol{k})\,|u_{\boldsymbol{k}}\rangle = E(\boldsymbol{k})\,|u_{\boldsymbol{k}}\rangle$, where $|u_{\boldsymbol{k}}\rangle$ is a Bloch cell function, and where we have dropped the band index n. Since $\big[\hat{H}(\boldsymbol{k}), \hat{U}(g)\big] = 0$, the state $\hat{U}(g)\,|u_{\boldsymbol{k}}\rangle$ is also an eigenstate of $\hat{H}(\boldsymbol{k})$ with eigenvalue $E(\boldsymbol{k})$. If $|u_{\boldsymbol{k}}\rangle$ is nondegenerate, then we must have $\hat{U}(g)\,|u_{\boldsymbol{k}}\rangle = \lambda_g(\boldsymbol{k})\,|u_{\boldsymbol{k}}\rangle$ for all $g \in \mathcal{P}_{\boldsymbol{k}}$. But then $\big[\hat{U}(g), \hat{U}(h)\big]|u_{\boldsymbol{k}}\rangle = 0$, which means

$$e^{i\phi_h(\boldsymbol{K}_g)}\,\hat{U}(gh)\,|u_{\boldsymbol{k}}\rangle = e^{i\phi_g(\boldsymbol{K}_h)}\,\hat{U}(hg)\,|u_{\boldsymbol{k}}\rangle \quad . \tag{5.105}$$

Thus, if $gh = hg$, we must have either (i) $\phi_h(\boldsymbol{K}_g) = \phi_g(\boldsymbol{K}_h)$ or else (ii) $|u_{\boldsymbol{k}}\rangle = 0$, *i.e.* there is no such nondegenerate eigenstate at wavevector $\boldsymbol{k}$. Therefore,

⋆ *If $gh = hg$ and $\phi_h(\boldsymbol{K}_g) \neq \phi_g(\boldsymbol{K}_h)$, all the eigenstates of $\hat{H}(\boldsymbol{k})$ appear in degenerate multiplets.*

That is, two or more bands become "stuck" together at these special $\boldsymbol{k}$ points. Note that the sticking conditions cannot be satisfied in a symmorphic space group, because the phase functions can all be set to zero by a choice of gauge (*i.e.* by a choice of origin for the point group operations). Note also that under a gauge transformation, the change in $\phi_h(\boldsymbol{K}_g) - \phi_g(\boldsymbol{K}_h)$ is

$$\Delta\big(\phi_h(\boldsymbol{K}_g) - \phi_g(\boldsymbol{K}_h)\big) = \chi(\boldsymbol{K}_g\, h - \boldsymbol{K}_g) - \chi(\boldsymbol{K}_h\, g - \boldsymbol{K}_h) = \chi(\boldsymbol{k}\, gh - \boldsymbol{k}\, hg) \quad , \tag{5.106}$$

which vanishes when $gh = hg$.

Since $\phi_g(\boldsymbol{0}) = 0$ for all g, the sticking conditions require that either $\boldsymbol{K}_g$ or $\boldsymbol{K}_h$ be nonzero. This is possible only when $\boldsymbol{k} \in \partial\hat{\Omega}$ lies on the boundary of the first Brillouin zone, for otherwise the vectors $\boldsymbol{K}_g$ and $\boldsymbol{K}_h$ are too short to be reciprocal lattice vectors[32]. Thus, in nonsymmorphic crystals, band sticking occurs only along the boundary. Consider, for example, the case of diamond, with nonsymmorphic space group $F\frac{4_1}{d}\bar{3}\frac{2}{m}$ ($Fd\bar{3}m$ in the short notation). The diamond structure consists of two interpenetrating

[32] My childhood dreams of becoming a reciprocal lattice vector were dashed for the same reason.

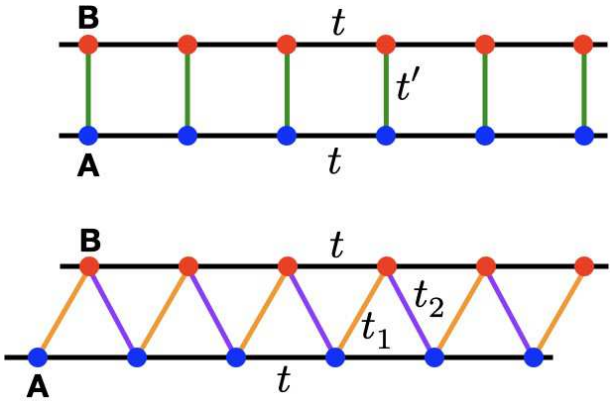


Figure 5.23: Two one-dimensional lattices: the ladder (top) and the trestle (bottom). The trestle is nonsymmorphic when the two classes of diagonal links are equivalent, *i.e.* when $t_1 = t_2$.

fcc Bravais lattices, and exhibits a 4_1 screw axis and a diamond (d) glide[33]. Let $\boldsymbol{k} = \frac{1}{2}\boldsymbol{K}$, where $\boldsymbol{K}$ is the shortest reciprocal lattice vector along the screw axis. Then $\boldsymbol{K}_r = \boldsymbol{k} - \boldsymbol{k}r = 0$ because $\boldsymbol{k}$ is along the invariant axis of the fourfold rotation r, hence r is in the little group. Diamond is centrosymmetric, meaning that its point group contains the inversion operator I, which commutes with all other point group elements. Clearly $\boldsymbol{K}_I = \boldsymbol{k} - I\boldsymbol{k} = 2\boldsymbol{k} = \boldsymbol{K}$, so I is in the little group as well. The sticking conditions then require $\phi_r(\boldsymbol{K}) \neq 0$, which is the condition we found for r to be a screw in the first place. So we have band sticking at $\boldsymbol{k} = \frac{1}{2}\boldsymbol{K}$. This is a special case of the following general rule: in nonsymmorphic centrosymmetric crystals, there is band sticking at every $\boldsymbol{k} = \frac{1}{2}\boldsymbol{K}$ where $\boldsymbol{K}$ is an extinguished reciprocal lattice (Bragg) vector.

Band sticking can also occur along *continuous lines* along the zone boundary. This is possible when the point group contains perpendicular mirrors, such as in the case D_{3h}. Let $\boldsymbol{k}$ lie along the line where the horizontal Brillouin zone surface intersects the vertical mirror plane. The vertical component of $\boldsymbol{k}$ is thus $\frac{1}{2}\boldsymbol{K}$, where $\boldsymbol{K}$ is the shortest vertical reciprocal lattice vector, but otherwise $\boldsymbol{k}$ can lie anywhere along this line. Then $\boldsymbol{K}_{m_h} = \boldsymbol{K}$ and $\boldsymbol{K}_{m_v} = 0$, for all $\boldsymbol{k}$ along the line, where $m_{h,v}$ are the horizontal and vertical mirror operations, respectively. The sticking condition is $\phi_{m_v}(\boldsymbol{K}) \neq 0$, which says that m_v is a glide mirror and $\boldsymbol{K}$ is extinguished. Introducing a perturbation which breaks the nonsymmorphic symmetries unsticks the bands and revives the extinguished Bragg vectors. An example is the hcp structure, shown in Fig. 5.22.

As an example, consider the two one-dimensional lattices in fig. 5.23. We shall call these the ladder (top) and the trestle (bottom). Their respective tight binding Hamiltonians are given by

$$\hat{H}^{\text{ladder}}(k) = -\begin{pmatrix} 2t\cos k & t' \\ t' & 2t\cos k \end{pmatrix} \quad , \quad \hat{H}^{\text{trestle}}(k) = -\begin{pmatrix} 2t\cos k & t_1 + t_2\, e^{-ik} \\ t_1 + t_2\, e^{ik} & 2t\cos k \end{pmatrix} \quad . \tag{5.107}$$

The dispersions are

$$\begin{aligned} E_\pm^{\text{ladder}}(k) &= -2t\cos k \pm t' \\ E_\pm^{\text{trestle}}(k) &= -2t\cos k \pm \left|t_1 + t_2 e^{-ik}\right| \quad . \end{aligned} \tag{5.108}$$

[33] Diamond has a diamond (d) glide. The d is for "duh".

d	Name	Examples	Space group	$\mathcal{S}$
2	Shastry–Sutherland	$SrCu_2(BO_3)_2$	*p*4*g*	2
3	hcp	Be, Mg, Zn	$P6_3/mmc$	2
3	Diamond	C, Si	$Fd\bar{3}m$	2
3	Pyrochlore	$Dy_2Ti_2O_7$ (spin ice)	$Fd\bar{3}m$	2
3	–	α-SiO_2, GeO_2	$P3_121$	3
3	–	$CrSi_2$	$P6_222$	3
3	–	$Pr_2Si_2O_7$, $La_2Si_2O_7$	$P4_1$	4
3	Hex. perovskite	$CsCuCl_3$	$P6_1$	6

Figure 5.24: Examples of space groups and their nonsymmorphic ranks.

The gaps $\Delta(k) = E_+(k) = E_-(k)$ are given by

$$\begin{aligned} \Delta^{\text{ladder}}(k) &= 2t' \\ \Delta^{\text{trestle}}(k) &= 2\left|t_1 + t_2 e^{-ik}\right| = 2\sqrt{(t_1 - t_2)^2 + 4t_1 t_2 \cos^2(\tfrac{1}{2}k)} \quad . \end{aligned} \tag{5.109}$$

Note that the ladder always has a direct gap, whereas the gap for the trestle vanishes at $k = \pi$ provided that $t_1 = t_2$. This latter condition ensures that the trestle is nonsymmorphic, where the nonsymmorphic space group element is reflection about the midline parallel to the two legs, followed by a lattice translation of half a unit cell.

A more detailed result was derived by Michel and Zak[34]. In nonsymmorphic crystals, energy bands stick together in groups of $\mathcal{S}$, where $\mathcal{S} = 2$, 3, 4, or 6 is the *nonsymmorphic rank* of the space group. In such cases, groups of $\mathcal{S}$ bands are stuck at high symmetry points or along high symmetry lines in the Brillouin zone, and one must fill an integer multiple of $\mathcal{S}$ bands of spinless electrons in order to construct a band insulating state.

[34] L. Michel and J. Zak, *Phys. Rev. B* **59**, 5998 (1999).

Chapter 6

Consequences of Crystallographic Symmetry

6.1 Atomic Physics and the Periodic Table

First, some atomic physics[1]. The eigenspectrum of single electron hydrogenic atoms is specified by quantum numbers $n \in \{1, 2, \ldots\}$, $l \in \{0, 1, \ldots, n-1\}$, $m_l \in \{-l, \ldots, +l\}$, and $m_s = \pm\frac{1}{2}$. The bound state energy eigenvalues $E_{nl} = -e^2/2na_{\text{B}}$, where $a_{\text{B}} = \hbar^2/me^2 = 0.529\,\text{Å}$ is the Bohr radius, depend only on the principal quantum number n. Accounting for electron-electron interactions using the Hartree-Fock method[2], the essential physics of *screening* is introduced, a result of which is that states of different l for a given n are no longer degenerate. Smaller l means lower energy since those states are localized closer to the nucleus, where the potential is less screened. Thus, for a given n, the smaller l states fill up first. For a given n and l, there are $(2s+1) \times (2l+1) = 4l+2$ states, labeled by m_l and m_s. This group of orbitals is called a *shell*.

6.1.1 Aufbau principle

Based on the HF energy levels, the order in which the electron shells are filled throughout the periodic table is roughly given by that in Tab. 6.1. This is known as the *Aufbau principle* from the German *Aufbau* = "building up". The order in which the orbitals are filled follows the *diagonal rule*, which says that orbitaPoisson bra ls with lower values of $n + l$ are filled before those with higher values, and that in the case of equal $n + l$ values, the orbital with the lower n is filled first. There are hiccups here and there. For example, in filling the 3d shell of the transition metal series (row four of the PT) , ^{21}Sc, ^{22}Ti, and ^{23}V, are configured as $[\text{Ar}]\,4\text{s}^2\,3\text{d}^1$, $[\text{Ar}]\,4\text{s}^2\,3\text{d}^2$, and $[\text{Ar}]\,4\text{s}^2\,3\text{d}^3$, respectively, but chromium's (dominant) configuration is $[\text{Ar}]\,4\text{s}^1\,3\text{d}^5$. Similarly, copper is $[\text{Ar}]\,4\text{s}^1\,3\text{d}^{10}$ rather than the expected $[\text{Ar}]\,4\text{s}^2\,3\text{d}^9$.

[1] An excellent discussion is to be found in chapter 20 of G. Baym's *Lectures on Quantum Mechanics*.

[2] Hartree-Fock theory tends to overestimate ground state atomic energies by on the order of 1 eV per pair of electrons. The reason is that electron-electron correlations are not adequately represented in the Hartree-Fock many-body wavefunctions, which are single Slater determinants.



Figure 6.1: The *Aufbau* principle and the diagonal rule. Image credit: Wikipedia.

For palladium, the diagonal rule predicts an electronic configuration $[\mathrm{Kr}]\,5\mathrm{s}^2\,4\mathrm{d}^8$ whereas experiments say it is $[\mathrm{Kr}]\,5\mathrm{s}^0\,4\mathrm{d}^{10}$. Go figure. Again, don't take this shell configuration stuff too seriously, because the atomic ground states are really linear combinations of different shell configurations, so we should really think of these various configurations as being the dominant ones among a more general linear combination of states. Row five pretty much repeats row four, with the filling of the 5s, 4d, and 5p shells. In row six, the lanthanide (4f) series interpolates between the 6s and 5d shells, as the 5f actinide series interpolates in row seven between 7s and 6d.

shell:	1s	2s	2p	3s	3p	4s	3d	4p	5s
termination:	^{2}He	^{4}Be	^{10}Ne	^{12}Mg	^{18}Ar	^{20}Ca	^{30}Zn	^{36}Kr	^{38}Sr
shell:	4d	5p	6s	4f	5d	6p	7s	5f/6d	
termination:	^{48}Cd	^{54}Xe	^{56}Ba	^{71}Lu	^{80}Hg	^{86}Rn	^{88}Ra	^{102}No	

Table 6.1: Rough order in which shells of the periodic table are filled.

6.1.2 Splitting of configurations: Hund's rules

The electronic configuration does not uniquely specify a ground state. Consider, for example, carbon, whose configuration is $1\mathrm{s}^2\,2\mathrm{s}^2\,2\mathrm{p}^2$. The filled 1s and 2s shells are inert. However, there are $\binom{6}{2} = 15$ possible ways to put two electrons in the 2p shell. It is convenient to label these states by total L, S, and J quantum numbers, where $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is the total angular momentum. It is standard to abbreviate each such multiplet as a *term* ${}^{2S+1}L_J$, where $L = \mathrm{S}, \mathrm{P}, \mathrm{D}, \mathrm{F}, \mathrm{G}$, *etc.*. For carbon, the largest L value we can get is $L = 2$, which requires $S = 0$ and hence $J = L = 2$. This 5-fold degenerate multiplet is then abbreviated ${}^{1}\mathrm{D}_2$. But we can also add together two $l = 1$ states to get total angular momentum $L = 1$ as well. The corresponding spatial wavefunction is antisymmetric, hence $S = 1$ in order to achieve a symmetric spin wavefunction. Since $|L - S| \leq J \leq |L + S|$ we have $J = 0$, $J = 1$, or $J = 2$ corresponding to multiplets ${}^{3}\mathrm{P}_0$, ${}^{3}\mathrm{P}_1$, and ${}^{3}\mathrm{P}_2$, with degeneracy 1, 3, and 5, respectively. The final state has $J = L = S = 0$: ${}^{1}\mathrm{S}_0$. The Hilbert space is then spanned by two $J = 0$ singlets, one $J = 1$ triplet, and two $J = 2$ quintuplets: $0 \oplus 0 \oplus 1 \oplus 2 \oplus 2$. That makes 15 states. Which of these terms corresponds to the

3d transition metal series ($[\mathrm{Ar}]$ core)									
^{21}Sc	^{22}Ti	^{23}V	^{24}Cr	^{25}Mn	^{26}Fe	^{27}Co	^{28}Ni	^{29}Cu	^{30}Zn
$4s^2\,3d^1$	$4s^2\,3d^2$	$4s^2\,3d^3$	$4s^1\,3d^5$	$4s^2\,3d^5$	$4s^2\,3d^6$	$4s^2\,3d^7$	$4s^2\,3d^8$	$4s^1\,3d^{10}$	$4s^2\,3d^{10}$

Table 6.2: Electronic configuration of 3d-series metals.

ground state?

The ordering of the multiplets is determined by the famous *Hund's rules*:

1. The LS multiplet with the *largest* S has the lowest energy.
2. If the largest value of S is associated with several multiplets, the multiplet with the *largest* L has the lowest energy.
3. If an incomplete shell is not more than half-filled, then the lowest energy state has $J = |L - S|$. If the shell is more than half-filled, then $J = L + S$.

Hund's rules are largely empirical, but are supported by detailed atomic quantum many-body calculations. Basically, rule #1 prefers large S because this makes the spin part of the wavefunction maximally symmetric, which means that the spatial part is maximally antisymmetric. Electrons, which repel each other, prefer to exist in a spatially antisymmetric state. As for rule #2, large L expands the electron cloud somewhat, which also keeps the electrons away from each other. For neutral carbon, the ground state has $S = 1$, $L = 1$, and $J = |L - S| = 0$, hence the ground state term is $^3\mathrm{P}_0$.

Let's practice Hund's rules on a couple of ions:

- P : The electronic configuration for elemental phosphorus is $[\mathrm{Ne}]\,3s^2\,3p^3$. The unfilled 3d shell has three electrons. First maximize S by polarizing all spins parallel (up, say), yielding $S = \frac{3}{2}$. Next maximize L consistent with Pauli exclusion, which says $L = -1 + 0 + 1 = 0$. Finally, since the shell is exactly half-filled, and not more, $J = |L - S| = \frac{3}{2}$, and the ground state term is $^4\mathrm{S}_{3/2}$.
- Mn^{4+} : The electronic configuration $[\mathrm{Ar}]\,4s^0\,3d^3$ has an unfilled 3d shell with three electrons. First maximize S by polarizing all spins parallel, yielding $S = \frac{3}{2}$. Next maximize L consistent with Pauli exclusion, which says $L = 2 + 1 + 0 = 3$. Finally, since the shell is less than half-filled, $J = |L - S| = \frac{3}{2}$. The ground state term is $^4\mathrm{F}_{3/2}$.
- Fe^{2+} : The electronic configuration $[\mathrm{Ar}]\,4s^0\,3d^6$ has an unfilled 3d shell with six electrons, or four holes. First maximize S by making the spins of the holes parallel, yielding $S = 2$. Next, maximize L consistent with Pauli exclusion, which says $L = 2 + 1 + 0 + (-1) = 2$ (adding L_z for the four holes). Finally, the shell is more than half-filled, which means $J = L + S = 4$. The ground state term is $^5\mathrm{D}_4$.
- Nd^{3+} : The electronic configuration $[\mathrm{Xe}]\,6s^0\,4f^3$ has an unfilled 4f shell with three electrons. First maximize S by making the electron spins parallel, yielding $S = \frac{3}{2}$. Next, maximize L consistent

n_p	0	1	2	3	4	5	6
L	0	1	1	0	1	1	0
S	0	$\frac{1}{2}$	1	$\frac{3}{2}$	1	$\frac{1}{2}$	0
J	0	$\frac{1}{2}$	0	$\frac{3}{2}$	2	$\frac{3}{2}$	0

n_d	0	1	2	3	4	5	6	7	8	9	10
L	0	2	3	3	2	0	2	3	3	2	0
S	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	2	$\frac{3}{2}$	1	$\frac{1}{2}$	0
J	0	$\frac{3}{2}$	2	$\frac{3}{2}$	0	$\frac{5}{2}$	4	$\frac{9}{2}$	4	$\frac{5}{2}$	0

n_f	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
L	0	3	5	6	6	5	3	0	3	5	6	6	5	3	0
S	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$	3	$\frac{5}{2}$	2	$\frac{3}{2}$	1	$\frac{1}{2}$	0
J	0	$\frac{5}{2}$	4	$\frac{9}{2}$	4	$\frac{5}{2}$	0	$\frac{7}{2}$	6	$\frac{15}{2}$	8	$\frac{15}{2}$	6	$\frac{7}{2}$	0

Table 6.3: Hund's rules applied to p, d, and f shells.

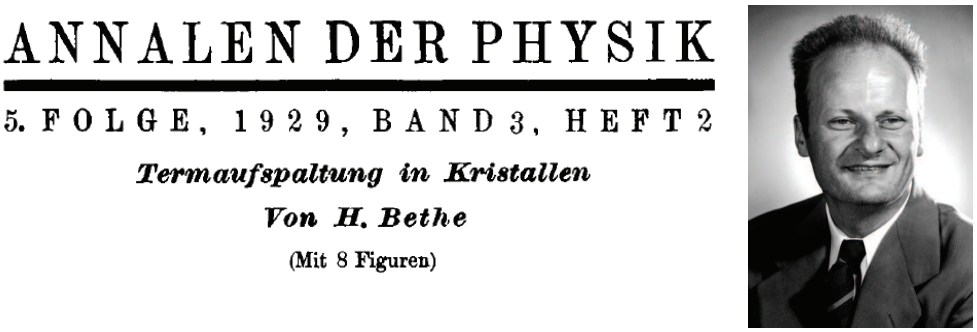
with Pauli exclusion: $L = 3 + 2 + 1 = 6$. Finally, because the shell is less than half-filled, we have $J = |L - S| = \frac{9}{2}$. The ground state term is ${}^4\mathrm{I}_{9/2}$.

For high Z ions, spin-orbit effects are very strong, and one cannot treat the angular momentum and spin degrees of freedom of the individual electrons separately. Rather, the electrons are characterized by their total angular momentum j, and the LS (Russell-Saunders) coupling scheme which gives rise to Hund's rules crosses over to another scheme called jj coupling[3]. In practice, pure jj coupling is rare, and the electronic structure of high Z atoms and ions reflects some intermediate situation between pure LS and pure jj schemes.

6.2 Crystal Field Theory

The Hamiltonian of an isolated atom or ion has the full rotational symmetry of $\mathsf{O}(3)$. In a crystalline environment, any electrons in an unfilled outer shell experience a *crystal electric field* due to the charges of neighboring ions. This breaks $\mathsf{O}(3)$ down to a discrete site group $\mathcal{P}(\boldsymbol{r})$, resulting in a new multiplet structure classified by the IRREPs of $\mathcal{P}(\boldsymbol{r})$. The program is therefore to identify the representation of $\mathsf{SO}(3)$ (possibly with half-odd-integer angular momentum) and decompose it into the IRREPs of the

[3]See, *e.g.*, P. H. Heckmann and E. Träbert, *Introduction to the Spectroscopy of Atoms* (North-Holland, 1989).


ANNALEN DER PHYSIK

5. FOLGE, 1929, BAND 3, HEFT 2

Termaufspaltung in Kristallen

Von H. Bethe

(Mit 8 Figuren)

Figure 6.2: Title from Bethe's original article on term splitting in crystals, *Ann. der Physik* **395**, 133-208 (1929), and a photo of Bethe.

appropriate site group using the decomposition formula

$$n_\Gamma(\Psi) = \frac{1}{N_G}\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma^*}(\mathcal{C})\,\chi^{\Psi}(\mathcal{C}) \quad . \tag{6.1}$$

If the crystal is symmorphic and the ion sits at a site of maximal symmetry, then the decomposition is with respect to the crystallographic point group $\mathcal{P}$. The foundations of this analysis were laid in 1929 by Hans Bethe in a seminal paper entitled *Termsaufspaltung in Kristallen* ("term splitting in crystals").

6.2.1 Decomposing IRREPs of O(3)

Our first order of business is to obtain the characters of the various point group class representatives in the representations of SO(3), $\chi^J(\mathcal{C})$, and then to invoke Eqn. 6.1 to decompose the terms ${}^{2S+1}L_J$ into the point group IRREPs[4] The individual classes $\mathcal{C}$ will contain elements which are either rotations $C(\alpha)$ through an angle α about an axis, inversion I, reflections in a plane $\sigma = I\,C(\pi)$, or rotoreflections $S(\alpha) = I\,C(\alpha - \pi)$. We consider each of these in turn:

- *Identity* : The character of the identity is the dimension of the O(3) IRREP. Thus $\chi^J(E) = 2J + 1$.
- *Proper rotations* : Recall how the group character, being the trace of a representation matrix, is invariant under a similarity transformation, and upon rotating to a frame where the invariant axis is $\hat{\boldsymbol{z}}$, the trace of the rotation matrix $D(\alpha, \hat{\boldsymbol{z}}) = \exp(-i\alpha J^z)$ is

$$\chi^J(\alpha) = \frac{\sin\,(J + \frac{1}{2})\alpha}{\sin\,\frac{1}{2}\alpha} \tag{6.2}$$

- *Inversion* : The inversion element I commutes with all other point group operations. Since $I^2 = 1$, the inversion eigenvalue is $\eta = \pm 1$. This is called the *parity*. For a single atomic orbital of angular momentum l, we have $\eta = (-1)^l$. But for the term ${}^{2S+1}L_J$, the parity is $\eta = \prod_i (-1)^{l_i}$, where l_i is

[4] When the ion is located at a site which is not of maximal symmetry, $\mathcal{P}$ will refer to the appropriate site group.

the angular momentum of the $i^{\rm th}$ electron state in the electron configuration associated with each term. Thus, if there are n electrons in the angular momentum l shell, the parity is $\eta = (-1)^{nl}$ which is not necessarily the same as $(-1)^L$. For example, the ground state term of nitrogen is ${}^4{\rm S}_{3/2}$, hence $L = 0$. But the corresponding electron configuration is $1{\rm s}^2\,2{\rm s}^2\,2{\rm p}^3$, hence $\eta = -1$. The character of the inversion operator is $\chi^J(I) = (2J+1)\,\eta$.

- *Reflections* : Every reflection can be written as $\sigma = I\,C(\pi)$. Therefore since I commutes with $C(\pi)$, their eigenvalues multiply and we have $\chi^J(\sigma) = \eta\,\sin(J+\frac{1}{2})\pi$.
- *Rotoreflections* : Since $S(\alpha) = I\,C(\alpha-\pi)$, we have $\chi^J(\widetilde{\alpha}) = \chi^J(\alpha-\pi)\,\eta$, where $\widetilde{\alpha}$ denotes rotoreflection through angle α.

We will first consider the case where $J \in \mathbb{Z}$, so we do not need to invoke the double groups. Another possible setting is that we might be neglecting spin-orbit effects and considering individual atomic orbitals of angular momentum l, in which case the parity is $\eta = (-1)^l$. For point group proper rotations, we have from Eqn. 6.2,

$$\chi^J(\pi) = \begin{cases} +1 & \text{if } J = 2k \\ -1 & \text{if } J = 2k+1 \end{cases} \quad , \quad \chi^J(2\pi/3) = \begin{cases} +1 & \text{if } J = 3k \\ 0 & \text{if } J = 3k+1 \\ -1 & \text{if } J = 3k+2 \end{cases} \tag{6.3}$$

and

$$\chi^J(\pi/2) = \begin{cases} +1 & \text{if } J = 4k \\ +1 & \text{if } J = 4k+1 \\ -1 & \text{if } J = 4k+2 \\ -1 & \text{if } J = 4k+3 \end{cases} \quad , \quad \chi^J(\pi/3) = \begin{cases} +1 & \text{if } J = 6k \\ +2 & \text{if } J = 6k+1 \\ +1 & \text{if } J = 6k+2 \\ -1 & \text{if } J = 6k+3 \\ -2 & \text{if } J = 6k+4 \\ -1 & \text{if } J = 6k+5 \end{cases} . \tag{6.4}$$

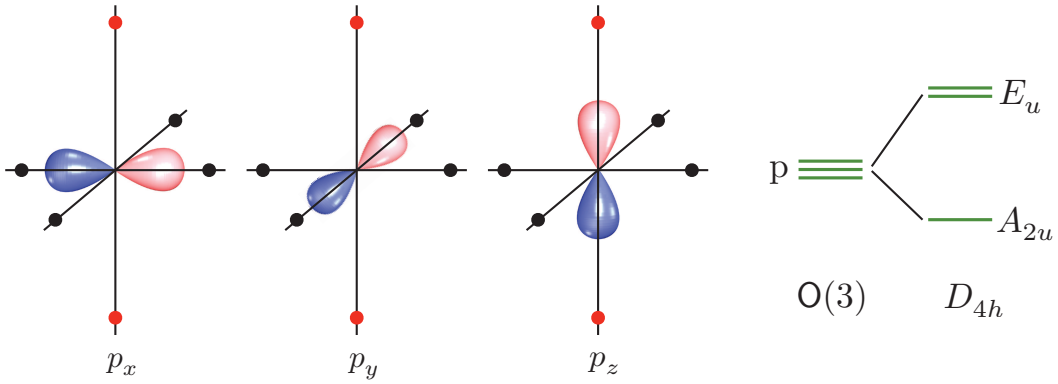


Figure 6.3: Atomic p orbital in a tetragonal environment with D_{4h} symmetry.

D_4	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	basis
A_1	1	1	1	1	1	x^2+y^2 or z^2
A_2	1	1	1	-1	-1	z or L_z
B_1	1	-1	1	1	-1	x^2-y^2
B_2	1	-1	1	-1	1	xy
E	2	0	-2	0	0	$\{x\,,\,y\}$ or $\{xz\,,\,yz\}$
1^- (p)	3	1	-1	-1	-1	$A_2 \oplus E$
2^+ (d)	5	-1	1	1	1	$A_1 \oplus B_1 \oplus B_2 \oplus E$

Table 6.4: Character table of D_4 and decomposition of atomic p- and d- levels in a D_4 environment. Note that $D_{4h} = D_4 \times C_i$.

6.2.2 Atomic levels in a tetragonal environment

Let's first consider a simple case of an atomic p-level placed in a tetragonal environment with D_4 symmetry, as depicted in Fig. 6.3. In free space, the p level is triply degenerate. Since D_4 is a proper point group, we only need the characters for the operations E, C_2, and C_4, which, according to the above computations, are

$$\chi^{l=1}(E) = 3 \quad , \quad \chi^{l=1}(C_2) = -1 \quad , \quad \chi^{l=1}(C_3) = 0 \quad , \quad \chi^{l=1}(C_4) = +1 \quad , \tag{6.5}$$

where we've included $\chi^{l=1}(C_3)$ as a bonus character. Using the representation decomposition formula of Eqn. 6.1, we then find $1^- = A_2 \oplus E$.

Suppose our environment has the full D_{4h} symmetry and not only D_4. Now $D_{4h} = D_4 \times C_i$, where $C_i = \{E, I\} \cong \mathbb{Z}_2$, and we know (see §2.4.6) that for an arbitrary group G, each conjugacy class $\mathcal{C}$ in G has a double $I\mathcal{C}$ in $G \times \mathbb{Z}_2$, and furthermore that each IRREP Γ of G spawns two IRREPs $\Gamma^\pm$ (also called Γ_g and Γ_u) for $G \times \mathbb{Z}_2$, with $\chi^{\Gamma^\pm}(\mathcal{C}) = \chi^\Gamma(\mathcal{C})$ and $\chi^{\Gamma^\pm}(I\,\mathcal{C}) = \pm\chi^\Gamma(\mathcal{C})$. Since p-states have parity $\eta = (-1)^l = -1$, we immediately know that in a D_{4h} environment, $1^- = A_{2u} \oplus E_u$.

What happens if we place an atomic d level in a tetragonal environment with D_{4h} symmetry? In this case we have

$$\chi^{l=2}(E) = 5 \quad , \quad \chi^{l=2}(C_2) = +1 \quad , \quad \chi^{l=2}(C_3) = -1 \quad , \quad \chi^{l=2}(C_4) = -1 \quad . \tag{6.6}$$

Accordingly we find $2^+ = A_1 \oplus B_1 \oplus B_2 \oplus E$ in D_4, and of course $2^+ = A_{1g} \oplus B_{1g} \oplus B_{1g} \oplus E_g$ in D_{4h}. Note that the labels u and g apply only when the site group symmetry includes inversion. Accordingly, in Tab. 6.6, the IRREPs for the two proper point groups T_d and D_3 do not include the g or u label.

6.2.3 Point charge model

We can understand the splitting of atomic levels in terms of the local crystal field potential due to the neighboring ions, which breaks the continuous $\mathrm{O}(3)$ atomic symmetry. Consider an electron at position

O	E	$8C_3$	$3C_2$	$6C_2'$	$6C_4$	basis
$\Gamma = A_1$	1	1	1	1	1	$x^2+y^2+z^2$
A_2	1	1	1	-1	-1	$L_x\,L_y\,L_z$ (sixth order in $\boldsymbol{r}$)
E	2	-1	2	0	0	$\{\sqrt{3}\,(x^2-y^2)\,,\,3z^2-r^2\}$
T_1	3	0	-1	-1	1	$\{x\,,\,y\,,\,z\}$
T_2	3	0	-1	1	-1	$\{yz\,,\,zx\,,\,xy\}$
$J^\eta = 0^\pm$	1	1	1	1	1	A_1
$1^\pm$	3	0	-1	-1	1	T_1
$2^\pm$	5	-1	1	1	-1	$E\oplus T_2$
$3^\pm$	7	1	-1	-1	-1	$A_2\oplus T_1\oplus T_2$
$4^\pm$	9	0	1	1	1	$A_1\oplus E\oplus T_1\oplus T_2$
$5^\pm$	11	-1	-1	-1	1	$E\oplus 2T_1\oplus T_2$

Table 6.5: Character table of O and decomposition of $\mathsf{O}(3)$ IRREPs in terms of O IRREPs.

$\boldsymbol{r}$ in the vicinity of the origin, and the electrostatic potential arising from a fixed ion at position $\boldsymbol{\Delta}$ (not necessarily a direct lattice vector). The Coulomb potential is proportional to

$$\frac{1}{|\boldsymbol{\Delta}-\boldsymbol{r}|} = \frac{1}{\Delta}\left(1-2\hat{\boldsymbol{\Delta}}\cdot\boldsymbol{u}+u^2\right)^{-1/2} \quad , \tag{6.7}$$

where $\boldsymbol{u}\equiv\boldsymbol{r}/\Delta$ and $\hat{\boldsymbol{\Delta}}\equiv\boldsymbol{\Delta}/\Delta$. Define $\varepsilon\equiv 2\hat{\boldsymbol{\Delta}}\cdot\boldsymbol{u}-u^2$. Then from Taylor's theorem,

$$(1-\varepsilon)^{-1/2} = 1+\tfrac{1}{2}\,\varepsilon+\tfrac{3}{8}\,\varepsilon^2+\tfrac{5}{16}\,\varepsilon^3+\tfrac{35}{128}\,\varepsilon^4+\ldots \quad . \tag{6.8}$$

We then have, keeping terms up to order u^4, and restoring the dimensionful variables,

$$\begin{aligned}\frac{1}{|\boldsymbol{\Delta}-\boldsymbol{r}|} = \frac{1}{\Delta}+\frac{\boldsymbol{\Delta}\cdot\boldsymbol{r}}{\Delta^3}+\frac{3\,(\boldsymbol{\Delta}\cdot\boldsymbol{r})^2-\Delta^2\,r^2}{2\Delta^5}+\frac{5(\boldsymbol{\Delta}\cdot\boldsymbol{r})^3-3\Delta^2\,(\boldsymbol{\Delta}\cdot\boldsymbol{r})\,r^2}{2\Delta^7}\\ +\frac{35(\boldsymbol{\Delta}\cdot\boldsymbol{r})^4-30\Delta^2\,(\boldsymbol{\Delta}\cdot\boldsymbol{r})^2\,r^2+3\Delta^4\,r^4}{8\Delta^9}+\ldots \quad .\end{aligned} \tag{6.9}$$

The local potential is given by

$$V(\boldsymbol{r}) = -\sum_{\boldsymbol{\Delta}}\frac{Z_{\boldsymbol{\Delta}}\,e^2}{\Delta}\,\frac{1}{|\hat{\boldsymbol{\Delta}}-\boldsymbol{u}|} \quad , \tag{6.10}$$

where the charge of the ion at position $\boldsymbol{\Delta}$ is $Z_{\boldsymbol{\Delta}}\,e$. The general result, using the spherical harmonic expansion, is

$$V_{\rm CF}(\boldsymbol{r}) = \sum_{\boldsymbol{\Delta}}\frac{4\pi Z_{\boldsymbol{\Delta}}e^2}{\Delta}\sum_{l=0}^{\infty}\frac{1}{2l+1}\left(\frac{r}{\Delta}\right)^l\sum_{m=-l}^{l}Y^*_{lm}(\hat{\boldsymbol{\Delta}})\,Y_{lm}(\hat{\boldsymbol{r}}) \quad . \tag{6.11}$$

In a tetragonal environment, the ions are located at $\boldsymbol{\Delta}=\pm a\,\hat{\boldsymbol{x}}$, $\pm a\,\hat{\boldsymbol{y}}$, and $\pm b\,\hat{\boldsymbol{z}}$. The isotropy of space is

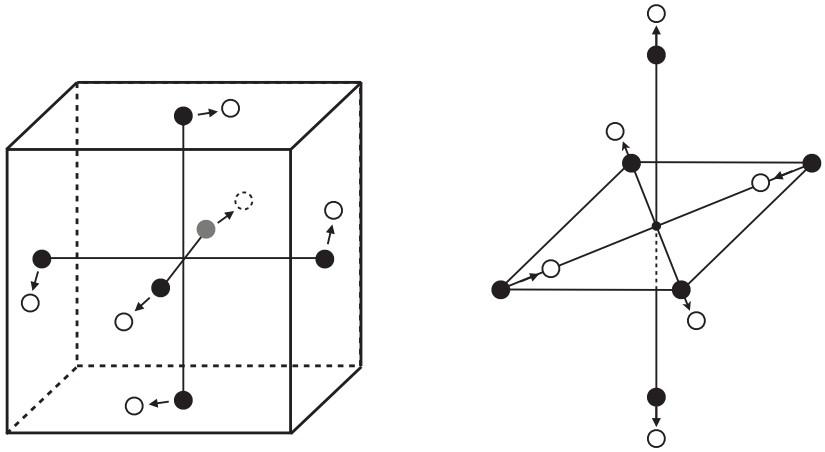


Figure 6.4: Trigonal and rhombic distortions of an octahedral environment.

already broken at $\mathcal{O}(r^2)$ of the expansion, and one finds, neglecting the constant piece,

$$V_{\rm tet}(\boldsymbol{r}) \ = \overbrace{-Ze^2\left(\frac{1}{a}-\frac{1}{b}\right)}^{A}\left(\frac{x^2}{a^2}+\frac{y^2}{a^2}-\frac{2z^2}{b^2}\right) \quad . \tag{6.12}$$

Here we have assumed that all the surrounding ions have charge $+Ze$, but the D_{4h} symmetry allows for the planar ions do have a different charge than the axial ions. Note that for $a = b$ the above potential vanishes. In this case the symmetry is cubic and we must go to fourth order. Suppose $Z < 0$ and that $a < b$. In this case the coefficient A is positive, and we see that the p_x and p_y orbitals incur an energy cost, since they are pointed directly toward the closest negative ions. These orbitals provide suitable basis functions for the E IRREP of D_4. The p_z orbital is then lower in energy, as Fig. 6.3 indicates, and corresponds to the A_2 IRREP. For d orbitals, clearly $d_{x^2-y^2}$ is going to be highest in energy, since its lobes are all pointing toward the planar ions. This transforms under the B_1 IRREP, as may be seen by inspection of the characters. The d_{xz} and d_{yz} orbitals clearly remain degenerate, since x may still be rotated into y. Accordingly they transform as the two-dimensional E IRREP. This leaves $d_{3z^2-r^2}$ and d_{xy} . There is no symmetry relating these orbitals, and they transform as the one-dimensional IRREPs A_1 and B_2, respectively.

6.2.4 Cubic and octahedral environments

Now let's implement the same calculation for the case of a cubic or octahedral environment. Centering each about the origin, one has that the eight cubic sites are located at $R\,(\pm1,\pm1,\pm1)$. The six octahedral sites are at $R\left\{(\pm1,0,0)\,,\ (0,\pm1,0)\,,\ (0,0,\pm1)\right\}$. If the side lengths are all a, then $R = \frac{\sqrt{3}}{2}\,a$ for the cube and $R = \frac{1}{\sqrt{2}}\,a$ for the octrahedron. One finds in each case that the local potential, neglecting the constant

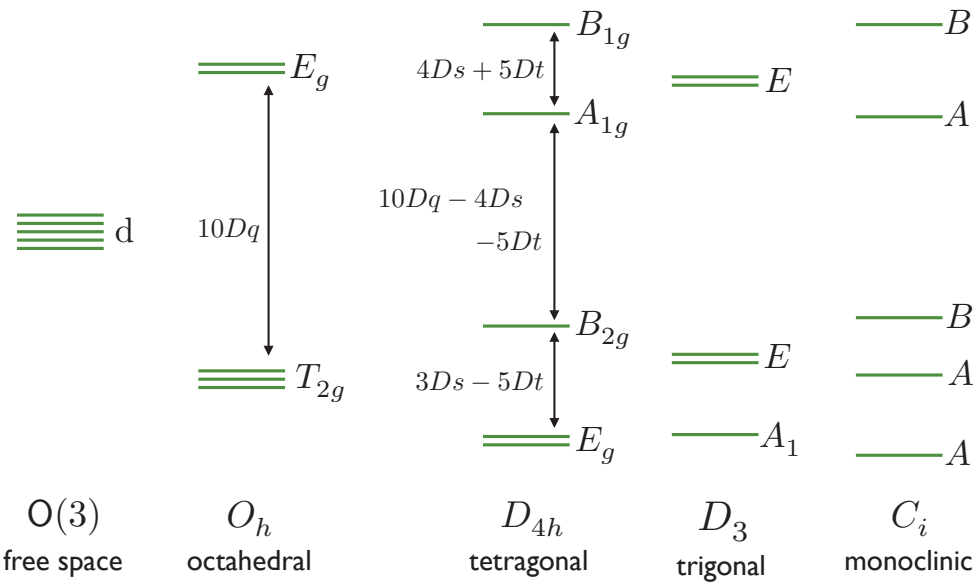


Figure 6.5: Splitting of an atomic d-level in different crystalline environments.

piece, may be written

$$V(\boldsymbol{r}) = \frac{A}{R^5}\Big(x^4 + y^4 + z^4 - \tfrac{3}{5}\,r^4\Big) \quad , \tag{6.13}$$

where $A_{\rm cube} = -\frac{70}{9}Ze^2$ and $A_{\rm octahedron} = +\frac{35}{4}Ze^2$. Thus, the cubic and octahedral environments have an opposite effect, and crystal field levels pushed up in a cubic environment are pushed down in an octahedral environment, all else being the same. A typical scenario is that our central ion is a transition metal, and the surrounding cage is made of O^{--} ions ($Z = -2$).

Consulting Tab. 6.5, we see that atomic p levels remain threefold degenerate in a cubic or octahedral environment, transforming as the T_2 representation. The fivefold degeneracy of the atomic d level is split, though, into $2^+ = E \oplus T_2$. If the site symmetry is O_h, we have $2^+ = E_g \oplus T_{2g}$. In a cubic environment, the T_{2g} levels are pulled lower, since the $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals point toward the face centers of the cube, *i.e.* away from the oxygen anions, and the E_g levels are pushed up. In an octahedral environment, the situation is reversed.

What happens in a tetragonal environment? Carrying out the above calculation of $V(\boldsymbol{r})$, one finds a nontrivial contribution at third order in $\boldsymbol{r}/R$, and

$$V_{\rm tet}(\boldsymbol{r}) = \frac{A}{R^4}\,xyz \quad , \tag{6.14}$$

with $A = -\frac{20}{\sqrt{3}}Ze^2$. Notice how in all cases the potential transforms according to the trivial representation Γ_1. The decomposition of the 2^+ IRREP of $\mathsf{O}(3)$ into IRREPs of T_d is pretty much identical, because T_d and O are isomorphic. One again has $2^+ = E \oplus T_2$. With respect to the 12 element group T, one has $s^+ = E \oplus T$. Tab. 6.6 indicates how electron shell levels up to $l = 4$ split in various crystal field environments. Note again how there is no g or u index on the IRREPs of the proper point groups, since they do not contain the inversion element I.

We can compute analytically the energy shifts using the point charge model. For the case of an atomic d level, we first resolve the d states into combinations transforming according to the E and T_2 IRREPs of O, writing the angular wavefunctions as

$$\begin{aligned} d_{xy}(\hat{\boldsymbol{r}}) &= \tfrac{i}{\sqrt{2}}\Big\{Y_{2,-2}(\hat{\boldsymbol{r}}) - Y_{2,2}(\hat{\boldsymbol{r}})\Big\} \\ d_{yz}(\hat{\boldsymbol{r}}) &= \tfrac{1}{\sqrt{2}}\Big\{Y_{2,-1}(\hat{\boldsymbol{r}}) + Y_{2,1}(\hat{\boldsymbol{r}})\Big\} \\ d_{xz}(\hat{\boldsymbol{r}}) &= \tfrac{i}{\sqrt{2}}\Big\{Y_{2,-1}(\hat{\boldsymbol{r}}) - Y_{2,1}(\hat{\boldsymbol{r}})\Big\} \quad , \end{aligned} \tag{6.15}$$

which transform as T_2, and

$$\begin{aligned} d_{x^2-y^2}(\hat{\boldsymbol{r}}) &= \tfrac{1}{\sqrt{2}}\Big\{Y_{2,-2}(\hat{\boldsymbol{r}}) + Y_{2,2}(\hat{\boldsymbol{r}})\Big\} \\ d_{3z^2-r^2}(\hat{\boldsymbol{r}}) &= Y_{2,0}(\hat{\boldsymbol{r}}) \quad , \end{aligned} \tag{6.16}$$

which transform as E. According to the Wigner-Eckart theorem, this already diagonalizes the 5×5 Hamiltonian within the atomic d basis, with

$$\varepsilon(E_g) = \big\langle\, d_{x^2-y^2} \,\big|\, V(\boldsymbol{r}) \,\big|\, d_{x^2-y^2} \,\big\rangle \qquad , \qquad \varepsilon(T_{2g}) = \big\langle\, d_{xy} \,\big|\, V(\boldsymbol{r}) \,\big|\, d_{xy} \,\big\rangle \quad . \tag{6.17}$$

One finds $\varepsilon^{\rm OCT}(E_g) = -4Dq$ and $\varepsilon^{\rm OCT}(T_{2g}) = +6Dq$, with

$$Dq = \frac{eq\,\langle r^4\rangle}{6a^5} \quad , \tag{6.18}$$

where $q = Ze$ is the ligand charge, a is the distance from the metal ion (where the d electrons live) to the ligand ions, and $\langle r^4\rangle = \langle\, R_{n2} \,|\, r^4 \,|\, R_{n2} \,\rangle$ is the expectation of r^4 with respect to the radial wavefunction $R_{nl}(r)$ with $l = 2$. For the cubic environment, one finds $\varepsilon^{\rm CUB}(E_g) = -\frac{8}{9}\times 6Dq$ and $\varepsilon^{\rm CUB}(T_{2g}) = +\frac{8}{9}\times 4Dq$, while in a tetrahedral environment $\varepsilon^{\rm THD}(E_g) = -\frac{4}{9}\times 6Dq$ and $\varepsilon^{\rm THD}(T_{2g}) = +\frac{4}{9}\times 4Dq$. In a tetragonal environment, one finds

$$\begin{aligned} \varepsilon^{\rm TTR}(E_g) &= -4Dq - Ds + 4Dt \\ \varepsilon^{\rm TTR}(B_{2g}) &= -4Dq + 2Ds - Dt \\ \varepsilon^{\rm TTR}(A_{1g}) &= 6Dq - 2Ds - 6Dt \\ \varepsilon^{\rm TTR}(B_{1g}) &= 6Dq + 2Ds - Dt \quad , \end{aligned} \tag{6.19}$$

where

$$Ds = \frac{2eq}{7}\left(\frac{1}{a^3} - \frac{1}{b^3}\right)\langle r^2\rangle \qquad , \qquad Dt = \frac{2eq}{21}\left(\frac{1}{a^5} - \frac{1}{b^5}\right)\langle r^4\rangle \quad . \tag{6.20}$$

Fig. 6.5 gives a schematic picture of how an atomic d level splits in various crystalline environments ($D > 0$ case is shown).

6.2.5 Matrix elements and selection rules

Recall the Wigner-Eckart theorem,

$$\big\langle\, \Gamma_c\,\gamma\,,\, l_c \,\big|\, \hat{Q}^{\Gamma_a}_{\alpha} \,\big|\, \Gamma_b\,\beta\,,\, l_b \,\big\rangle = \sum_s \begin{pmatrix} \Gamma_a & \Gamma_b & \Gamma_c\,,s \\ \alpha & \beta & \gamma \end{pmatrix} \big\langle\, \Gamma_c\,,\, l_c \,\big\|\, \hat{Q}^{\Gamma_a} \,\big\|\, \Gamma_b\,,\, l_b \,\big\rangle_s \quad , \tag{6.21}$$

L^η	O_h cubic	T_d tetrahedral	D_{4h} tetragonal	D_3 trigonal	D_{2h} orthorhombic
0^+ (s)	A_{1g}	A_1	A_{1g}	A_1	A_{1g}
1^- (p)	T_{1u}	T_2	$A_{2u} \oplus E_u$	$A_2 \oplus E$	$B_{2u} \oplus E_u$
2^+ (d)	$E_g \oplus T_{2g}$	$E \oplus T_2$	$A_{1g} \oplus B_{1g}$ $\oplus B_{2g} \oplus E_g$	$A_1 \oplus 2E$	$A_{1g} \oplus B_{1g}$ $\oplus B_{2g} \oplus E_g$
3^- (f)	$A_{2u} \oplus T_{1u} \oplus T_{2u}$	$A_2 \oplus T_1 \oplus T_2$	$A_{2u} \oplus B_{1u}$ $\oplus B_{2u} \oplus 2E_u$	$A_1 \oplus 2A_2$	$A_{1u} \oplus A_{2u}$ $\oplus B_{2u} \oplus 2E_u$
4^+ (g)	$A_{1g} \oplus E_g$ $\oplus T_{1g} \oplus T_{2g}$	$A_1 \oplus E$ $\oplus T_1 \oplus T_2$	$2A_{1g} \oplus A_{2g} \oplus B_{1g}$ $\oplus B_{2g} \oplus 2E_g$	$2A_1 \oplus A_2 \oplus 3E$	$2A_{1g} \oplus A_{2g} \oplus B_{1g}$ $\oplus B_{2g} \oplus 2E_g$

Table 6.6: Splitting of one-electron levels in crystal fields of different symmetry.

where $l_{b,c}$ labels different subspaces transforming according to the $\Gamma_{b,c}$ IRREPs of the symmetry group G, and s is the multiplicity index necessary when G is not simply reducible. Operators $\hat{Q}$ such as the Hamiltonian transform according to the trivial representation, in which case

$$\left\langle \Gamma_c\,\gamma\,,\,l_c \,\middle|\, \hat{Q} \,\middle|\, \Gamma_b\,\beta\,,\,l_b \right\rangle = \delta_{\Gamma_b\,\Gamma_c}\,\delta_{\beta\gamma}\left\langle \Gamma_c\,,\,l_c \,\middle\|\, \hat{Q} \,\middle\|\, \Gamma_b\,,\,l_b \right\rangle \quad , \tag{6.22}$$

where

$$\left\langle \Gamma_c\,,\,l_c \,\middle\|\, \hat{Q} \,\middle\|\, \Gamma_b\,,\,l_b \right\rangle = \frac{1}{d_{\Gamma_b}} \sum_\beta \left\langle \Gamma_b\,\beta\,,\,l_c \,\middle|\, \hat{Q} \,\middle|\, \Gamma_b\,\beta\,,\,l_b \right\rangle \quad . \tag{6.23}$$

In order that $\left(\begin{smallmatrix} \Gamma_a & \Gamma_b \\ \alpha & \beta \end{smallmatrix} \middle|\, \begin{smallmatrix} \Gamma_c, s \\ \gamma \end{smallmatrix}\right) \neq 0$, we must have $\Gamma_c \subset \Gamma_a \times \Gamma_b$, *i.e.*

$$n_{\Gamma_c}(\Gamma_a \times \Gamma_b) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\Gamma_c^*}(\mathcal{C})\,\chi^{\Gamma_a}(\mathcal{C})\,\chi^{\Gamma_b}(\mathcal{C}) \tag{6.24}$$

must be nonzero. Equivalently, the condition may be stated as $\Gamma_b \subset \Gamma_a^* \times \Gamma_c$ or $\Gamma_a \subset \Gamma_b^* \times \Gamma_c$.

Let's apply these considerations to the problem of radiative transitions in atoms. We follow the treatment in chapter 3 of Lax, following a brief review of quantum radiation theory. The single electron Hamiltonian is

$$\hat{H} = \frac{1}{2m}\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)^2 + V(\boldsymbol{r}) + g\mu_{\rm B}\boldsymbol{H}\cdot\boldsymbol{s}/\hbar + \frac{1}{2m^2c^2}\,\boldsymbol{s}\cdot\boldsymbol{\nabla}V \times \left(\boldsymbol{p} + \tfrac{e}{c}\boldsymbol{A}\right) \quad , \tag{6.25}$$

where $\boldsymbol{A}$ is the vector potential of the electromagnetic field, $V(\boldsymbol{r})$ is the scalar potential due to the ionic nucleus, and $\boldsymbol{s} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ is the electron spin operator. $\mu_{\rm B} = \frac{e\hbar}{2mc} = 5.788 \times 10^{-9}$ eV/G is the Bohr magneton, and $g = 2 + \frac{\alpha}{\pi} + \mathcal{O}(\alpha^2)$ with $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the so-called g-factor[5], which is $g = 2$ at "tree level" within

[5] Like, duh.

	E	C_2	C_3	C_4	C_6	I	σ	S_6	S_4	S_3
$1^-\,(\boldsymbol{P})$	3	−1	0	1	2	−3	1	0	−1	−2
$1^+\,(\boldsymbol{M})$	3	−1	0	1	2	3	−1	0	1	2

Table 6.7: Characters for the electric and magnetic dipole operators.

quantum electrodynamics[6]. The last term above is due to the spin-orbit interaction and we will neglect the contribution of $\boldsymbol{A}$ therein. The quantized electromagnetic field is described by the vector potential[7]

$$\boldsymbol{A}(\boldsymbol{r}) = \sum_{\boldsymbol{k},\lambda} \sqrt{\frac{2\pi\hbar c}{V|\boldsymbol{k}|}} \left(a_{\boldsymbol{k}\lambda}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, \hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{k}) + a^\dagger_{\boldsymbol{k}\lambda}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, \hat{\boldsymbol{e}}_\lambda(\boldsymbol{k}) \right) \quad , \tag{6.26}$$

where $\hat{\boldsymbol{e}}_\lambda(\boldsymbol{k})$ is the polarization vector, with $\left\{ \hat{\boldsymbol{e}}_1(\boldsymbol{k})\,,\, \hat{\boldsymbol{e}}_2(\boldsymbol{k})\,,\, \hat{\boldsymbol{k}} \right\}$ an orthonormal triad for each $\boldsymbol{k}$.

The matrix element one must compute is that of $\boldsymbol{p}\cdot\boldsymbol{A}(\boldsymbol{r})$, where $\boldsymbol{p}$ is the electron momentum and $\boldsymbol{A}(\boldsymbol{r})$ is the quantized electromagnetic vector potential. Writing $\boldsymbol{A}(\boldsymbol{r})$ as the above Fourier sum, we need to evaluate

$$\left\langle\, 0 \,\middle|\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, \boldsymbol{p}\cdot\hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{k}) \,\middle|\, n \,\right\rangle \quad , \tag{6.27}$$

where the atomic transition is from $|\,n\,\rangle$ to the ground state $|\,0\,\rangle$, $\boldsymbol{k}$ is the wavevector of the emitted photon, and $\hat{\boldsymbol{e}}_\lambda(\boldsymbol{k})$ is the photon polarization vector (with λ the polarization index). If $ka_{\rm B} \ll 1$, we may approximate $e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \approx 1$, and we then need the matrix element of

$$\hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{k}) \cdot \left\langle\, 0 \,\middle|\, \boldsymbol{p} \,\middle|\, n \,\right\rangle = \frac{m}{i\hbar}\,(E_n - E_0)\,\hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{k}) \cdot \left\langle\, 0 \,\middle|\, \boldsymbol{r} \,\middle|\, n \,\right\rangle \quad . \tag{6.28}$$

If the states $|\,0\,\rangle$ and $|\,n\,\rangle$ are of the same parity, then the transition is forbidden within the electric dipole approximation, and one must expand $\exp(-i\boldsymbol{k}\cdot\boldsymbol{r}) = 1 - i\boldsymbol{k}\cdot\boldsymbol{r} - \frac{1}{2}(\boldsymbol{k}\cdot\boldsymbol{r})^2 + \ldots$ to next order, *i.e.* to the magnetic dipole and electric quadrupole terms. Magnetic dipole transitions involve the matrix element $\boldsymbol{k}\times\hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{k})\cdot\langle\,0\,|\,\boldsymbol{l}+2\boldsymbol{s}\,|\,n\,\rangle$, where $\boldsymbol{l}=\boldsymbol{r}\times\boldsymbol{p}$ and $\boldsymbol{s}$ is the electron spin. Summing over all the electrons in the unfilled shell, we have the electric and magnetic dipole operators,

$$\boldsymbol{P} = e\sum_i \boldsymbol{r}_i \qquad , \qquad \boldsymbol{M} = \frac{e\hbar}{2mc}\sum_i (\boldsymbol{l}_i + 2\boldsymbol{s}_i) \quad . \tag{6.29}$$

We see that these operators transform as an axial vector ($\boldsymbol{P}$, or 1^-) and a pseudovector ($\boldsymbol{M}$, or 1^+), respectively. This has profound consequences for the allowed matrix elements.

Site group C_{3v}

Lax[8] considers the case of an ion in an environment with a C_{3v} site group. The characters for the vector and pseudovector representations of the $\boldsymbol{P}$ and $\boldsymbol{M}$ operators are given in Tab. 6.7. Consulting the

[6] Radiative corrections to $g_{\rm tree} = 2$ may be cast in the form of an asymptotic power series in the fine structure constant $\alpha = e^2/\hbar c \approx \frac{1}{137}$.

[7] See, *e.g.*, J. J. Sakurai, *Advanced Quantum Mechanics*, §2.3.

[8] See the subsection "Dipole Radiation Selection Rules" on pp. 88-89 in Lax, *Symmetry Principles*.

character table for C_{3v} (Tab. 2.1), we decompose their respective O(3) IRREPs $1^{\mp}$ into C_{3v} IRREPs, and find $1^- = A_1 \oplus E$ and $1^+ = A_2 \oplus E$, with P_z transforming as A_1 and $P_{x,y}$ as E. Similarly, M_z transforms as A_2 and $M_{x,y}$ as E. We now need to know how the products of the C_{3v} IRREPs decompose, which is summarized in Tab. 6.9. Since $A_1 \times A_2 = A_2 \times A_1 = A_2$, and we see that no component of $\boldsymbol{P}$ can have a nonzero matrix elements between these corresponding IRREPs, *i.e.* $\langle A_1 \,|\, \boldsymbol{P} \,|\, A_2 \rangle = 0$. Similarly, since $A_1 \times A_1 = A_2 \times A_2 = A_1$, we have $\langle A_1 \,|\, \boldsymbol{M} \,|\, A_1 \rangle = \langle A_2 \,|\, \boldsymbol{M} \,|\, A_2 \rangle = 0$. Further restrictions apply when we consider the longitudinal (Q_z) and transverse ($Q_{x,y}$) parts of these operators, and we find that $\langle A_i \,|\, Q_z \,|\, E \rangle = \langle A_i \,|\, Q_{x,y} \,|\, A_j \rangle = 0$ where $\boldsymbol{Q}$ is either $\boldsymbol{P}$ or $\boldsymbol{M}$, for all i and j.

Site group D_{3d}

Now consider the problem of dipole radiation in a D_{3d} environment. haracter table for D_{3d}, including the decomposition of the $\boldsymbol{P}$ and $\boldsymbol{M}$ representations, is provided in Tab. 6.8. Unlike C_{3v}, the group D_{3d} contains the inversion I, hence its IRREPs are classified as either g or u, according to whether $\chi^{\Gamma}(I) = \pm d_{\Gamma}$. From Tab. 6.8, we find $1^- = A_{2u} \oplus E_u$ and $1^+ = A_{2g} \oplus E_g$. Next, we decompose the products of the D_{3d} IRREPs, in Tab. 6.9, and we obtain $1^- = A_{2u} \oplus E_u$ and $1^+ = A_{2g} \oplus E_g$. Since I commutes with

D_{3d}	E	$2C_3$	$3C_2'$	I	$2IC_3$	$3IC_2'$	
A_{1g}	1	1	1	1	1	1	
A_{2g}	1	1	−1	1	1	−1	
E_g	2	−1	0	2	−1	0	
A_{1u}	1	1	1	−1	−1	−1	
A_{2u}	1	1	−1	−1	−1	1	
E_u	2	−1	0	−2	1	0	
1^- ($\boldsymbol{P}$)	3	0	−1	−3	0	1	$A_{2u} \oplus E_u$
1^+ ($\boldsymbol{M}$)	3	0	−1	3	0	−1	$A_{2g} \oplus E_g$

Table 6.8: Character table for D_{3d}.

all group elements, its eigenvalue is a good quantum number, and accordingly $\langle \Gamma_g \,|\, \boldsymbol{M} \,|\, \Gamma_u' \rangle = 0$ for any IRREPs Γ_g and Γ_u', since $\boldsymbol{M}$ is even under inversion and can have no finite matrix element between states of different parity. Similarly, $\boldsymbol{P}$ is odd under inversion, so $\langle \Gamma_g \,|\, \boldsymbol{P} \,|\, \Gamma_g' \rangle = \langle \Gamma_u \,|\, \boldsymbol{P} \,|\, \Gamma_u' \rangle = 0$. Again, matrix elements of the longitudinal and transverse components are subject to additional restrictions, and the general rule is that some IRREP Γ_a contained in the decomposition of a given operator $\hat{Q}$ must also be contained in the decomposition of the product representation $\Gamma_b^* \times \Gamma_c$ in order that $\langle \Gamma_c \,|\, \hat{Q} \,|\, \Gamma_b \rangle$ be nonzero[9].

[9]Note how we are using an abbreviated notation $|\, \Gamma \,\rangle$ for the more complete $|\, \Gamma\, \mu\, , l \,\rangle$.

C_{3v}	A_1	A_2	E
A_1	A_1	A_2	E
A_2	A_2	A_1	E
E	E	E	$A_1 \oplus A_2 \oplus E$

D_{3d}	A_{1g}	A_{2g}	E_g	A_{1u}	A_{2u}	E_u
A_{1g}	A_{1g}	A_{2g}	E_g	A_{1u}	A_{2u}	E_u
A_{2g}	A_{2g}	A_{1g}	E_g	A_{2u}	A_{1u}	E_u
E_g	E_g	E_g	$A_{1g} \oplus A_{2g} \oplus E_g$	E_u	E_u	$A_{1u} \oplus A_{2u} \oplus E_u$
A_{1u}	A_{1u}	A_{2u}	E_u	A_{1g}	A_{2g}	E_g
A_{2u}	A_{2u}	A_{1u}	E_u	A_{2g}	A_{1g}	E_g
E_u	E_u	E_u	$A_{1u} \oplus A_{2u} \oplus E_u$	E_g	E_g	$A_{1g} \oplus A_{2g} \oplus E_g$

Table 6.9: Decomposition of products of IRREPs in C_{3v} and D_{3d}. Red entries indicate cases where $\langle\, \Gamma \,|\, \boldsymbol{P} \,|\, \Gamma' \,\rangle = 0$ for all components of $\boldsymbol{P}$, and blue entries where $\langle\, \Gamma \,|\, \boldsymbol{M} \,|\, \Gamma' \,\rangle = 0$ for all components of $\boldsymbol{M}$, where Γ and Γ' are the row and column IRREP labels, respectively. Additional constraints apply to matrix elements of the longitudinal (z) and transverse (x, y) components individually (see text).

6.2.6 Crystal field theory with spin

Thus far we have considered how the $2l+1$ states in a single-electron orbital of angular momentum l, which form an IRREP of $\mathsf{O}(3)$, split in the presence of a crystal field and reorganize into IRREPs of the local site group, according to Eqn. 6.1. This formalism may be applied to many-electron states described by terms ${}^{2S+1}L_J$, provided $J \in \mathbb{Z}$. Or it may be applied to terms on the basis of their L values alone, if we neglect the atomic spin-orbit coupling which is the basis of Hund's third rule. In this section, we consider term splitting in more detail, exploring how it can be approached either from the strong spin-orbit coupling side or the strong crystal field potential side. We shall show how a given term ${}^{2S+1}L_J$ may be analyzed by either of the following procedures:

(i) First decompose the spin S and angular momentum L multiplets into IRREPs $\Gamma_a(S)$ and $\Gamma_b(L)$ of $\mathcal{P}(\boldsymbol{r})$, respectively. Then decompose the products $\Gamma_a(S) \times \Gamma_b(L)$, again into IRREPs of $\mathcal{P}(\boldsymbol{r})$. This is appropriate when $V_{\rm CF} \gg V_{\rm RS}$, where $V_{\rm CF}$ is the scale of the crystal field potential, and $V_{\rm RS}$ the scale of the atomic Russell-Saunders L-S coupling.

(ii) First decompose ${}^{2S+1}L$ within $\mathsf{O}(3)$ into IRREPs according to their total angular momentum J. Then decompose these $\mathsf{O}(3)$ IRREPs into IRREPs of $\mathcal{P}(\boldsymbol{r})$. This is appropriate when $V_{\rm RS} \gg V_{\rm CF}$.

We illustrate the salient features by means of two examples.

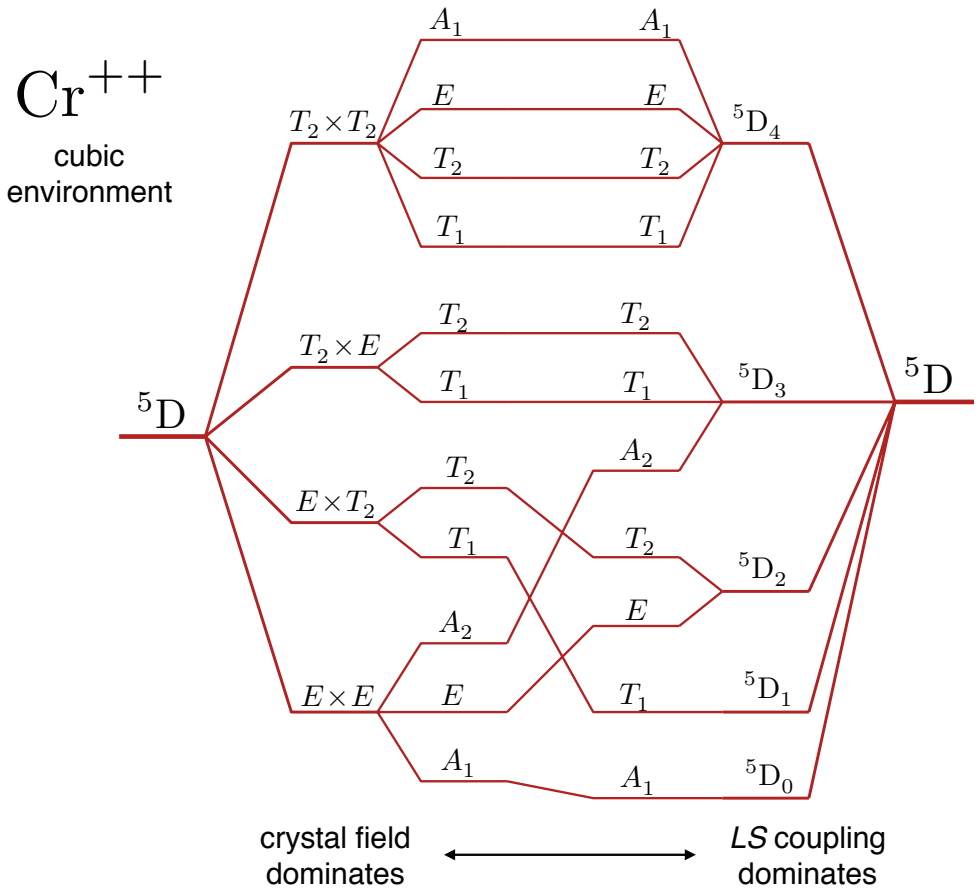


Figure 6.6: Decomposition of the ^{5}D states of Cr^{++} into IRREPs of O.

Cr^{++} in a cubic environment

The first is that of the Cr^{++} ion, whose electronic configuration is $[\mathrm{Ar}]\,4s^0\,3d^4$. The ground state term in free space is $^5\mathrm{D}_0$, *i.e.* $S = L = 2$. According to Tab. 6.5, each of these degenerate multiplets, for both spin and angular momentum, decomposes as $\mathrm{D} = E \oplus T_2$ within O. Thus,

$$^5\mathrm{D} = \Gamma_{S=2} \times \Gamma_{L=2} = \big(E \oplus T_2\big) \times \big(E \oplus T_2\big) = E \times E \;\oplus\; E \times T_2 \;\oplus\; T_2 \times E \;\oplus\; T_2 \times T_2 \quad . \tag{6.30}$$

Appealing again to the character table for O, from Eqn. 6.1 we compute

$$\begin{aligned} E \times E &= A_1 \oplus A_2 \oplus E \\ E \times T_2 = T_2 \otimes E &= T_1 \oplus T_2 \\ T_2 \times T_2 &= A_1 \oplus E \oplus T_1 \oplus T_2 \quad . \end{aligned} \tag{6.31}$$

The resulting tally of O IRREPs and their multiplicities:

$$^5\mathrm{D} = 2\,A_1 \oplus A_2 \oplus 2\,E \oplus 3\,T_1 \oplus 3\,T_2 \quad . \tag{6.32}$$

T_d'	E	$\overline{E}$	$8C_3$	$8\overline{C}_3$	$\begin{matrix}3C_2\\3\overline{C}_2\end{matrix}$	$6S_4$	$6\overline{S}_4$	$\begin{matrix}6\sigma_d\\6\overline{\sigma}_d\end{matrix}$		
O'	E	$\overline{E}$	$8C_3$	$8\overline{C}_3$	$\begin{matrix}3C_2\\3\overline{C}_2\end{matrix}$	$6C_4$	$6\overline{C}_4$	$\begin{matrix}6C_2'\\6\overline{C}_2'\end{matrix}$	O' basis	T_d' basis
$\Delta_1 = A_1$	1	1	1	1	1	1	1	1	r^2	r^2 or xyz
$\Delta_2 = A_2$	1	1	1	1	1	−1	−1	−1	xyz	$L_x\,L_y\,L_z$
$\Delta_{12} = E$	2	2	−1	−1	2	0	0	0	$\left\{\sqrt{3}\,(x^2-y^2)\,, 3z^2-r^2\right\}$	$\left\{\sqrt{3}\,(x^2-y^2)\,, 3z^2-r^2\right\}$
$\Delta_{15} = T_1$	3	3	0	0	−1	1	1	−1	$\left\{L_x\,, L_y\,, L_z\right\}$	$\left\{L_x\,, L_y\,, L_z\right\}$
$\Delta_{25} = T_2$	3	3	0	0	−1	−1	−1	1	$\left\{yz\,,\, zx\,,\, xy\right\}$	$\left\{x\,, y\,, z\right\}$
Δ_6	2	−2	1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	0	$\left\{\vert\,\frac{1}{2}\,,\,\pm\frac{1}{2}\,\rangle\right\}$	$\left\{\vert\,\frac{1}{2}\,,\,\pm\frac{1}{2}\,\rangle\right\}$
Δ_7	2	−2	1	−1	0	$-\sqrt{2}$	$\sqrt{2}$	0	$\left\{xyz\otimes\vert\,\frac{1}{2}\,,\,\pm\frac{1}{2}\,\rangle\right\}$	$\left\{L_x\,L_y\,L_z\otimes\vert\,\frac{1}{2}\,,\,\pm\frac{1}{2}\,\rangle\right\}$
Δ_8	4	−4	−1	1	0	0	0	0	$\left\{\vert\,\frac{3}{2}\,,\,m\,\rangle\right\}$	$\left\{\vert\,\frac{3}{2}\,,\,m\,\rangle\right\}$
$\Gamma_{1/2}$	2	−2	1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	0	Δ_6	
$\Gamma_{3/2}$	4	−4	−1	1	0	0	0	0	Δ_8	
$\Gamma_{5/2}$	6	−6	0	0	0	$-\sqrt{2}$	$\sqrt{2}$	0	$\Delta_7\oplus\Delta_8$	
$\Gamma_{7/2}$	8	−8	1	−1	0	0	0	0	$\Delta_6\oplus\Delta_7\oplus\Delta_8$	
$\Gamma_{9/2}$	10	−10	−1	1	0	$\sqrt{2}$	$-\sqrt{2}$	0	$\Delta_6\oplus 2\,\Delta_8$	
$\Delta_8\times\Delta_2$	4	−4	−1	1	0	0	0	0	Δ_8	
$\Delta_8\times\Delta_{15}$	12	−12	0	0	0	0	0	0	$\Delta_6\oplus\Delta_7\oplus 2\,\Delta_8$	
$\Delta_8\times\Delta_{25}$	12	−12	0	0	0	0	0	0	$\Delta_6\oplus\Delta_7\oplus 2\,\Delta_8$	

Table 6.10: Character table for the double groups O' and T_d'.

Note that a sum of their dimensions yields $2+1+4+9+9=25$, which of course is consistent with $S=2$ and $L=2$. Now let's approach this from the spin-orbit side. That is, we first multiply the $S=2$ and $L=2$ IRREPs within $\mathsf{O}(3)$, yielding

$$2\times 2 = 0\oplus 1\oplus 2\oplus 3\oplus 4 \quad . \tag{6.33}$$

A check of the bottom half of Tab. 6.5 reveals that this once again results in the same final tally of O IRREPs. This situation is illustrated in Fig. 6.6.

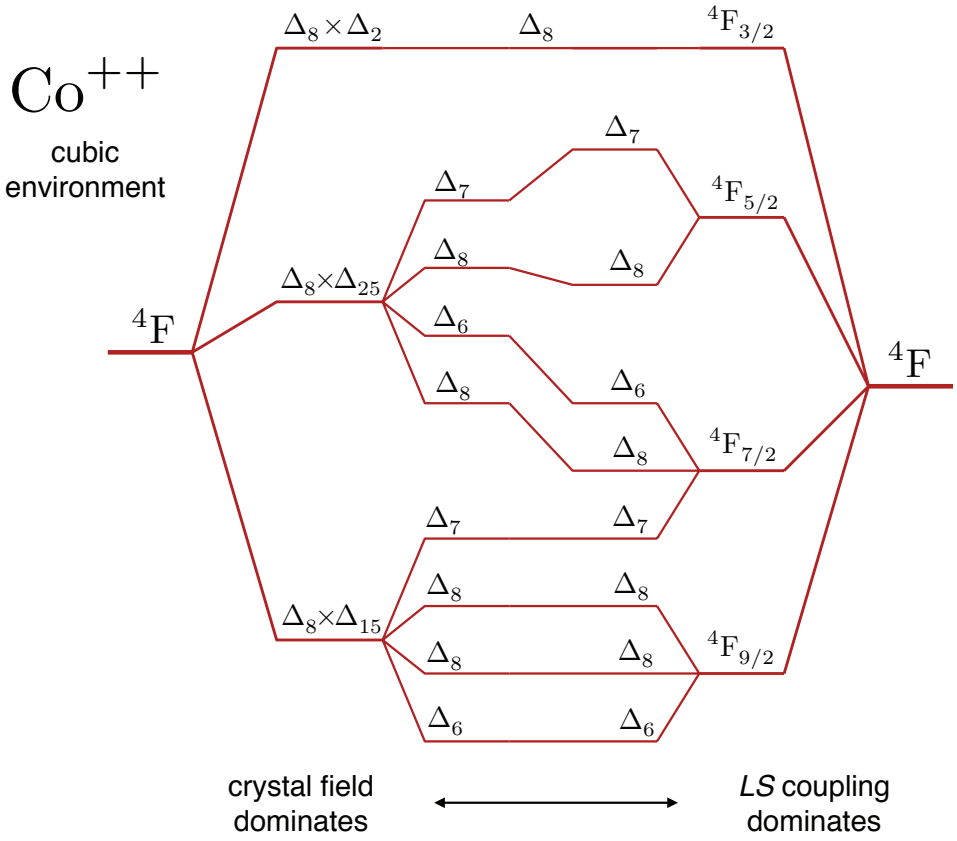


Figure 6.7: Decomposition of the ^{4}F states of Co^{++} into IRREPs of the double group O'.

Co^{++} in a cubic environment

Next, consider the case of Co^{++}, whose ground state term is $^4\mathrm{F}_{9/2}$, corresponding to $S = \frac{3}{2}$ and $L = 3$. We first ignore spin-orbit, and we decompose the $L = 3$ multiplet of O(3) as $\mathrm{F} = A_2 \oplus T_1 \oplus T_2$. We adopt the alternate labels Δ_2, Δ_{15}, and Δ_{25} for these IRREPs of O (see Tab. 6.10[10]) because we will need to invoke the double group O' and its IRREPs presently. We next decompose the $S = \frac{3}{2}$ spin component, and here is where we need the double group O' and its IRREPs. We see from the table that $\Gamma_{3/2} = \Delta_8$. We now must decomposing the product representations of the double group O', and we find

$$\begin{aligned} \Delta_8 \times \Delta_2 &= \Delta_8 \\ \Delta_8 \times \Delta_{15} &= \Delta_6 \oplus \Delta_7 \oplus 2\,\Delta_8 \\ \Delta_8 \times \Delta_{25} &= \Delta_6 \oplus \Delta_7 \oplus 2\,\Delta_8 \quad . \end{aligned} \tag{6.34}$$

Therefore we conclude

$$^4\mathrm{F} = 2\,\Delta_6 \oplus 2\,\Delta_7 \oplus 5\,\Delta_8 \quad . \tag{6.35}$$

Since Δ_6 and Δ_7 are two-dimensional, and Δ_8 is four-dimensional, the total dimension of all the terms in ^{4}F is $2 \times 2 + 2 \times 2 + 4 \times 5 = 28 = (2S+1)(2L+1)$, with $S = \frac{3}{2}$ and $L = 3$.

[10] Tab. 3.6.2 on p. 95 of Lax contains a rare error: $\chi^{\Gamma_{5/2}}(6C_4) = -\sqrt{2}$ while $\chi^{\Gamma_{9/2}}(6C_4) = +\sqrt{2}$.

Had we first decomposed into O(3) IRREPs, writing

$$\tfrac{3}{2} \times 3 = \tfrac{3}{2} \oplus \tfrac{5}{2} \oplus \tfrac{7}{2} \oplus \tfrac{9}{2} \quad , \tag{6.36}$$

and decomposing these half-odd-integer spin IRREPs of O(3) into double group IRREPs of O', we have

$$\begin{aligned} \Gamma_{3/2} &= \Delta_8 \\ \Gamma_{5/2} &= \Delta_7 \oplus \Delta_8 \\ \Gamma_{7/2} &= \Delta_6 \oplus \Delta_7 \oplus \Delta_8 \\ \Gamma_{9/2} &= \Delta_6 \oplus 2\,\Delta_8 \quad . \end{aligned} \tag{6.37}$$

Again we arrive at the same crystal field levels as in Eqn. 6.35, now labeled by IRREPs of the double group O'. The agreement between the two procedures is shown in Fig. 6.7.

Figs. 6.6 and 6.7 are not intended to convey an accurate ordering of energy levels, although in each case the ground state ${}^{2S+1}L_J$ term is placed on the bottom right. Due to level repulsion (see §3.2.6), multiplets corresponding to the same IRREP cannot cross as the ratio of $V_{\rm CF}$ to $V_{\rm RS}$ is varied. Note how in Fig. 6.6 there is level crossing, but between different IRREPs.

Dominant crystal field

We have seen how accounting for crystal field splittings either before or after accounting for spin-orbit coupling yields the same set of levels classified by IRREPs of the local site group. Our starting point in both cases was the partial term ${}^{2S+1}L$, where S and L are obtained from Hund's first and second rules, respectively. Phenomenologically, we can think of Hund's first rule as minimizing the intraatomic ferromagnetic exchange energy $-J_{\rm H}\,\boldsymbol{S}^2$, where $\boldsymbol{S}$ is the total atomic spin. What happens, though, if $V_{\rm CF}$ is so large that it dominates the energy scale $J_{\rm H}$? Consider, for example, the case of Co^{4+}, depicted in Fig. 6.8. The electronic configuration is $[{\rm Ar}]\,4{\rm s}^0\,4{\rm d}^5$, and according to Hund's rules the atomic ground state term is ${}^6{\rm S}_{5/2}$. In a weak crystal field, this resolves into IRREPs of O' according to Tab. 6.10 : $\Gamma_{5/2} = \Delta_7 \oplus \Delta_8$, each multiple of which consists of linear combinations of the original $J = S = \frac{5}{2}$ atomic levels. As shown in the figure, there are three electrons in the T_2 orbital and two in the E orbital. The strong Hund's rules coupling $J_{\rm H}$ keeps the upper two electrons from flipping and falling into the lower single particle states. This is the *high spin state*. If $V_{\rm CF} \gg J_{\rm H}$, though, the E electrons cannot resist the energetic advantage of the T_2 states, and the electrons reorganize into the *low spin state*, with $S = \frac{1}{2}$. Unlike the high spin state, the low spin state cannot be written as a linear combination of states from the original ground state term. Rather, one must start with the configuration, which contains $\binom{10}{5} = 252$ states. After some tedious accounting, one finds these states may be resolved into the following O(3) product representations

$$\begin{aligned} [{\rm Ar}]\,4{\rm s}^0\,4{\rm d}^5 = {}&{}^2{\rm I} \oplus {}^2{\rm H} \oplus {}^4{\rm G} \oplus {}^2{\rm G} \oplus {}^2{\rm G} \oplus {}^4{\rm F} \oplus {}^2{\rm F} \oplus {}^2{\rm F} \\ &\oplus {}^4{\rm D} \oplus {}^2{\rm D} \oplus {}^2{\rm D} \oplus {}^2{\rm D} \oplus {}^4{\rm P} \oplus {}^2{\rm P} \oplus {}^6{\rm S} \oplus {}^2{\rm S} \quad . \end{aligned} \tag{6.38}$$

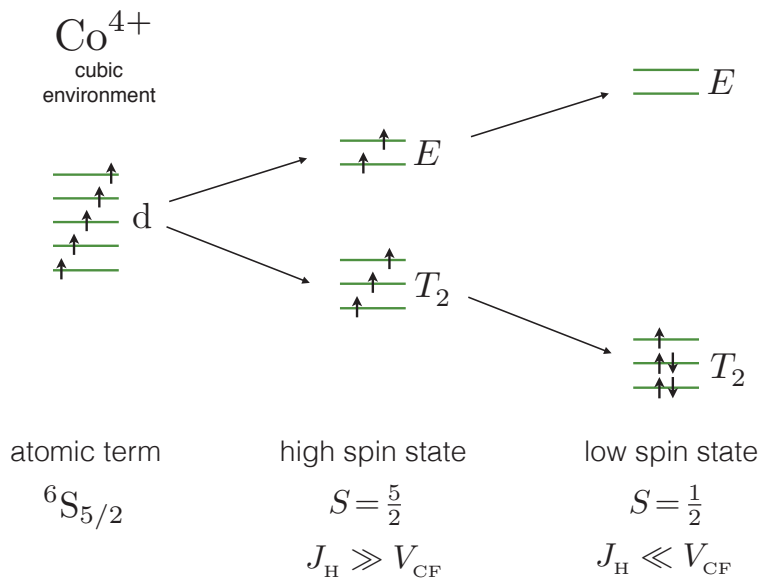


Figure 6.8: High spin and low spin states of the Co^{4+} ion in a cubic environment.

These may be each arranged into full terms by angular momentum addition to form $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, which yields ${}^2\mathrm{I} = {}^2\mathrm{I}_{13/2} \oplus {}^2\mathrm{I}_{11/2}$, ${}^4\mathrm{F} = {}^4\mathrm{F}_{9/2} \oplus {}^4\mathrm{F}_{7/2} \oplus {}^4\mathrm{F}_{5/2} \oplus {}^4\mathrm{F}_{3/2}$, *etc.*[11] The high spin state came from the term ${}^6\mathrm{S}_{5/2}$. The low spin states must then be linear combinations of the ${}^4\mathrm{D}_{1/2}$, ${}^4\mathrm{P}_{1/2}$, ${}^2\mathrm{P}_{1/2}$, and ${}^2\mathrm{S}_{1/2}$ terms. These latter states all transform according to the Δ_6 IRREP of O', whereas ${}^6\mathrm{S}_{5/2} = \Delta_7 \oplus \Delta_8$. Therefore, there must be a level crossing as V_{CF} is increased and we transition from high spin state to low spin state.

The oxides of Mn, Fe, Cu, and Co are quite rich in their crystal chemistry, as these ions may exist in several possible oxidation states (*e.g.* Co^{2+}, Co^{3+}, Co^{4+}) as well as various coordinations such as tetrahedral, pyramidal, cubic/octahedral. The cobalt oxides are particularly so because Co may exist in high spin, low spin, and even intermediate spin states. Co^{2+} is always in the high spin state $T_2^5\,E^2$ ($S = \frac{3}{2}$), while Co^{4+}, which we have just discussed, is usually in the low spin state $T_2^5\,E^0$ ($S = \frac{1}{2}$). Co^{3+} exists in three possible spin states: high ($T_2^4\,E^2$, $S = 2$), intermediate ($T_2^5\,E^1$, $S = 1$), and low ($T_2^6\,E^0$, $S = 0$). Such a complex phenomenology derives from the sensitivity of V_{CF} to changes in the Co-O bond length and Co-O-Co bond angle[12].

[11] The full decomposition of the $[\mathrm{Ar}]\,4\mathrm{s}^0\,4\mathrm{d}^5$ configuration into terms is then

$$[\mathrm{Ar}]\,4\mathrm{s}^0\,4\mathrm{d}^5 = {}^2\mathrm{I}_{13/2} \oplus {}^2\mathrm{I}_{11/2} \oplus {}^2\mathrm{H}_{11/2} \oplus {}^2\mathrm{H}_{9/2} \oplus {}^4\mathrm{G}_{11/2} \oplus {}^4\mathrm{G}_{9/2} \oplus {}^4\mathrm{G}_{7/2} \oplus {}^4\mathrm{G}_{5/2} \oplus 2\cdot{}^2\mathrm{G}_{9/2} \oplus 2\cdot{}^2\mathrm{G}_{7/2} \oplus {}^4\mathrm{F}_{9/2} \oplus {}^4\mathrm{F}_{7/2} \oplus {}^4\mathrm{F}_{5/2} \oplus {}^4\mathrm{F}_{3/2} \oplus 2\cdot{}^2\mathrm{F}_{7/2} \oplus 2\cdot{}^2\mathrm{F}_{5/2} \oplus {}^4\mathrm{D}_{7/2} \oplus {}^4\mathrm{D}_{5/2} \oplus {}^4\mathrm{D}_{3/2} \oplus {}^4\mathrm{D}_{1/2} \oplus 3\cdot{}^2\mathrm{D}_{5/2} \oplus 3\cdot{}^2\mathrm{D}_{3/2} \oplus {}^4\mathrm{P}_{5/2} \oplus {}^4\mathrm{P}_{3/2} \oplus {}^4\mathrm{P}_{1/2} \oplus {}^2\mathrm{P}_{3/2} \oplus {}^2\mathrm{P}_{1/2} \oplus {}^6\mathrm{S}_{5/2} \oplus {}^2\mathrm{S}_{1/2} \quad .$$

[12] See B. Raveau and M. M. Seikh, *Cobalt Oxides: From Crystal Chemistry to Physics* (Wiley, 2012).

C_3	E	C_3	C_3^2	
A	1	1	1	
E	1	ω	ω^2	
E^*	1	ω^2	ω	
$\boldsymbol{P}\ (1^-)$	3	0	0	$A \oplus E \oplus E^*$
$\boldsymbol{M}\ (1^+)$	3	0	0	$A \oplus E \oplus E^*$

C_{3v}	E	$2C_3$	$3\sigma_v$	
A_1	1	1	1	
A_2	1	1	-1	
E	2	1	0	
$\boldsymbol{P}\ (1^-)$	3	0	1	$A_1 \oplus E$
$\boldsymbol{M}\ (1^+)$	3	0	-1	$A_2 \oplus E$

Table 6.11: Character tables for C_3 and C_{3v} and decomposition of $\boldsymbol{P}$ and $\boldsymbol{M}$. Here $\omega = e^{2\pi i/3}$.

6.3 Macroscopic Symmetry

Macroscopic properties of crystals[13] are described by *tensors*. The general formulation is

$$\theta_{a_1 \cdots a_k} = T^{j_1 \cdots j_n}_{a_1 \cdots a_k} \, h_{j_1 \cdots j_n} \quad . \tag{6.39}$$

where $\theta_{a_1 \cdots a_k}$ is an observable, $h_{j_1 \cdots j_n}$ is an applied field, and $T^{j_1 \cdots j_n}_{a_1 \cdots a_k}$ is a *generalized susceptibility tensor*. The *rank* of a tensor is the number of indices it carries. Examples include dielectric response, which is a second rank tensor:

$$D_\mu(\boldsymbol{k}, \omega) = \varepsilon_{\mu\nu}(\boldsymbol{k}, \boldsymbol{\omega}) \, E_\nu(\boldsymbol{k}, \omega) \quad . \tag{6.40}$$

Nonlinear response such as second harmonic generation is characterized by a rank three tensor,

$$D^{(2)}_\mu(2\omega) = \chi_{\mu\nu\lambda}(2\omega, \omega, \omega) \, E_\nu(\omega) \, E_\lambda(\omega) \quad . \tag{6.41}$$

Another example comes from the theory of elasticity, where the *stress tensor* $\sigma_{\alpha\beta}(\boldsymbol{r})$ is linearly related to the local *strain tensor* $\varepsilon_{\mu\nu}(\boldsymbol{r})$ by a fourth rank *elastic modulus tensor* $C_{\alpha\beta\mu\nu}$,

$$\sigma_{\alpha\beta}(\boldsymbol{r}) = C_{\alpha\beta\mu\nu} \, \varepsilon_{\mu\nu}(\boldsymbol{r}) \quad . \tag{6.42}$$

We shall discuss the elastic modulus tensor in greater detail further below.

These various tensors must be invariant under all point group operations, a statement known as *Neumann's principle*. Note that this requires that the symmetry group $\mathcal{Y}$ of a given tensor T must contain the crystallographic point group, *i.e.* $\mathcal{P} \subset \mathcal{Y}$, but does not preclude the possibility that $\mathcal{Y}$ may contain additional symmetries. One might ask what happens in nonsymmorphic crystals, when the space group is generated by translations and by elements $\{ g \,|\, \boldsymbol{\tau}_g \}$ with $\boldsymbol{\tau}_g \neq 0$. The answer is that macroscopic properties of crystals cannot depend on these small translations within each unit cell.

6.3.1 Ferroelectrics and ferromagnets

A crystal may also exhibit a permanent electric ($\boldsymbol{P}$) or magnetic ($\boldsymbol{M}$) polarization. Any such vector must be invariant under all point group operations, *i.e.* $\boldsymbol{P} = \hat{g}\boldsymbol{P}\ \forall\ g \in \mathcal{P}$, with the same holding for $\boldsymbol{M}$[14]. In

[13] See C. S. Smith, *Solid State Physics* **6**, 175 (1958) for a review.

[14] We write $\hat{g}\boldsymbol{P}$ for the action of the group operation g on the quantity $\boldsymbol{P}$.

$\boldsymbol{P}\ (1^-)$	C_1	C_2	C_3	C_4	C_6	C_s	C_{2v}	C_{3v}	C_{4v}	C_{6v}
	1	2	3	4	6	m	$mm2$	$3m$	$4mm$	$6mm$
$\boldsymbol{M}\ (1^+)$	C_1	C_2	C_3	C_4	C_6	C_i	C_{2h}	S_6	C_{4h}	C_{6h}
	1	2	3	4	6	$\overline{1}$	$2/m$	$\overline{3}$	$4/m$	$6/m$

Table 6.12: Point groups supporting ferroelectricity and ferromagnetism.

component notation, we have

$$(\hat{g}\boldsymbol{P})_\nu = P_\mu\, D_{\mu\nu}(g) \quad , \tag{6.43}$$

where $D_{\alpha\beta}(g)$ is the matrix representation of g. Clearly any point group $\mathcal{P}$ which contains the inversion element I does not allow for a finite polarization, since $D_{\mu\nu}(I) = -\delta_{\mu\nu}$.

If Ψ is the (generally reducible) representation under which $\boldsymbol{P}$ or $\boldsymbol{M}$ or indeed any susceptibility tensor $X^{j_1\cdots j_n}_{a_1\cdots a_k}$ transforms, then the number of real degrees of freedom associated with the tensor is the number of times it contains the trivial IRREP of $\mathcal{P}$, *i.e.* the number of degrees of freedom is

$$n(\Psi) = \frac{1}{N_G}\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^\Psi(\mathcal{C}) \quad . \tag{6.44}$$

Recall that $\chi(\mathcal{C}) = 1$ for all classes in the trivial representation. Examining the character tables for C_3 and C_{3v}, we see that $n(1^\pm) = 1$ in C_3, but in C_{3v} we have $n(1^-) = 1$ but $n(1^+) = 0$. We conclude that any crystal with a nonzero magnetization density $\boldsymbol{M} \neq 0$ cannot be one of C_{3v} symmetry. In general, the condition for a point group to support ferroelectricity is that it be *polar*, *i.e.* that it preserve an axis, which is the axis along which $\boldsymbol{P}$ lies. Of the 32 crystallographic point groups, ten are polar. The cyclic groups C_n support ferromagnetism, and since 1^+ is even under inversion, adding I to these groups is also consistent with finite $\boldsymbol{M}$. For all point groups other than those listed in Tab. 6.12, we have $n(1^\pm) = 0$. For example, in D_{3d}, we found $1^\pm = A_{2\pm} \oplus E_\pm$ (see Tab. 6.8). In O_h, we found $1^\pm = T_{1\pm}$ (see Tab. 6.5 and add $\pm = g/u$ when inversion is present). In neither case is the trivial representation present in the decomposition. Note that $C_s \cong C_{1v}$.

If we orient the symmetry axis of these groups along $\hat{\boldsymbol{z}}$, we find, upon using the character tables and the decomposition formula in Eqn. 6.44,

$$\boldsymbol{P}(C_1) = \begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix} \quad , \quad \boldsymbol{P}(C_s) = \begin{pmatrix} P_x \\ P_y \\ 0 \end{pmatrix} \quad , \quad \boldsymbol{P}(C_{n>2}\,,\, C_{n>2\,v}) = \begin{pmatrix} 0 \\ 0 \\ P_z \end{pmatrix} \tag{6.45}$$

and

$$\boldsymbol{M}(C_1) = \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} \quad , \quad \boldsymbol{M}(C_i) = \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} \quad , \quad \boldsymbol{M}(C_{n>2}\,,\, C_{n>2}\times C_i) = \begin{pmatrix} 0 \\ 0 \\ M_z \end{pmatrix} \quad , \tag{6.46}$$

with $\boldsymbol{P} = \boldsymbol{M} = 0$ in the case of all other groups.

6.3.2 Spontaneous symmetry breaking

Homage to Socrates, Galileo, Coleman, and Zee:

> *Sagredo* : This thing you have demanded, *i.e.* that $\hat{g}\boldsymbol{M} = \boldsymbol{M}$ for all point group operations $g \in \mathcal{P}$, I fear is asking too much. For I learned in Professor McX's class about the wondrous phenomenon of *spontaneous symmetry breaking*, the whole point of which is that as a parameter is varied, if our crystal be in the thermodynamic limit, the symmetry of the ground state may indeed become lower than that of the Hamiltonian itself. Should not we then expect $\hat{g}\boldsymbol{M} \neq \boldsymbol{M}$ when g corresponds to the action of one of the so-called *broken generators* of the symmetry group?
>
> *Salviati* : Thou hast learnt well, and McX ought be well pleased by your understanding. But thy question contains the seeds of its own answer. For surely the symmetry group of the Hamiltonian, that which describes all the particles in a crystal, is indeed that most sublime and continuous group $\mathsf{O}(3)$, appended, if need be, by the $\mathsf{SU}(2)$ of spin. The very fact that a crystal hath a point group $\mathcal{P}$ with symmetry lower than that of $\mathsf{O}(3)$ heralds the spontaneous symmetry breaking which resulted in that crystalline phase in the first place. When we demand $\hat{g}\boldsymbol{M} = \boldsymbol{M}$ for all $g \in \mathcal{P}$, we are saying that a spontaneous moment $\boldsymbol{M}$ is consistent only with certain point groups.
>
> *Sagredo* : Master, thou didst remove the scales from before my eyes, that I might see what the gods have ordained! For if a spontaneous moment $\boldsymbol{P}$ or $\boldsymbol{M}$ were to develop felicitously in a crystal, it would, through electroelastic or magnetoelastic couplings, by necessity induce some small motions of the ions. Thus, any transition where a spontaneous polarization or magnetization ensues must be concomitant with a *structural deformation* if the high symmetry phase doth not permit a finite $\boldsymbol{P}$ or $\boldsymbol{M}$.
>
> *Salviati* : Indeed it is so. Your words are excellent.
>
> *Sagredo* : And therefore, a material of the cubic affiliation, such as iron, whose point group abhoreth a spontaneous magnetization, is held accurs'd, for surely it could never become a ferromagnet!
>
> *Salviati* : Well, um. . .you see. . .
>
> *Simplicio* : I'm hungry. Let's get sushi.

Simplicio has pulled Salviati's chestnuts out of the fire with his timely suggestion, but to Sagredo's last point, it is generally understood that a tetragonal deformation in α-Fe must accompany its ferromagnetic transition at $T_{\rm C} = 1043\,\mathrm{K}$. However, the resulting value of $(c-a)/a$ is believed to be on the order of 10^{-6}, based on magnetostriction measurements[15], which is to say a shift in the c-axis length by a distance smaller than a nuclear diameter. So far as I understand, the putative tetragonal distortion is too weak to be observed at present[16].

[15] See E. du Tremolet *et al., J. Mag. Magn. Mat.* **31**, 837 (1983).

[16] In fact, since D_{4h} does not accommodate a nonzero $\boldsymbol{M}$, the ferromagnetic phase of α-Fe must have C_{4h} symmetry, which is not a holohedral point group. *I.e.* α-Fe below $T_{\rm C}$ is either not a Bravais lattice, or its crystallographic symmetry is further broken down to monoclinic, *i.e.* C_{2h}.

6.3.3 Pyroelectrics, thermoelectrics, ferroelectrics, and piezoelectrics

Let's just get all this straight right now, people:

- *Pyroelectric* : A pyroelectric material possesses a spontaneous polarization $\boldsymbol{P}$ below a critical temperature $T_{\rm c}$. This is due to the formation of a dipole moment $\boldsymbol{p}$ within each unit cell of the crystal. The Greek root *pyr-* means "fire", and the pyroelectric coefficient is defined to be $\boldsymbol{\gamma} = d\boldsymbol{P}/dT$. In the presence of an external electric field $\boldsymbol{E}$, one has $\boldsymbol{P} = \boldsymbol{P}_{\rm ind} + \boldsymbol{P}_{\rm s}$, where $\boldsymbol{P}_{\rm ind} = \chi \boldsymbol{E}$ is the *induced polarization*, with χ the polarization tensor, and $\boldsymbol{P}_{\rm s}$ is the *spontaneous polarization*. One then has $\boldsymbol{\gamma} = d\boldsymbol{P}_{\rm s}/dT$. We regard $\boldsymbol{\gamma}$ as a rank one tensor, since T is a scalar. Pyroelectric crystals were known to the ancient Greeks, and in the $18^{\rm th}$ century it was noted that tourmaline crystals develop charges at their faces upon heating or cooling.

- *Thermoelectric* : The thermoelectric effect is the generation of an electric field due in a sample with a fixed temperature *gradient*. One has $\boldsymbol{\mathcal{E}} = \rho \boldsymbol{j} + Q \boldsymbol{\nabla} T$, where $\boldsymbol{\mathcal{E}} = -\boldsymbol{\nabla}(\phi - e^{-1}\mu)$ is the gradient of the electrochemical potential and $\boldsymbol{j}$ is the electrical current. The response tensors ρ and Q are the electrical resistivity and the *thermopower* (also called the *Seebeck coefficient*), respectively. The units of thermopower are $k_{\rm B}/e$, and Q has the interpretation of the entropy carried per charge.

  Note that despite the similarity in their names (*thermo-* is the Greek root for "heat"), thermoelectricity and pyroelectricity are distinct phenomena. In a pyroelectric, the change in temperature ΔT is uniform throughout the sample. A change in temperature will result in a change of the dipole moment per cell, and the accumulation of surface charges and a potential difference which gradually decays due to leakage. Almost every material, whether a metal or an insulator, whether or not a polar crystal, will exhibit a thermoelectric effect[17]. The electric field will remain so long as the temperature gradient $\boldsymbol{\nabla} T$ is maintained across the sample.

- *Ferroelectric* : For our purposes, there is no distinction between a ferroelectric and a pyroelectric. However, in the literature, the distinction lies in the behavior of each in an external electric field $\boldsymbol{E}$. The spontaneous polarization $\boldsymbol{P}_{\rm s}$ of a ferroelectric can be reversed by the application of a sufficiently strong $\boldsymbol{E}$ field. In a pyroelectric, this coercive field exceeds the breakdown field, so the dipole reversal cannot be accomplished. In a ferroelectric, the dipole moment can be reversed.

- *Piezoelectric* : Piezoelectricity occurs in 20 of the 21 noncentrosymmetric crystallographic point groups, the exception being the cubic group O (432). The polarization of a piezoelectric is changed by applying stress: $\Delta P_\mu = d_{\mu\nu\lambda}\,\sigma_{\nu\lambda}$, where $\Delta \boldsymbol{P} = \boldsymbol{P} - \boldsymbol{P}_{\rm s}$ and $\sigma_{\nu\lambda}$ is the stress tensor. We shall discuss the piezoelectric tensor $d_{\mu\nu\lambda}$ more below. The hierarchy of these phenomena is then

$$\text{ferroelectric} \subset \text{pyroelectric} \subset \text{piezoelectric} \quad ,$$

  with thermoelectricity being unrelated to the other three.

  The Ginzburg-Landau free energy for an isotropic pyroelectrics or ferroelectrics is modeled by

$$f(P,E) = f_0 + aP^2 + bP^4 + cP^6 - EP \quad , \tag{6.47}$$

[17] The exception is the case of superconductors, which have zero Seebeck coefficient because the Cooper pairs carry zero entropy.

where $E = \boldsymbol{E} \cdot \hat{\boldsymbol{n}}$ is the projection of the external electric field along the invariant axis of the pyroelectric's point group, $a \propto T - T_{\rm c}$, and $c > 0$. If $b > 0$ the transition at $T = T_{\rm c}$ is second order, while if $b < 0$ the second order transition is preempted by a first order one at $a = \frac{3}{16}(b^2/c)$. But what do we mean by P in eqn. 6.47? If the high symmetry (*i.e.* $\boldsymbol{P} = 0$ when $\boldsymbol{E} = 0$) crystalline phase is of cubic symmetry, we should write

$$\begin{aligned} f(\boldsymbol{P}, \boldsymbol{E}) = f_0 &+ a(P_x^2 + P_y^2 + P_z^2) + b_1(P_x^4 + P_y^4 + P_z^4) + b_2(P_x^2 P_y^2 + P_y^2 P_z^2 + P_x^2 P_z^2) \\ &+ c_1(P_x^6 + P_y^6 + P_z^6) + c_2(P_x^4 P_y^2 + P_x^4 P_z^2 + P_y^4 P_x^2 + P_y^4 P_z^2 + P_z^4 P_x^2 + P_z^4 P_y^2) \\ &+ c_3 P_x^2 P_y^2 P_z^2 - \boldsymbol{E} \cdot \boldsymbol{P} + \mathcal{O}(\boldsymbol{P}^8) \quad . \end{aligned} \tag{6.48}$$

Ferroelectricity in barium titanate

A parade example of ferroelectricity is barium titanate depicted in Fig. 6.9. $BaTiO_3$ has four structural phases:

(i) a high temperature cubic phase (C) for $T \gtrsim 393\,\mathrm{K}$

(ii) an intermediate temperature tetragonal phase (T) for $T \in [\sim 282\,\mathrm{K}\,,\ \sim 393\,\mathrm{K}]$

(iii) a second intermediate temperature orthorhombic phase (O) for $T \in [\sim 183\,\mathrm{K}\,,\ \sim 282\,\mathrm{K}]$

(iv) a low temperature rhombohedral (trigonal) phase (R) for $T \lesssim 183\,\mathrm{K}$.

All but the high temperature cubic phase exhibit ferroelectricity, *i.e.* spontaneous polarization which may be reversed by the application of an external electric field. These phases have traditionally been

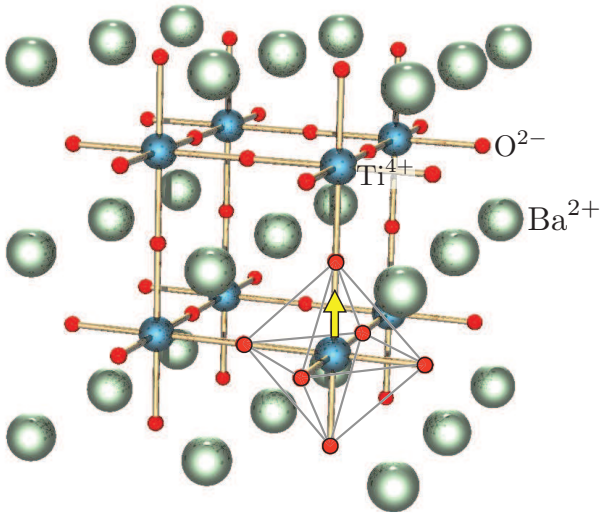


Figure 6.9: High temperature cubic perovskite crystal structure of $BaTiO_3$. Ba^{2+} sites are in green, Ti^{4+} in blue, and O^{2-} in red. The yellow arrow shows the direction in which the Ti^{4+} ion moves as the material is cooled below $T_{\rm c}$ within the displacive model. Image credit: Wikipedia.

understood in terms of the displacement of the Ti^{4+} ion within each unit cell. In the cubic phase, each Ti^{4+} ion sits in the center of an oxygen octahedron, and the free energy density from eqn. 6.48 is $f_{\rm C} = f_0$. The three ordered phases have $\boldsymbol{P} = P\hat{\boldsymbol{n}}$, where $\hat{\boldsymbol{n}}_{\rm C} = (0,0,1)$, $\hat{\boldsymbol{n}}_{\rm O} = \frac{1}{\sqrt{2}}(0,1,1)$, and $\hat{\boldsymbol{n}}_{\rm R} = \frac{1}{\sqrt{3}}(1,1,1)$. Each of these phases is described by a sixth order Landau free energy of the form of eqn. 6.47, with

$$b_{\rm T} = b_1 \quad , \quad b_{\rm O} = \tfrac{1}{2}b_1 + \tfrac{1}{4}b_2 \quad , \quad b_{\rm R} = \tfrac{1}{3}b_1 + \tfrac{1}{3}b_2 \tag{6.49}$$

and

$$c_{\rm T} = c_1 \quad , \quad c_{\rm O} = \tfrac{1}{2}c_1 + \tfrac{1}{2}c_2 \quad , \quad c_{\rm R} = \tfrac{1}{9}c_1 + \tfrac{2}{9}c_2 + \tfrac{1}{27}c_3 \quad . \tag{6.50}$$

Minimizing the free energy in phase $j \in \{{\rm T}, {\rm O}, {\rm R}\}$ yields the equation $a + 2b_jP_j^2 + 3c_jP_j^4 = 0$, with solution

$$P_j(T) = \frac{-b_j + \sqrt{b_j^2 - 3ac_j}}{3c_j} \quad , \tag{6.51}$$

where $a = \alpha(T - T_{\rm c})$ and $T_{\rm c} \approx 393\,{\rm K}$. The free energy in phase j is then obtained by substituting the result for $P = P_j$ into $f_j(T) = f_0 + a_jP^2 + b_jP^4 + c_jP^6$.

Provided $b_{\rm T} > b_{\rm O}$ and $b_{\rm R}$, the second order transition at $a = 0$ (*i.e.* $T = T_{\rm c}$) is from cubic to tetragonal. As one lowers the temperature further, one encounters two first order transitions, first from tetragonal to orthorhombic, and second from orthorhombic to rhombohedral (trigonal)[18]. These transitions occur at temperatures where $f_{\rm T}(T_{\rm c}') = f_{\rm O}(T_{\rm c}')$ and $f_{\rm O}(T_{\rm c}'') = f_{\rm R}(T_{\rm c}'')$.

The standard displacive model of ferroelectricity in $BaTiO_3$ is unable to explain several experiments, however. In the displacive model the high temperature cubic phase has point group O_h. This would mean that first order Raman scattering is forbidden, because, as we shall see below in §6.4.3, Raman scattering preserves parity, and thus the low energy, odd parity long wavelength phonons are all Raman inactive. Yet a healthy first order Raman signal is observed[19]. A second problem is that one expects on general grounds soft modes with frequencies tending toward zero as one approaches a second order phase transition. Yet experiments show damped but finite frequency modes at the cubic to tetragonal transition[20]. Finally, aspects of the observed x-ray scattering are difficult to understand within the displacive model. In particular , x-ray fine structure measurements show in all phases that the Ti^{4+} ions are displaced along different $\langle 111\rangle$ directions[21]. In 2006, Zhang, Cagin, and Goddard[22] (ZCG) presented results from a density functional calculation the results of which differed from those of the displacive model. Rather than an undistorted cubic phase, ZCG found that the C phase is *antiferroelectric*, with a $2 \times 2 \times 2$ unit cell (see Fig. 6.10). In the T and O phases, there is mixed ferroelectric and antiferroelectric order, and only in the R phase is the material purely ferroelectric. The associated space and point group symmetries are listed in tab. 6.13.

Note that while C_{4v} is a subgroup of O_h, it is not a subgroup of T_d. Thus, the C to T transition is predicted to be first order according to ZCG. Their identification of the symmetries of the various phases also resolves the aforementioned difficulties in reconciling the displacive model with experimental data.

[18] Within Landau theory, the order of the transitions will depend on details of the Landau parameters.
[19] A. M. Quittet and M. Lambert, *Solid State Comm.* **12**, 1053 (1973).
[20] Y. Luspin, J. L. Servoin, and F. Gervais, *J. Phys. C Solid State* **13**, 3761 (1980).
[21] B. Ravel *et al.*, *Ferroelectrics* **206**, 407 (1998).
[22] Q. Zhang, T. Cagin, and W. A. Goddard III, *Proc. Natl. Acad. Sci.* **103**, 14695 (2006).

phase	displacive model		DFT results	
	$\mathcal{S}$	$\mathcal{P}$	$\mathcal{S}$	$\mathcal{P}$
cubic	$Pm\overline{3}m$	$m\overline{3}m = O_h$	$I\overline{4}3m$	$\overline{4}3m = T_d$
tetrahedral	$P4mm$	$4mm = C_{4v}$	$I4cm$	$4mm = C_{4v}$
orthorhombic	$Amm2$	$mm2 = C_{2v}$	$Pmn2_1$	$mm2 = C_{2v}$
rhombohedral	$R3m$	$3m = C_{3v}$	$R3m$	$3m = C_{3v}$

Table 6.13: Phases of $BaTiO_3$ and their space and point groups.

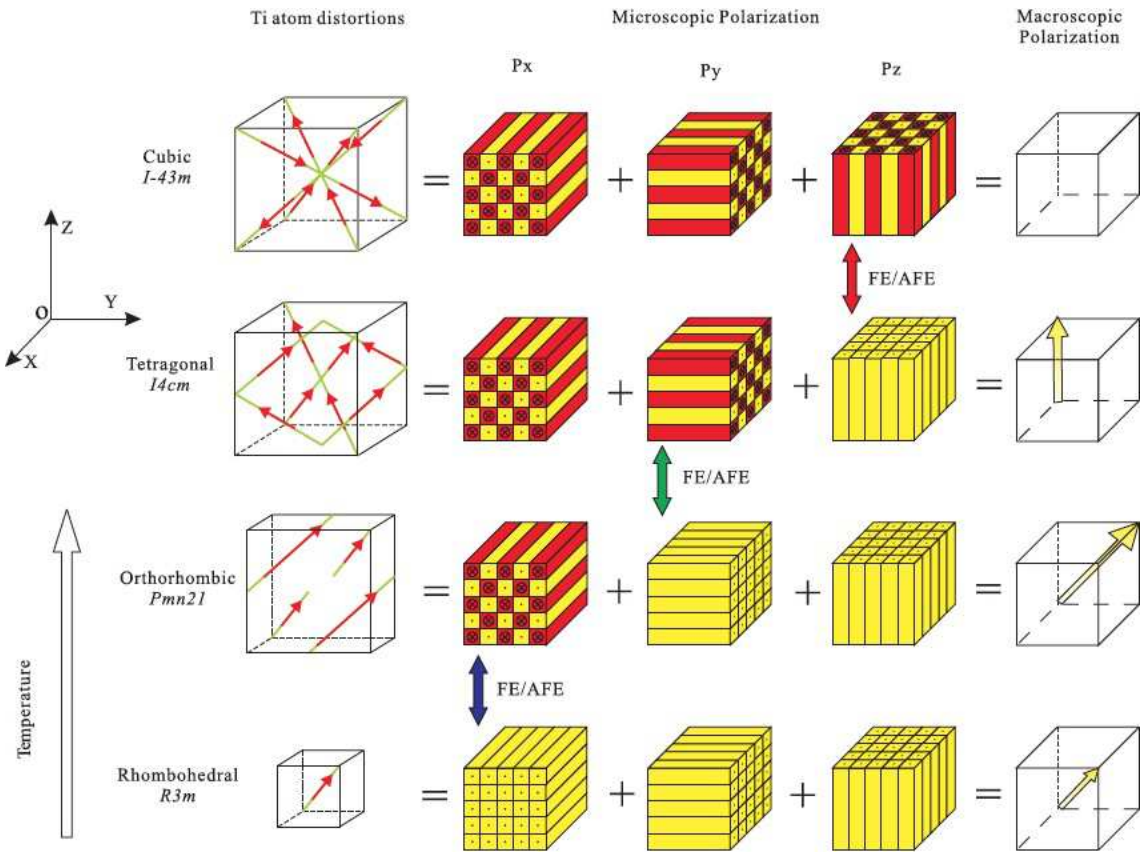


Figure 6.10: Fig. 1 from Zhang, Cagin, and Goddard (2006) showing Ti^{4+} ion distortions and polarizations in $BaTiO_3$, as determined from density functional calculations.

6.3.4 Second rank tensors : conductivity

The conductivity $\sigma_{\mu\nu}$ and dielectric susceptibility $\varepsilon_{\mu\nu}$ are examples of second rank tensors, *i.e.* matrices, which relate a vector cause ($\boldsymbol{E}$) to a vector effect ($\boldsymbol{j}$ or $\boldsymbol{D}$)[23]. The action of a group element g on a second rank tensor $T_{\mu\nu}$ is given by

$$(\hat{g}\,T)_{\alpha\beta} = T_{\mu\nu}\,D_{\mu\alpha}(g)\,D_{\nu\beta}(g) \quad . \tag{6.52}$$

Thus the tensor $T_{\mu\nu}$ transforms according to the product representation $\Psi(G) = D(G) \times D(G)$. Recall that product representations were discussed earlier in §2.4.7 and §3.2.

The product representation can be reduced to the symmetric (S) and antisymmetric (A) representations, which themselves may be further reduced within a given symmetry group G. Recall the characters in these representations are given by (see §3.2.2)

$$\chi^{\mathsf{S,A}}(g) = \tfrac{1}{2}\big[\chi(g)\big]^2 \pm \tfrac{1}{2}\,\chi(g^2) \quad . \tag{6.53}$$

Note that any equilibrium thermodynamic response function $T_{\mu\nu} = -\partial^2 F/\partial h_\mu\,\partial h_\nu$, where $\boldsymbol{h}$ is an applied field, will necessarily transform according to the symmetric product representation Ψ^{S}. The number of independent components of a general response tensor will then be given by

$$n(\Psi^{\mathsf{S,A}}) = \frac{1}{N_G}\sum_{\mathcal{C}} N_{\mathcal{C}}\,\chi^{\mathsf{S,A}}(\mathcal{C}) \quad . \tag{6.54}$$

Let's work this out for the group C_{3v}, the vector representation 1^- of which has characters $\chi(E) = 3$, $\chi(2C_3) = 0$, and $\chi(3\sigma_v) = 1$ (see Tab. 6.11). From these values, we obtain

$$\chi^{\mathsf{S}}(E) = 6 \quad , \quad \chi^{\mathsf{S}}(2C_3) = 0 \quad , \quad \chi^{\mathsf{S}}(3\sigma_v) = 2 \tag{6.55}$$

$$\chi^{\mathsf{A}}(E) = 3 \quad , \quad \chi^{\mathsf{A}}(2C_3) = 0 \quad , \quad \chi^{\mathsf{A}}(3\sigma_v) = -1 \quad , \tag{6.56}$$

and we then compute $n(\Psi^{\mathsf{S}}) = 2$ and $n(\Psi^{\mathsf{A}}) = 0$. The full decomposition into C_{3v} IRREPs is found to be $\Psi^{\mathsf{S}} = 2A_1 \oplus 2E$ and $\Psi^{\mathsf{A}} = A_2 \oplus E$. We conclude that the most general symmetric tensor invariant under C_{3v} is of the form $\mathsf{diag}(a, a, c)$, where $\hat{\boldsymbol{z}}$ is the symmetry axis. The antisymmetric component vanishes entirely, because $\Psi^{\mathsf{A}} = 1^+$ does not contain the trivial A_1 IRREP. However, note that $n_{A_2}(\Psi^{\mathsf{A}}) = 1$, which means that the tensor

$$T = \begin{pmatrix} a & d & 0 \\ -d & a & 0 \\ 0 & 0 & c \end{pmatrix} \tag{6.57}$$

is permissible with nonzero a, c, and d *if and only if* a *and* c *transform as* A_1 *and* d *transforms as* A_2. For example, the conductivity tensor may be of the form

$$\sigma = \begin{pmatrix} \sigma_\perp(H_z) & f(H_z) & 0 \\ -f(H_z) & \sigma_\perp(H_z) & 0 \\ 0 & 0 & \sigma_\parallel(H_z) \end{pmatrix} \quad , \tag{6.58}$$

where $f(H_z)$ is an odd function of the magnetic field component along the symmetry axis. The quantities $\sigma_{\perp\,,\parallel}(H_z)$ are constants invariant under all C_{3v} operations and are even functions of H_z.

[23] Of course the dielectric and conductivity tensors are related by $\varepsilon_{\mu\nu}(\boldsymbol{k},\omega) = \delta_{\mu\nu} + (4\pi i/\omega)\,\sigma_{\mu\nu}(\boldsymbol{k},\omega)$.

	elements of $T_{\mu\nu} = T_{\nu\mu}$					
crystal system	11	22	33	23	31	12
triclinic	a	b	c	f	e	d
monoclinic	a	b	c	0	0	d
orthorhombic	a	b	c	0	0	0
trigonal	a	a	c	0	0	0
tetragonal	a	a	c	0	0	0
hexagonal	a	a	c	0	0	0
cubic	a	a	a	0	0	0

Table 6.14: Allowed nonzero entries of symmetric rank two tensors by crystal system. Crystallographic axes are assumed.

C_{3v} is a trigonal point group. For the others, the allowed nonzero elements of a symmetric tensor T are given in Tab. 6.14. Note that cubic symmetry requires that any symmetric rank two tensor be a multiple of the identity. This means, for example, that the inertia tensor $I_{\alpha\beta}$, with the origin at the center of a uniform cube, is a multiple of the identity[24], and thus independent of the cube's orientation. This entails, for example, that if a cube is used to construct a torsional pendulum, the frequency of the oscillations will be the same whether the torsional fiber runs through a face center, a corner, an edge center, or indeed any point on the cube's surface, so long as it also runs through the cube's center.

Representation ellipsoid

Given a dimensionless rank two tensor $T_{\mu\nu}$, one can form the function $T(\boldsymbol{r}) = T_{\mu\nu}\, x^\mu\, x^\nu$. The locus of points $\boldsymbol{r}$ for which $T(\boldsymbol{r}) = \pm 1$ is called the *representation ellipsoid* of $T_{\mu\nu}$. Clearly any antisymmetric part of T will be projected out in forming the function $T(\boldsymbol{r})$ and will not affect the shape of the representation ellipsoid. In fact, $T(\boldsymbol{r}) = \pm 1$ defines an ellipsoid only if all the eigenvalues of T are of the same sign. Else it defines a hyperboloid. For any real symmetric matrix, the eigenvalues are real and the eigenvectors are mutually orthogonal, or may be chosen to be so in the case of degeneracies.

For triclinic systems, the ellipsoid axes are under no restriction. For monoclinic systems, one of the ellipsoid's axes must be the twofold axis of the crystal. For orthorhombic systems, all three axes of the ellipsoid are parallel to the crystalline axes. For trigonal, tetragonal, and hexagonal crystals, two of the eigenvalues are degenerate (see Tab. 6.14), which means that the ellipsoid is a surface of revolution along the high symmetry axis of the crystal. *I.e.* the ellipsoid has an $\mathsf{O}(2)$ symmetry about this axis. Finally, for cubic systems, the representation ellipsoid is a sphere S^2.

[24] $I_{\alpha\beta} = \frac{1}{6} M a^2\, \delta_{\alpha\beta}$ where M is the cube's mass and a its side length.

6.3.5 Third rank tensors : piezoelectricity

A common example of a third rank tensor comes from the theory of the piezoelectric effect. An applied stress $\sigma_{\nu\lambda}$ leads to a polarization density P_μ, where

$$P_\mu = d_{\mu\nu\lambda}\,\sigma_{\nu\lambda} \quad , \tag{6.59}$$

where $d_{\mu\nu\lambda}$ is the piezoelectric tensor. We can immediately say that if the point group $\mathcal{P}$ contains the inversion element I, then $d_{\mu\nu\lambda} = 0$, because $D_{\mu\mu'}(I) = -\delta_{\mu\mu'}$ and therefore $\hat{I}\, d_{\mu\nu\lambda} = -d_{\mu\nu\lambda}$.

Since the stress tensor σ is symmetric (see below), it contains six independent elements, the piezoelectric tensor $d_{\mu\nu\lambda}$ is itself symmetric in its last two indices[25], *i.e.* $d_{\mu\nu\lambda} = d_{\mu\lambda\nu}$. Accordingly one may define the composite index $(\nu\lambda) \to a$, as defined in the following table:

$(\nu\lambda)$:	(11)	(22)	(33)	(23)	(31)	(12)
a :	1	2	3	4	5	6

Table 6.15: Composite indices for symmetric rank two tensors.

If we then define $d_{\mu 4} \equiv d_{\mu 23} = d_{\mu 32}$, $d_{\mu 5} \equiv d_{\mu 31} = d_{\mu 13}$, and $d_{\mu 6} \equiv d_{\mu 12} = d_{\mu 21}$, we may represent the tensor multiplication in Eqn. 6.59 as an ordinary matrix multiplication, *viz.*

$$\begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ 2\sigma_4 \\ 2\sigma_5 \\ 2\sigma_6 \end{pmatrix} \quad , \quad \sigma = \begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{pmatrix} \quad . \tag{6.60}$$

Note the appearance of a factor of two in the last three elements of the column vector of stresses.

Now let's consider how the symmetry under a point group $\mathcal{P}$ restricts the form of $d_{\mu a}$.

- For triclinic crystals with point group C_1, there is no restriction, and $d_{\mu a}$ contains 18 independent elements. If $\mathcal{P} = C_i$, which contains inversion, then of course $d_{\mu a} = 0$ for all (μ, a).
- For monoclinic crystals, the highest symmetry without inversion is C_s, which is generated by the identity and reflections $z \to -z$. All piezoelectric tensor elements $d_{\mu\nu\lambda}$ in which the index $3(z)$ appears an odd number of times must vanish. For the rectangular 3×6 matrix $d_{\mu a}$, this means that the following eight elements vanish by symmetry:

  $$d_{14} = d_{15} = d_{24} = d_{25} = d_{31} = d_{32} = d_{33} = d_{36} = 0 \quad . \tag{6.61}$$

  We are left with ten independent piezoelectric constants for the group C_s , which is also a polar point group, and hence can support ferroelectricity or ferromagnetism. The general form of the

[25] Thus $d_{\mu\nu\lambda}$ is not the most general rank three tensor possible.

3×6 piezoelectric tensor is

$$d_{\mu a}^{\text{MONO}}[C_s] = \begin{pmatrix} d_{11} & d_{12} & d_{13} & 0 & 0 & d_{16} \\ d_{21} & d_{22} & d_{23} & 0 & 0 & d_{26} \\ 0 & 0 & 0 & d_{34} & d_{35} & 0 \end{pmatrix} \quad . \tag{6.62}$$

- For orthorhombic crystals, the only point groups without inversion C_{2v} and D_2. Consider first C_{2v}, in which $x \to -x$ and $y \to -y$ are symmetries, though not $z \to -z$[26]. The only nonzero piezoelectric tensor elements are those with an even number of indices of 1(x) and 2(y), which means that only five elements of $d_{\mu a}$ may be nonzero, and the general form for $d_{\mu a}$ within C_{2v} is

$$d_{\mu a}^{\text{ORTHO}}[C_{2v}] = \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{24} & 0 & 0 \\ d_{31} & d_{32} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.63}$$

  Note that C_{2v} is polar. For D_2, which is nonpolar, the only nonzero elements are d_{14} , d_{25} , and d_{36} .

- For tetragonal crystals, the highest symmetries not containing inversion are D_{2d} , C_{4v} , D_4 , and C_{4h}. Consider the case D_{2d}. Any point (x, y, z) has symmetry-related images at $(-x, -y, z)$, (y, x, z), and $(x, -y, -z)$, which allows only for two independent nonzero piezoelectric tensor elements: $d_{14} = d_{25}$ and d_{36} . The group D_{2d} is nonpolar. For D_4, there is only one independent nonzero element: $d_{14} = -d_{25}$. The lowest point group symmetry in the tetragonal system is C_4, which relates (x, y, z) to $(-y, x, z)$. This allows for the four independent nonzero piezoelectric tensor elements:

$$d_{\mu a}^{\text{TET}}[C_4] = \begin{pmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & -d_{14} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.64}$$

  Reducing the symmetry to C_{4v} eliminates d_{14}, and there are only three independent moduli. For S_4, relative to C_4, we have $d_{32} = -d_{31}$, we lose d_{33} but gain d_{36}, so again there are four independent moduli.

- For trigonal crystals, the highest symmetry noncentrosymmetric point group is D_3 The implementation of the symmetry restrictions here is a little bit more involved because of the threefold rotations and is left as an exercise to the student. There are three independent piezoelectric coefficients:

$$d_{\mu a}^{\text{TRIG}}[D_3] = \begin{pmatrix} d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.65}$$

  The lowest within the trigonal class is C_3, for which there are six independent moduli:

$$d_{\mu a}^{\text{TRIG}}[C_3] = \begin{pmatrix} d_{11} & -d_{11} & 0 & d_{14} & d_{15} & -2d_{22} \\ -d_{22} & d_{22} & 0 & d_{15} & -d_{14} & -2d_{11} \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.66}$$

[26] If we would include a third orthogonal reflection, we'd then have inversion, in which case all $d_{\mu\nu\lambda} = 0$.

Increasing the symmetry to C_{3v}, we lose d_{14} and d_{26}, so there are four independent moduli:

$$d_{\mu a}^{\text{TRIG}}[C_{3v}] = \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15} & -2d_{22} \\ -d_{22} & d_{22} & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.67}$$

Both C_{3v} and C_3 are polar.

- For hexagonal crystals, we begin with the lowest symmetry group in the system, C_6. There are four independent elastic moduli, with

$$d_{\mu a}^{\text{HEX}}[C_6] = \begin{pmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & -d_{14} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.68}$$

Increasing the symmetry to C_{6v}, one loses a modulus, with $d_{14} = 0$. Starting with C_{3h}, one has two independent moduli:

$$d_{\mu a}^{\text{HEX}}[C_{3h}] = \begin{pmatrix} d_{11} & -d_{11} & 0 & 0 & 0 & -2d_{22} \\ -d_{22} & d_{22} & 0 & 0 & 0 & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad . \tag{6.69}$$

Increasing the symmetry to D_{3h}, we lose d_{11} due to the twofold axis which sends (x, y, z) to $(-x, y, -z)$, and the only nonzero elements are $d_{16} = 2d_{21} = -2d_{22}$. Finally, for D_6, the only nonzero elements are $d_{14} = -d_{25}$.

- Finally we arrive at the cubic system. The centrosymmetric cubic point groups O_h and T_h of course do not support piezoelectricity. Surprisingly, while O is noncentrosymmetric, its symmetries are sufficient to disallow piezoelectricity as well, and $d_{\mu a} = 0$ for all elements. Thus, O is the sole example among the 21 noncentrosymmetric crystallographic point groups which does not allow for piezoelectric behavior. The point groups T and T_d support piezoelectricity, with one independent constant $d_{14} = d_{25} = d_{36}$. Neither is polar.

6.3.6 Fourth rank tensors : elasticity

Another example comes from the theory of elasticity, where an elastic medium is described by a local deformation field $\boldsymbol{u}(\boldsymbol{r})$, corresponding to the elastic displacement of the solid at $\boldsymbol{r}$. The *strain tensor* is defined by the dimensionless expression

$$\varepsilon_{ij}(\boldsymbol{r}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \quad . \tag{6.70}$$

Note that $\varepsilon = \varepsilon^{\mathsf{T}}$ is a symmetric tensor by definition. Similarly, the *stress tensor* $\sigma_{ij}(\boldsymbol{r})$ is defined by

$$dF_i(\boldsymbol{r}) = -\sigma_{ij}(\boldsymbol{r})\, n_j\, d\Sigma \quad , \tag{6.71}$$

where $d\boldsymbol{F}(\boldsymbol{r})$ is the differential force on a surface element $d\Sigma$ whose normal is the vector $\hat{\boldsymbol{n}}$. Angular momentum conservation requires that the stress tensor also be symmetric[27]. The stress and strain tensors are related by the rank four *elastic modulus tensor*, *viz.*

$$\sigma_{ij}(\boldsymbol{r}) = C_{ijkl}\,\varepsilon_{kl}(\boldsymbol{r}) = \frac{\delta f}{\delta \varepsilon_{ij}(\boldsymbol{r})} \quad , \tag{6.72}$$

where the second equality is a statement of thermal equilibrium akin to $p = -\partial F/\partial V$. Here,

$$f(\boldsymbol{r}) = f_0 + \tfrac{1}{2}\,C_{ijkl}\,\varepsilon_{ij}(\boldsymbol{r})\,\varepsilon_{kl}(\boldsymbol{r}) + \mathcal{O}(\varepsilon^3) \tag{6.73}$$

is the local free energy density. Since ε is a dimensionless tensor, the elastic moduli have dimensions of energy density, typically expressed in cgs units as $\mathrm{dyn/cm^2}$. For an *isotropic* material, the only $\mathsf{O}(3)$ invariant terms in the free energy to order ε^2 are proportional to either $(\mathsf{Tr}\,\varepsilon)^2$ or to $\mathsf{Tr}(\varepsilon^2)$. Thus,

$$f = f_0 + \tfrac{1}{2}\,\lambda\,(\mathsf{Tr}\,\varepsilon)^2 + \mu\,\mathsf{Tr}\,(\varepsilon^2) \quad . \tag{6.74}$$

The parameters λ and μ are called the *Lamé coefficients*[28]. For isotropic elastic materials, then,

$$\sigma_{ij} = \frac{\partial f}{\partial \varepsilon_{ij}} = \lambda\,\mathsf{Tr}\,\varepsilon\,\delta_{ij} + 2\mu\,\varepsilon_{ij} \quad . \tag{6.75}$$

In the literature, one often meets up with the quantity $K \equiv \lambda + \frac{2}{3}\mu$, in which case the free energy density becomes

$$f = f_0 + \tfrac{1}{2}K\,(\mathsf{Tr}\,\varepsilon)^2 + \mu\,\mathsf{Tr}\big(\varepsilon - \tfrac{1}{3}\,\mathsf{Tr}\,\varepsilon\big)^2 \tag{6.76}$$

The reason is that the tensor $\widetilde{\varepsilon} \equiv \varepsilon - \frac{1}{3}(\mathsf{Tr}\,\varepsilon)\cdot\mathbb{1}$ is traceless, and therefore the constant K tells us about *bulk deformations* while μ tells us about *shear deformations*. One then requires $K > 0$ and $\mu > 0$ for thermodynamic stability. We then may write, for isotropic materials,

$$\begin{aligned} \sigma &= K\,(\mathsf{Tr}\,\varepsilon)\cdot\mathbb{1} + 2\mu\,\widetilde{\varepsilon} \\ \varepsilon &= \frac{1}{9K}\,(\mathsf{Tr}\,\sigma)\cdot\mathbb{1} + \frac{1}{2\mu}\,\widetilde{\sigma} \quad , \end{aligned} \tag{6.77}$$

with $\widetilde{\sigma} \equiv \sigma - \frac{1}{3}(\mathsf{Tr}\,\sigma)\cdot\mathbb{1}$ the traceless part of the stress tensor[29].

If one solves for the homogeneous deformation[30] of a rod of circular cross section, the only nonzero element of the stress tensor is $\sigma_{zz} = p$, where p is the pressure on either of the circular faces of the rod. One then finds that $\varepsilon_{xx} = \varepsilon_{yy} = \big(\frac{1}{9K} - \frac{1}{6\mu}\big)p$ and $\varepsilon_{zz} = \big(\frac{1}{9K} + \frac{1}{3\mu}\big)p$ are the only nonzero elements of the strain tensor. Thus,

$$Y \equiv \frac{\sigma_{zz}}{\varepsilon_{zz}} = \frac{9K\mu}{3K+\mu} \qquad , \qquad \beta \equiv -\frac{\varepsilon_{xx}}{\varepsilon_{zz}} = \frac{3K-2\mu}{2(3K+\mu)} \quad . \tag{6.78}$$

[27] Integrate the differential torque $d\boldsymbol{N} = \boldsymbol{r} \times d\boldsymbol{F}$ over the entire body. Integrating by parts, one obtains a surface term and a volume term. The volume torque density is $-\epsilon_{ijk}\,\sigma_{jk}$, which must vanish, thereby entailing the symmetry $\sigma = \sigma^{\mathsf{T}}$.

[28] If you were wondering why we've suddenly switched to roman indices C_{ijkl} instead of Greek $C_{\alpha\beta\mu\nu}$, it is to obviate any confusion with the Lamé parameter μ.

[29] In d space dimensions, one has $K = \lambda + 2d^{-1}\mu$ and $\widetilde{m} = m - d^{-1}\mathsf{Tr}\,m$ is the traceless part of any matrix m.

[30] In a homogeneous deformation, the strain and stress tensors are constant throughout the body.

The quantity Y is called the *Young's modulus*, and must be positive. The quantity β is the *Poisson ratio* β and satisfies $\beta \in \big[-1, \frac{3}{2}\big]$. A material like tungsten carbide has a very large Young's modulus of $Y = 53.4 \times 10^{11}\,\mathrm{dyn/cm^2}$ at STP, which means that you have to pull like hell in order to get it to stretch a little. Normally, when you stretch a material, it narrows in the transverse directions, which corresponds to a positive Poisson ratio. Materials for which $\beta < 0$ are called *auxetics*. When stretched, an auxetic becomes thicker in the directions perpendicular to the applied force. Examples include various porous foams and artificial macrostructures.

Elasticity and symmetry

Since

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij} \quad , \tag{6.79}$$

we may use the composite index notation in Tab. 6.15 to write the rank four tensor $C_{ijkl} \equiv C_{ab} = C_{ba}$ as a symmetric 6×6 matrix, with 21 independent elements before accounting for symmetry considerations. The linear stress-strain relation is then given by

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ 2\varepsilon_4 \\ 2\varepsilon_5 \\ 2\varepsilon_6 \end{pmatrix} \quad . \tag{6.80}$$

Since the elastic tensor is rank four, it is symmetric under inversion.

And now, let the symmetry commence!

- For triclinic crystals with point group C_1 or C_i, there are no symmetries to apply to C_{ab}, hence there are 21 independent elastic moduli. However, one can always rotate axes, and given the freedom to choose three Euler angles, this means we can always choose axes in such a way that three of the 21 moduli vanish, leaving 18. Again, this requires a nongeneric choice of axes.
- For monoclinic crystals, there is symmetry under $z \to -z$, and as in the example of the piezoelectric tensor $d_{\mu\nu\lambda}$, we have that C_{ijkl} vanishes if the index 3(z) appears an odd number of times, which means, in composite index notation,

  $$C_{14} = C_{15} = C_{24} = C_{25} = C_{34} = C_{35} = C_{46} = C_{56} = 0 \quad , \tag{6.81}$$

  leaving 13 independent elastic moduli for point groups C_2, C_s, and C_{2h}. The 6×6 matrix C_{ab} thus takes the form

  $$C_{ab}^{\text{MONO}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\ C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\ 0 & 0 & 0 & C_{44} & C_{45} & 0 \\ 0 & 0 & 0 & C_{45} & C_{55} & 0 \\ C_{16} & C_{26} & C_{36} & 0 & 0 & C_{66} \end{pmatrix} \quad . \tag{6.82}$$

- For orthorhombic crystals, $x \to -x$ and $y \to -y$ are each symmetries. Adding $z \to -z$ in the case of D_{2h} doesn't buy us any new restrictions since C is symmetric under inversion. We then have $C_{ab} = 0$ whenever $a \in \{1,2,3\}$ and $b \in \{4,5,6\}$. The general form of C_{ab} is then

$$C_{ab}^{\text{ORTHO}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix} \quad . \tag{6.83}$$

- For the tetragonal system, we can rotate (x, y, z) to $(-y, x, z)$. For the lower symmetry point groups among this system, namely C_4, S_4, and C_{4h}, the most general form is

$$C_{ab}^{\text{TET}}[C_4, S_4, C_{4h}] = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{11} & C_{13} & 0 & 0 & -C_{16} \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ C_{16} & -C_{16} & 0 & 0 & 0 & C_{66} \end{pmatrix} \quad , \tag{6.84}$$

  which has seven independent moduli. For the higher symmetry tetragonal point groups D_4, C_{4v}, D_{2d}, and D_{4h}, we have $C_{16} = 0$ because of the twofold axes which send (x, y, z) into $(x, -y, -z)$ and $(-x, y, -z)$, and there are only six independent moduli.

- For the trigonal point groups, our lives are again complicated by the C_3 rotations. One convenient way to deal with this is to define $\xi \equiv x + iy$ and $\bar{\xi} \equiv x - iy$, with

$$\begin{aligned} \varepsilon_{\xi\xi} &= \xi_i \, \xi_j \, \varepsilon_{ij} = \varepsilon_{xx} - \varepsilon_{yy} + 2i \, \varepsilon_{xy} \\ \varepsilon_{\xi\bar{\xi}} &= \xi_i \, \bar{\xi}_j \, \varepsilon_{ij} = \varepsilon_{xx} + \varepsilon_{xy} \\ \varepsilon_{z\xi} &= \xi_i \, \varepsilon_{zi} = \varepsilon_{zx} + i \, \varepsilon_{zy} \\ \varepsilon_{z\bar{\xi}} &= \bar{\xi}_i \, \varepsilon_{zi} = \varepsilon_{zx} - i \, \varepsilon_{zy} \quad , \end{aligned} \tag{6.85}$$

  where $\xi_i = \partial_i \xi$ where $x_1 = x$ and $x_2 = y$, and $\bar{\xi}_i = \partial_i \bar{\xi}$. A C_3 rotation then takes $\xi \to e^{2\pi i/3} \, \xi$ and $\bar{\xi} \to e^{-2\pi i/3} \, \bar{\xi}$. The only allowed elements of C_{ijkl} are

$$C_{zzzz} \quad , \quad C_{zz\xi\bar{\xi}} \quad , \quad C_{\xi\xi\bar{\xi}\bar{\xi}} \quad , \quad C_{\xi\bar{\xi}\xi\bar{\xi}} \quad , \quad C_{z\xi z\bar{\xi}} \quad , \quad C_{z\xi\xi\xi} \quad , \quad C_{z\bar{\xi}\bar{\xi}\bar{\xi}} \quad , \tag{6.86}$$

  and their corresponding elements obtained by permuting $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$. The first five of these are real, and the last two are complex conjugates: $C_{z\bar{\xi}\bar{\xi}\bar{\xi}} = C^*_{z\xi\xi\xi}$. So there are seven independent elastic moduli for the point groups C_3 and S_6. Note the general rule that we must have either no complex indices, one ξ and one $\bar{\xi}$ index, two each of ξ and $\bar{\xi}$, three ξ, or three $\bar{\xi}$. All other coefficients vanish by C_3 symmetry. We may now construct the elastic free energy density,

$$\begin{aligned} f = f_0 + \tfrac{1}{2} C_{zzzz} \, \varepsilon_{zz}^2 + C_{\xi\xi\bar{\xi}\bar{\xi}} \, \varepsilon_{\xi\xi} \, \varepsilon_{\bar{\xi}\bar{\xi}} + 2 \, C_{\xi\bar{\xi}\xi\bar{\xi}} \, \varepsilon_{\xi\bar{\xi}}^2 + 2 \, C_{zz\xi\bar{\xi}} \, \varepsilon_{zz} \, \varepsilon_{\xi\bar{\xi}} \\ + 4 \, C_{z\xi z\bar{\xi}} \, \varepsilon_{z\xi} \, \varepsilon_{z\bar{\xi}} + 2 \, C_{z\xi\xi\xi} \, \varepsilon_{z\xi} \, \varepsilon_{\xi\xi} + 2 \, C_{z\bar{\xi}\bar{\xi}\bar{\xi}} \, \varepsilon_{z\bar{\xi}} \, \varepsilon_{\bar{\xi}\bar{\xi}} \quad . \end{aligned} \tag{6.87}$$

Note the coefficient of four in front of the $C_{z\xi z\bar{\xi}}$ term, which arises from summing over the eight equal contributions,

$$\tfrac{1}{2}\big(C_{z\xi z\bar{\xi}} + C_{z\xi\bar{\xi}z} + C_{\xi zz\bar{\xi}} + C_{\xi z\bar{\xi}z} + C_{z\bar{\xi}z\xi} + C_{z\bar{\xi}\xi z} + C_{\bar{\xi}zz\xi} + C_{\bar{\xi}z\xi z}\big)\,\varepsilon_{z\xi}\,\varepsilon_{z\bar{\xi}} = 4\,C_{z\xi z\bar{\xi}}\,\varepsilon_{z\xi}\,\varepsilon_{z\bar{\xi}} \quad . \tag{6.88}$$

From the free energy, one can identify the coefficients of $\varepsilon_a\,\varepsilon_b$, where a and b are composite indices, and thereby determine the general form for C_{ab}, which is

$$C_{ab}^{\text{TRIG}}[C_3, S_6] = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & -C_{25} & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & C_{25} & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & C_{25} \\ -C_{25} & C_{25} & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & C_{25} & C_{14} & \frac{1}{2}(C_{11}-C_{12}) \end{pmatrix} \quad , \tag{6.89}$$

Adding in reflections or twofold axes, as we have in the higher symmetry groups in this system, *i.e.* D_3, C_{3v}, and D_{3d} allows for $\xi \leftrightarrow \bar{\xi}$, in which case $C_{z\xi\xi\xi} = C_{z\bar{\xi}\bar{\xi}\bar{\xi}}$, reducing the number of independent moduli to six, with $C_{25} = 0$.

There's another way to compute the number of independent moduli, using Eqn. 6.44. This applies to all cases, but it is particularly instructive to work it out for C_3 since the threefold rotations make its analysis more tedious than other cases where the symmetry operations merely permute the Cartesian indices. We start by decomposing the representation by which the symmetric rank two tensor ε_{ij} transforms into IRREPs of C_3. From Tab. 6.11, we have that $1 = A \oplus E \oplus E^*$, where 1 denotes the vector ($l = 1$) IRREP of $\mathsf{O}(3)$. Since the strain tensor ε is symmetric, we decompose $\Gamma_\varepsilon \equiv (1\times 1)^{\mathsf{sym}}$ into C_3 IRREPs using $\chi^{\mathsf{sym}}(g) = \frac{1}{2}\big[\chi(g)\big]^2 + \frac{1}{2}\,\chi(g^2)$, according to which $\chi^{\Gamma_\varepsilon}(E) = 6$ and $\chi^{\Gamma_\varepsilon}(C_3) = \chi^{\Gamma_\varepsilon}(C_3^2) = 0$. Thus we have $\Gamma_\varepsilon = 2A \oplus 2E \oplus 2E^*$, whose total dimension is six, as is appropriate for a symmetric 3×3 matrix. We next must decompose $\Gamma_C \equiv (\Gamma_\varepsilon \times \Gamma_\varepsilon)^{\mathsf{sym}}$. into C_3 IRREPs. But this is a snap since we've computed the characters for Γ_ε[31]. Accordingly, we have $\chi^{\Gamma_C}(E) = \frac{1}{2}\big[\chi^{\Gamma_\varepsilon}(E)\big]^2 + \frac{1}{2}\chi^{\Gamma_\varepsilon}(E^2) = \frac{1}{2}\cdot 6^2 + \frac{1}{2}\cdot 6 = 21$ and $\chi^{\Gamma_C}(C_3) = \chi^{\Gamma_C}(C_3^2) = 0$. Therefore $\Gamma_C = 7A \oplus 7E \oplus 7E^*$ and we conclude from $n_A(\Gamma) = 7$ that there are seven independent elastic constants for C_3.

- For all seven hexagonal system point groups, we have $C_{z\xi\xi\xi} = C_{z\bar{\xi}\bar{\xi}\bar{\xi}} = 0$, because C_6 rotations take ξ to $\xi\,e^{i\pi/3}$, hence $C_{z\xi\xi\xi}$ to $-C_{z\xi\xi\xi}$. C_{3h} and D_{3h} don't contain this element, but do contain the mirror reflection $z \to -z$, hence in all cases the elastic tensor resembles that for the trigonal case, but with $C_{14} = C_{25} = 0$. Hence there are five independent moduli, with

$$C_{ab}^{\text{HEX}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(C_{11}-C_{12}) \end{pmatrix} \quad , \tag{6.90}$$

[31] We work directly with the reducible representation Γ_ε and only decompose into C_3 IRREPs at the end of our calculation.

- For the cubic system (five point groups), the only independent elements are C_{xxxx}, C_{xxyy}, C_{xyxy}, and their symmetry-related counterparts such as C_{zzzz}, C_{yzyz}, *etc.* Thus,

$$C_{ab}^{\text{CUB}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \quad , \tag{6.91}$$

- For an isotropic material, $C_{11} = C_{22} + 2C_{44}$. The Lamé parameters are $\lambda = C_{12}$ and $\mu = C_{44}$.

6.3.7 Summary of tensor properties of the crystallographic point groups

At this point in the notes, we pause for a lengthy table, Tab. 6.16.

6.4 Vibrational and Electronic States of Molecules

6.4.1 Small oscillations of molecules

In §2.6 we considered the planar oscillations of a linear triatomic molecule of C_{3v} symmetry. We now consider the general case. First we consider the classical problem of N interacting point masses. Expanding the potential energy about equilibrium, the Hamiltonian is

$$H = \sum_{i,\alpha} \frac{(p_i^\alpha)^2}{2m_i} + \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} \Phi_{ij}^{\alpha\beta}\, u_i^\alpha\, u_j^\beta + \mathcal{O}(u^3) \quad , \tag{6.92}$$

where $\boldsymbol{u}_i$ is the vector displacement of ion i from its equilibrium position, $\boldsymbol{p}_i$ is its momentum, and m_i its mass. The indices α and β range over $\{1, \ldots, d\}$, where d is the dimension of space. The quantity $\Phi_{ij}^{\alpha\beta}$ is known as the *dynamical matrix*, and it is defined to be

$$\Phi_{ij}^{\alpha\beta} = \left. \frac{\partial^2 V}{\partial u_i^\alpha\, \partial u_j^\beta} \right|_{\text{EQ}} \quad , \tag{6.93}$$

where $V = V(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ is the potential, and $\boldsymbol{r}_j = \boldsymbol{r}_j^0 + \boldsymbol{u}_j$ with $\boldsymbol{r}_j^0$ the equilibrium position of the jth ion. We now make a simple canonical transformation $p_i^\alpha = m_i^{1/2}\, \tilde{p}_i^\alpha$ and $u_i^\alpha = m_i^{-1/2} \tilde{u}_i^\alpha$ for all i and α. Clearly this preserves the Poisson bracket $\left\{ u_i^\alpha\, ,\, p_j^\beta \right\}_{\text{PB}} = \delta_{ij}\, \delta^{\alpha\beta}$. The Hamiltonian is then

$$H = \sum_{i,\alpha} \frac{(\tilde{p}_i^\alpha)^2}{2} + \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} \tilde{\Phi}_{ij}^{\alpha\beta}\, \tilde{u}_i^\alpha\, \tilde{u}_j^\beta + \mathcal{O}(u^3) \quad , \tag{6.94}$$

crystal system	group symbol Schoenflies	HM	tensor order 1st	2nd	3rd	4th
triclinic	C_1	1	3	6	18	21
	S_2	$\overline{1}$	0	6	0	21
monoclinic	C_2	2	1	4	8	13
	C_{1h}	m	2	4	10	13
	C_{2h}	$2/m$	0	4	0	13
orthorhombic	D_2	222	0	3	3	9
	C_{2v}	$mm2$	1	3	5	9
	D_{2h}	mmm	0	3	0	9
tetragonal	C_4	4	1	2	4	7
	S_4	$\overline{4}$	0	2	4	7
	C_{4h}	$4/m$	0	2	0	7
	D_4	422	0	2	1	6
	C_{4v}	$4mm$	1	2	3	6
	D_{2d}	$\overline{4}2m$	0	2	2	6
	D_{4h}	$4/mmm$	0	2	0	6
trigonal	C_3	3	1	2	6	7
	S_6	$\overline{3}$	0	2	0	7
	D_3	32	0	2	2	6
	C_{3v}	$3m$	1	2	4	6
	D_{3d}	$\overline{3}m$	0	2	0	6
hexagonal	C_6	6	1	2	4	5
	C_{3h}	$\overline{6}$	0	2	2	5
	C_{6h}	$6/m$	0	2	0	5
	D_6	622	0	2	1	5
	C_{6v}	$6mm$	1	2	3	5
	D_{3h}	$\overline{6}m2$	0	2	1	5
	D_{6h}	$6/mmm$	0	2	0	5
cubic	T	23	0	1	1	3
	T_h	$m\overline{3}$	0	1	0	3
	O	432	0	1	0	3
	T_d	$\overline{4}3m$	0	1	1	3
	O_h	$m\overline{3}m$	0	1	0	3
isotropic			0	1	0	2

Table 6.16: Tensor properties of the 32 crystallographic point groups.

where $\tilde\Phi_{ij}^{\alpha\beta} = m_i^{-1/2}\Phi_{ij}^{\alpha\beta}m_j^{-1/2}$ remains a real symmetric matrix in the composite indices $(i\alpha)$ and $(j\beta)$ and can therefore be diagonalized by an orthogonal transformation $S_{\sigma,i\alpha}$, where $\sigma \in \{1,\ldots,dN\}$ indexes the normal modes of the molecule. That means

$$\sum_{i,\alpha,j\beta} S_{\sigma,i\alpha}\,\tilde\Phi_{ij}^{\alpha\beta}\,S^{\mathsf T}_{j\beta,\sigma'} = \omega_\sigma^2\,\delta_{\sigma\sigma'} \quad , \tag{6.95}$$

where ω_σ has the dimensions of T^{-2}, *i.e.* frequency squared[32]. If the equilibrium is a stable one, then $\omega_\sigma^2 \geq 0$ for all σ. This orthogonal transformation induces a second canonical transformation, from $\{\tilde u_{i\alpha},\tilde p_{i\alpha}\}$ to $\{\xi_\sigma,\pi_\sigma\}$, with

$$\xi_\sigma = S_{\sigma,i\alpha}\,\tilde u_i^\alpha \qquad , \qquad \pi_\sigma = \tilde p_i^\alpha\,S^{-1}_{i\alpha,\sigma} = S_{\sigma,i\alpha}\,\tilde p_i^\alpha \quad , \tag{6.96}$$

and the final form of the Hamiltonian is then

$$H = \sum_{\sigma=1}^{dN}\left(\tfrac12\pi_\sigma^2 + \tfrac12\omega_\sigma^2\,\xi_\sigma^2\right) \quad . \tag{6.97}$$

Hamilton's equations of motion, which are of course preserved by the canonical transformations, are then $\dot\xi_\sigma = \partial H/\partial\pi_\sigma = \pi_\sigma$ and $\dot\pi_\sigma = -\partial H/\partial\xi_\sigma = -\omega_\sigma^2\,\xi_\sigma$, hence $\ddot\xi_\sigma = -\omega_\sigma^2\,\xi_\sigma$ and ω_σ is the oscillation frequency for the normal mode label σ.

6.4.2 Group theory and the dynamical matrix

To solve the general small oscillations problem, one must diagonalize the symmetric matrix $\tilde\Phi_{ij}^{\alpha\beta}$, which is of rank dN. While today this is a simple computational task, even for large molecules, such crank-turning is oblivious to the consequences of point group symmetries that are relevant to many physically relevant cases. The resulting multiplet structure in the spectrum is inscrutable without group theory.

To determine the IRREPs of the molecular point group $\mathcal{P}$ under which energy multiplets transform, just follow these simple steps:

(i) First, identify the point group $\mathcal{P}$ which describes the full symmetry of the equilibrium configuration.

(ii) Second, construct for each element $g \in \mathcal{P}$ the *permutation matrix* $D^{\mathsf{per}}(g)$, defined to be

$$D^{\mathsf{per}}_{ij}(g) = \langle\, i\,|\,g\,|\,j\,\rangle = \begin{cases} 1 & \text{if } g \text{ takes ion } j \text{ to ion } i \\ 0 & \text{otherwise} \quad . \end{cases} \tag{6.98}$$

These matrices, which are all rank N, form a representation which we call Γ^{per}.

(iii) Find the characters $\chi^{\mathsf{per}}(g)$. Note that

$$\chi^{\mathsf{per}}(g) = \text{number of ions remaining invariant under the operation } g \tag{6.99}$$

can be ascertained without computing all the matrix elements of $D^{\mathsf{per}}_{ij}(g)$.

[32]The original $\Phi_{ij}^{\alpha\beta}$ had dimensions of $EL^{-2} = MT^{-2}$, hence $\tilde\Phi_{ij}^{\alpha\beta}$ has dimensions of T^{-2}.

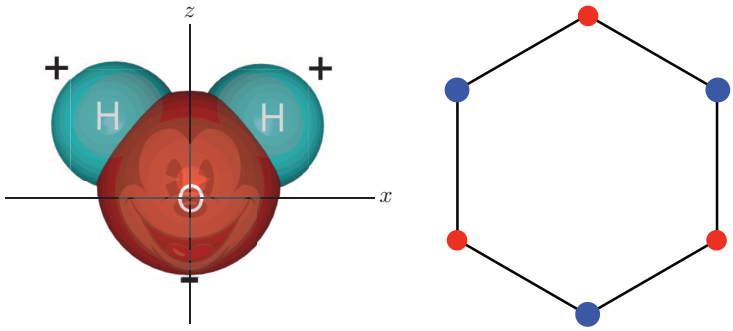


Figure 6.11: Left panel: the water molecule. Right panel: a molecule with C_{3v} symmetry. Rotations by an odd multiple of 60° are not a symmetry. Image credits: NCLab.com and ClipArtPanda.com.

(iv) For each $g \in \mathcal{P}$, construct the matrices $D^{\rm vec}(g) \in O(d)$, which is the $d \times d$ orthogonal matrix corresponding to the symmetry operation g.

(v) The symmetry operations operate on both the ion labels as well as their displacements from equilibrium. The corresponding representation of $\mathcal{P}$ is thus $\Psi = \Gamma^{\rm vec} \times \Gamma^{\rm per}$. From this, we must subtract one copy of $\Gamma^{\rm vec}$ corresponding to translational zero modes, and one copy of $\Gamma^{\rm rot}$, corresponding to rotational zero modes. Note that $\Gamma^{\rm rot}$ is the 1^+ representation of $\mathsf{O}(3)$, whose matrices are given by $D^{\rm rot}(g) = \det\big[D^{\rm vec}(g)\big] \cdot D^{\rm vec}(g)$

(vi) To find the IRREPs for the $d(N-2)$ finite frequency vibrational modes, decompose $\Gamma^{\rm per}$, $\Gamma^{\rm vec}$, and $\Gamma^{\rm rot}$ into IRREPs of $\mathcal{P}$. The vibrational representations of the molecule are then given by

$$\Gamma^{\rm vib} = \overbrace{\Gamma^{\rm vec} \times \Gamma^{\rm per}}^{\Psi} - \Gamma^{\rm vec} - \Gamma^{\rm rot} \quad . \tag{6.100}$$

(vii) Starting with an arbitrary (*e.g.* random) vector ψ, one can project onto the IRREPs Γ contained in $\Gamma^{\rm vib}$ using the projectors

$$\Pi^\Gamma = \frac{d_\Gamma}{N_G} \sum_{g\in G} \chi^{\Gamma^*}(g)\, D^\Psi(g) \qquad \text{or} \qquad \Pi^\Gamma_{\mu\nu} = \frac{d_\Gamma}{N_G} \sum_{g\in G} D^{\Gamma^*}_{\mu\nu}(g)\, D^\Psi(g) \quad , \tag{6.101}$$

where Π^Γ projects onto the IRREP Γ, and $\Pi^\Gamma_{\mu\nu}$ projects onto the $\mu^{\rm th}$ row of Γ.

(viii) The projected vectors $\Pi^\Gamma \psi$ form a basis for all occurrences of the IRREP Γ in the decomposition of the dN-dimensional representation Ψ. One then must project out the zero modes in $\Gamma^{\rm vec}$ and $\Gamma^{\rm rot}$.

Water molecule

Let's test this scheme on the simple water molecule in Fig. 6.11. The group is C_{2v}, with elements E (identity), C_2 (rotation by π about z-axis), σ_v (reflection in x-z plane), and σ_v' (reflection in y-z plane):

$$C_2\,(x,y,z) = (-x,-y,z) \quad , \quad \sigma_v\,(x,y,z) = (x,-y,z) \quad , \quad \sigma_v'\,(x,y,z) = (-x,y,z) \quad . \tag{6.102}$$

Choosing the ion site labels O = 1, H = 2, and H′ = 3, the permutation matrices are

$$D^{\mathsf{per}}(E) = D^{\mathsf{per}}(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad D^{\mathsf{per}}(C_2) = D^{\mathsf{per}}(\sigma_v') = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \tag{6.103}$$

which may readily be checked by inspection.

The matrices of Γ^{vec} are

$$\begin{aligned} D^{\mathsf{vec}}(E) &= \begin{pmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{pmatrix} \quad , \quad D^{\mathsf{vec}}(C_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{pmatrix} \\ D^{\mathsf{vec}}(\sigma_v) &= \begin{pmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{pmatrix} \quad , \quad D^{\mathsf{vec}}(\sigma_v') = \begin{pmatrix} -1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{pmatrix} \quad . \end{aligned} \tag{6.104}$$

We may now compute the characters of the matrices $D^{\mathsf{per}}(g)$ and $D^{\mathsf{vec}}(g)$; they are reported in Tab. 6.17. Multiplying the characters to compute $\chi^{\Psi}(g) = \chi^{\Gamma^{\mathsf{vec}}}(g)\,\chi^{\Gamma^{\mathsf{per}}}(g)$, and decomposing into IRREPs of C_{2v}, we find

$$\Psi = \Gamma^{\mathsf{vec}} \times \Gamma^{\mathsf{per}} = 3A_1 \oplus A_2 \oplus 3B_1 \oplus 2B_2 \quad . \tag{6.105}$$

From these IRREPs we must exclude

$$\begin{aligned} \Gamma^{\mathsf{vec}} &= A_1 \oplus B_1 \oplus B_2 \\ \Gamma^{\mathsf{rot}} &= A_2 \oplus B_1 \oplus B_2 \quad , \end{aligned} \tag{6.106}$$

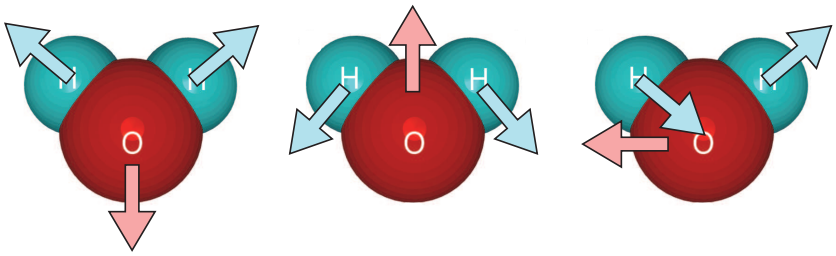
resulting in

$$\Gamma^{\mathsf{vib}} = 2A_1 \oplus B_1 \quad . \tag{6.107}$$

C_{2v}	E	C_2	σ_v	σ_v'	basis
A_1	1	1	1	1	z
A_2	1	1	−1	−1	xy
B_1	1	−1	1	−1	x
B_2	1	−1	−1	1	y
Γ^{vec}	3	−1	1	1	$A_1 \oplus B_1 \oplus B_2$
Γ^{rot}	3	−1	−1	−1	$A_2 \oplus B_1 \oplus B_2$
Γ^{per}	3	1	3	1	$2A_1 \oplus B_1$
$\Gamma^{\mathsf{vec}} \times \Gamma^{\mathsf{per}}$	9	−1	3	1	$3A_1 \oplus A_2 \oplus 3B_1 \oplus 2B_2$

$\Gamma \times \Gamma'$	A_1	A_2	B_1	B_2
A_1	A_1	A_2	B_1	B_2
A_2	A_2	A_1	B_2	B_1
B_1	B_1	B_2	A_1	A_2
B_2	B_2	B_1	A_2	A_1

Table 6.17: Character and representation product tables for C_{2v}.



A_1 A_1 B_1

Figure 6.12: Normal modes of the H_2O molecule and their C_{2v} IRREP labels. Image credit: NCLab.com.

Recall we started with nine degrees of freedom for the water molecule, corresponding to three translations for each of its constituent atoms. Subtracting three translational and three rotational zero modes, we are left with three finite frequency vibrational modes, two of which transform according to A_1 and one according to B_1. These vibrations are depicted in Fig. 6.12.

Buckyball

Flush with success after identifying the IRREPs or the vibrational spectrum of H_2O, let's try something with a bigger symmetry group – the buckyball C_{60}. The buckyball is depicted in Fig. 6.13. Its symmetry group is the icosahedral group with inversion, $I_h = I \times C_i$, which has 120 elements. A character tableis provided in Tab. 6.18. It should come as no surprise that $\Gamma^{\rm vec} = T_{1u}$ and $\Gamma^{\rm rot} = T_{1g}$.

When it comes to constructing $\Gamma^{\rm per}$, we are in luck. Eight of the ten classes of symmetry operations leave no sites fixed, hence for these classes we have $\chi^{\rm per}(\mathcal{C}) = 0$. The only operations which leave fixed points are the identity, which leaves every site invariant, hence $\chi^{\rm per}(E) = 60$, and the reflections 15σ, each of which leaves four sites invariant, hence $\chi^{\rm per}(15\sigma) = 4$[33]. Taking the product with $\Gamma^{\rm vec}$ to form $\Psi = \Gamma^{\rm vec} \times \Gamma^{\rm per}$, we have $\chi^{\Psi}(E) = 180$ and $\chi^{\Psi}(15\sigma) = 4$, hence thus, the number of times each IRREP Γ appears in the product representation Ψ is

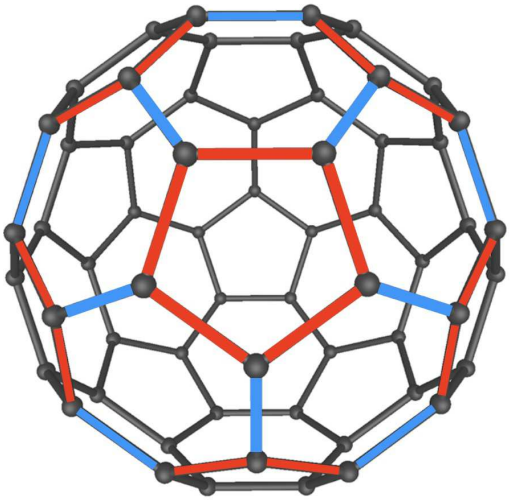
$$\begin{aligned} n_\Gamma(\Psi) &= \frac{1}{120}\Big(180 \cdot \chi^\Gamma(E) + 4 \cdot 15 \cdot \chi^\Gamma(15\sigma)\Big) \\ &= \tfrac{3}{2}\,\chi^\Gamma(E) + \tfrac{1}{2}\,\chi^\Gamma(15\sigma) \quad . \end{aligned} \tag{6.108}$$

The resulting $n_\Gamma(\Psi)$ values are given in the table within Fig. 6.13. Summing the dimensions of the IRREPs times their multiplicities, one finds

$$\sum_\Gamma n_\Gamma(\Psi)\, d_\Gamma = 180 \quad , \tag{6.109}$$

which is the total number of vibrational degrees of freedom of the buckyball (including zero modes). From the decomposition of Ψ into I_h IRREPs, one must subtract the translational and rotational zero

[33] See how a reflection plane bisecting the buckyball of Fig. 6.13 contains two links, *i.e.* four sites.



Γ	d_Γ	n_Γ	$n_\Gamma d_\Gamma$
A_g	1	2	2
T_{1g}	3	4	12
T_{2g}	3	4	12
G_g	4	6	24
H_g	5	8	40
A_u	1	1	1
T_{1u}	3	5	15
T_{2u}	3	5	15
G_u	4	6	24
H_u	5	7	35

Figure 6.13: The buckyball C_{60}, its IRREPs, and the decomposition of $\Psi = \Gamma^{\rm vec} \times \Gamma^{\rm per}$.

modes, which is to say one copy each of T_{1u} and T_{1g}, respectively. This leaves

$$\Gamma^{\rm vib} = 2A_g \oplus 3T_{1g} \oplus 4T_{2g} \oplus 6G_g \oplus 8H_g \oplus A_u \oplus 4T_{1u} \oplus 5T_{2u} \oplus 6G_u \oplus 7H_u \quad . \tag{6.110}$$

Animations of each of these normal modes may be viewed at

http://www.public.asu.edu/~cosmen/C60_vibrations/mode_assignments.htm

6.4.3 Selection rules for infrared and Raman spectroscopy

Recall that electromagnetic radiation can excite modes via dipole transitions, and that a general matrix element of the form $\langle\, \Gamma_{\rm f}\, \beta \,|\, \hat{Q}^\Gamma_\mu \,|\, \Gamma_{\rm i}\, \alpha \,\rangle$ can be nonzero only if $\Gamma_{\rm f} \in \Gamma_{\rm i} \times \Gamma$. Usually the initial state is the ground state, in which case $\Gamma_{\rm i}$ is the trivial representation, and in our case $\Gamma = \Gamma^{\rm vec}$, corresponding to an electric dipole transition. Then our condition for the possibility of a nonzero matrix element becomes simply $\Gamma_{\rm f} \in \Gamma^{\rm vec}$. Such modes are said to be *IR-active*. For example, for H_2O, all three vibrational modes are IR-active, because $\Gamma^{\rm vib} = 2A_1 \oplus B_1$ and $\Gamma^{\rm vec} = A_1 \oplus B_1 \oplus B_2$. For C_{60}, only the five T_{1u} multiplets are IR-active.

Raman spectroscopy involves the detection of inelastically scattered light. Thus, there is an incoming electromagnetic wave $\boldsymbol{\mathcal{E}}_{\rm i}$ and an outgoing wave $\boldsymbol{\mathcal{E}}_{\rm f}$. These are coupled through a 3×3 symmetric polarization tensor, $\alpha_{\mu\nu}$. We shall therefore be interested in symmetric, rank-two tensor representations of the molecular point group $\mathcal{P}$.

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	I	$12S_{10}^3$	$12S_{10}$	$20S_6$	15σ
A_g	1	1	1	1	1	1	1	1	1	1
T_{1g}	3	τ	$1-\tau$	0	-1	3	τ	$1-\tau$	0	-1
T_{2g}	3	$1-\tau$	τ	0	-1	3	$1-\tau$	τ	0	-1
G_g	4	-1	-1	1	0	4	-1	-1	1	0
H_g	5	0	0	-1	1	5	0	0	-1	1
A_u	1	1	1	1	1	-1	-1	-1	-1	-1
T_{1u}	3	τ	$1-\tau$	0	-1	-3	$-\tau$	$-1+\tau$	0	1
T_{2u}	3	$1-\tau$	τ	0	-1	-3	$-1+\tau$	$-\tau$	0	1
G_u	4	-1	-1	1	0	-4	1	1	-1	0
H_u	5	0	0	-1	1	-5	0	0	1	-1
$\Gamma^{\rm vec}$	3	τ	$1-\tau$	0	-1	-3	$-\tau$	$-1+\tau$	0	1
$\Gamma^{\rm rot}$	3	τ	$1-\tau$	0	-1	3	τ	$1-\tau$	0	-1
$\Gamma^{\rm per}$	60	0	0	0	0	0	0	0	0	4
Ψ	180	0	0	0	0	0	0	0	0	4

Table 6.18: Character table for the icosahedral group $I_{\rm h}$. Note $\tau = 2\cos\frac{\pi}{5} = \frac{1}{2}\big(1+\sqrt{5}\big)$ satisfies $\tau^2 = 1+\tau$. $\Gamma^{\rm per}$ is the permutation representation for the buckyball C_{60}.

The derivation of the effective Raman Hamiltonian is somewhat involved, and we include here a brief discussion for the sake of completeness. The goal is to compute the effective molecular Hamiltonian up to second order in the external *time-dependent* electric field $\boldsymbol{\mathcal{E}}(t)$, within a restricted manifold of molecular states consisting of the ground state $|\,{\rm g}\,\rangle$, assumed to transform trivially under point group operations, and an excited state multiplet $|\,\Gamma\,\gamma\,\rangle$, where γ is the partner label, transforming as the IRREP Γ. The effective Hamiltonian is found to be[34]

$$\hat{H}_{\rm eff}(t) = \hat{H}_0 - \hat{\boldsymbol{\mu}}\cdot\boldsymbol{\mathcal{E}}(t) + \tfrac{1}{2}\,\mathcal{E}_\rho(t)\int\limits_{-\infty}^{t} dt'\;\hat{\alpha}_{\rho\lambda}(t-t')\,\mathcal{E}_\lambda(t') + \mathcal{O}(\mathcal{E}^3) \quad , \tag{6.111}$$

where

$$\hat{H}_0 = E_{\rm g}\,|\,{\rm g}\,\rangle\langle\,{\rm g}\,| + {\sum_{\Gamma}}' E_\Gamma \sum_{\gamma=1}^{d_\Gamma} |\,\Gamma\,\gamma\,\rangle\langle\,\Gamma\,\gamma\,| \tag{6.112}$$

includes the molecular ground state and all vibrational excitation multiplets, and

$$\hat{\boldsymbol{\mu}} = -e\sum_{a,b} |\,b\,\rangle\,\langle\,b\,|\,\hat{\boldsymbol{d}}\,|\,a\,\rangle\,\langle\,a\,| \quad , \tag{6.113}$$

[34] See, *e.g.*, chapter 4 of R. Long, *The Raman Effect: A Unified Treatment of the Theory of Raman Scattering by Molecules* (Wiley, 2002).

where $|\,a\,\rangle$ and $|\,b\,\rangle$ are taken from the low-lying states $|\,\mathrm{g}\,\rangle$ and $|\,\Gamma\,\gamma\,\rangle$, and $\hat{\boldsymbol{d}}$ is the dipole moment operator of the molecule. If the molecular point group $\mathcal{P}$ contains the inversion element I, then $\hat{\boldsymbol{d}}$ can only have matrix elements between representations of different parity. The second order term involves the polarization tensor, which is obtained from time-dependent perturbation theory, *viz.*

$$\hat{\alpha}_{\rho\lambda}(s) = \frac{i}{\hbar}\left[\hat{P}\,e^{i\hat{H}_0 s/\hbar}\,\hat{d}_\rho\,e^{-i\hat{H}_0 s/\hbar}\,\hat{Q}\,\hat{d}_\lambda\,\hat{P} - \hat{P}\,\hat{d}_\lambda\,\hat{Q}\;e^{i\hat{H}_0 s/\hbar}\,\hat{d}_\rho\,e^{-i\hat{H}_0 s/\hbar}\,\hat{P}\right]\Theta(s) \quad , \tag{6.114}$$

where $\hat{P} = \sum_a |\,a\,\rangle\langle\,a\,|$ is the projector onto the ground state and low-lying vibrational multiplets, and $\hat{Q} \equiv \hat{\mathbb{1}} - \hat{P} = \sum_m{}' |\,m\,\rangle\langle\,m\,|$ is the orthogonal projector onto all other eigenstates (hence the prime on the sum) of the $\boldsymbol{\mathcal{E}} = 0$ molecular Hamiltonian. $\Theta(s)$ is the step function. The Fourier transform of $\hat{H}_{\rm eff}(t)$ is

$$\hat{H}_{\rm eff}(\omega) = \hat{H}_0\,\delta(\omega) - \boldsymbol{\mathcal{E}}(\omega)\cdot\hat{\boldsymbol{\mu}} + \tfrac{1}{2}\int\limits_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\mathcal{E}_\rho(\omega-\omega')\,\mathcal{E}_\lambda(\omega')\,\hat{\alpha}_{\rho\lambda}(\omega') \quad , \tag{6.115}$$

where

$$\hat{\alpha}_{\rho\lambda}(\omega) = \sum_{a,b}\sum_n{}'\,|\,b\,\rangle\left\{\frac{\langle\,b\,|\,\hat{d}_\rho\,|\,n\,\rangle\langle\,n\,|\,\hat{d}_\lambda\,|\,a\,\rangle}{E_n - E_b - \hbar\omega - i0^+} + \frac{\langle\,b\,|\,\hat{d}_\lambda\,|\,n\,\rangle\langle\,n\,|\,\hat{d}_\rho\,|\,a\,\rangle}{E_n - E_a + \hbar\omega + i0^+}\right\}\langle\,a\,| \quad . \tag{6.116}$$

To be clear about what it is we are doing here, we are endeavoring to derive a low-energy effective Hamiltonian for the vibrational states of a molecule. In general a given molecular state has electronic, vibrational, and rotational quantum numbers. In many relevant cases, there is a hierarchy of energy scales, with $\Delta E_{\rm rot} \ll \Delta E_{\rm vib} \ll \hbar\omega \ll \Delta E_{\rm el}$, which we shall assume. We'll ignore here the rotational modes, *i.e.* we'll treat them as zero modes of the vibrational spectrum. All states may be decomposed as

$$|\,n\,\rangle = |\,\mathrm{v}_n\,\rangle\otimes|\,\mathrm{e}_n\,\rangle \quad , \tag{6.117}$$

i.e. into a direct product of nuclear coordinate (vibrational) and electronic wavefunctions, where the electronic wavefunctions are eigenfunctions of the Born-Oppenheimer Hamiltonian in which the nuclear coordinates are frozen. Thus $|\,\mathrm{e}_n\,\rangle = |\,\mathrm{e}_n(Q)\,\rangle$ depends explicitly on the nuclear coordinates. Although the Born-Oppenheimer energies $E_n^{\mathsf{BO}}(Q)$ will then depend on Q, the electronic energies dominate and we may take $E_n^{\mathsf{BO}}(Q) \approx E_n^{\mathsf{BO}}(Q^0)$ at the equilibrium nuclear coordinates. The dipole moment operator $\hat{\boldsymbol{d}} = -e\sum_{i,l}\boldsymbol{r}_{i,l}$ is a sum over electron displacements with respect to the fixed origin of the point group,where $\boldsymbol{r}_{i,l}$ for a given electron is a sum of terms including the equilibrium position $\boldsymbol{Q}_i^0$ of the $i^{\rm th}$ ion, its displacement $\boldsymbol{u}_i = \boldsymbol{Q}_i - \boldsymbol{Q}_i^0$ from equilibrium, and the electronic position $\boldsymbol{\xi}_{i,l}$ of the $l^{\rm th}$ electron on that ion with respect to its nucleus. We may now write[35]

$$\hat{\alpha}_{\rho\lambda}(Q,\omega) = \frac{1}{\hbar}\sum_n{}'\left\{\frac{\langle\,\mathrm{e_g}(Q)\,|\,\hat{d}_\rho\,|\,\mathrm{e}_n(Q)\,\rangle\langle\,\mathrm{e}_n(Q)\,|\,\hat{d}_\lambda\,|\,\mathrm{e_g}(Q)\,\rangle}{\omega_{n\mathrm{g}} - \omega - i0^+} + \frac{\langle\,\mathrm{e_g}(Q)\,|\,\hat{d}_\lambda\,|\,\mathrm{e}_n(Q)\,\rangle\langle\,\mathrm{e}_n(Q)\,|\,\hat{d}_\rho\,|\,\mathrm{e_g}(Q)\,\rangle}{\omega_{n\mathrm{g}} + \omega + i0^+}\right\} \quad , \tag{6.118}$$

[35] In deriving Eqn. 6.118, we use the fact that the Q-dependent part of the energy $E_n(Q)$ may be dropped in the denominator because of the aforementioned energy scale hierarchy. We may then collapse the sum on the vibrational component of the high energy excited states using completeness.

which acts as an operator on the vibrational wavefunctions $|\, v_a \,\rangle$. The matrix elements $\langle\, \mathrm{e_g}(Q) \,|\, \hat{d}_\rho \,|\, \mathrm{e}_n(Q) \,\rangle$ *etc.* involve integration over the electronic coordinates alone, and therefore are functions of the ionic coordinates Q. Similarly, we define

$$\hat{\mu}_\rho(Q) = -e \left\langle\, \mathrm{e_g}(Q) \,\middle|\, \hat{d}_\rho \,\middle|\, \mathrm{e_g}(Q) \,\right\rangle \quad . \tag{6.119}$$

We arrive at an effective time-dependent Hamiltonian for the low-lying vibrational levels, which when expressed in the frequency domain is[36]

$$\begin{aligned} \left\langle\, \mathrm{v}_b \,\middle|\, \hat{H}_{\rm eff}(\omega) \,\middle|\, \mathrm{v}_a \,\right\rangle &= E_a\, \delta_{ab}\, \delta(\omega) - \mathcal{E}_\rho(\omega) \left\langle\, \mathrm{v}_b \,\middle|\, \hat{\mu}_\rho(Q) \,\middle|\, \mathrm{v}_a \,\right\rangle \\ &\quad + \tfrac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\, \mathcal{E}^*_\rho(\omega' - \omega)\, \mathcal{E}_\lambda(\omega') \left\langle\, \mathrm{v}_b \,\middle|\, \hat{\alpha}_{\rho\lambda}(Q, \omega') \,\middle|\, \mathrm{v}_a \,\right\rangle \quad . \end{aligned} \tag{6.120}$$

Finally, if the wavefunctions can be taken to be real, we see from Eqn. 6.118 that the polarizability matrix is symmetric, *i.e.* $\alpha_{\rho\lambda}(Q,\omega) = \alpha_{\lambda\rho}(Q,\omega)$. Note that the nuclear part $|\, \mathrm{e_g}(Q) \,\rangle\langle\, \mathrm{e_g}(Q) \,|$ is a one-dimensional projector common to all terms in the effective vibrational Hamiltonian, and can hence be set to unity.

At this point the electric field $\mathcal{E}_\rho(\omega)$ may be quantized and written in terms of photon creation and annihilation operators. The second term corresponds to *Rayleigh scattering* in which a photon of frequency $\omega = (E_b - E_a)/\hbar$ is absorbed. We assume here that a is the ground state. If a represents an occupied excited state, as may be the case at finite temperature, a photon can be emitted. Regarding the third term in $\hat{H}_{\rm eff}$, which corresponds to Raman scattering, we can read off from the form of the Hamiltonian that if $\mathcal{E}_\lambda(\omega')$ destroys an incoming photon of frequency ω', then $\mathcal{E}^*_\rho(\omega' - \omega)$ creates an outgoing photon of frequency $\omega' - \omega$, where $\hbar\omega = E_b - E_a$. When $E_b > E_a$ this is called *Stokes scattering*. In Stokes scattering, the frequency of the emitted radiation is less than that of the incident radiation. When $E_b < E_a$, the emitted radiation is at a higher frequency, and the process is called *anti-Stokes* scattering[37].

For Rayleigh scattering, the selection rules are as we discussed above. The operator $\hat{\boldsymbol{\mu}}$ transforms as a vector, hence $\langle\, b \,|\, \hat{\boldsymbol{\mu}} \,|\, a \,\rangle$ can be nonzero only if $\Gamma_b \in \Gamma^{\mathsf{vec}} \times \Gamma_a$. For Raman scattering, $\hat{\alpha}_{\rho\lambda}$ transforms as the symmetric product of two vectors, *i.e.* as $\Psi = (\Gamma^{\mathsf{vec}} \times \Gamma^{\mathsf{vec}})^{\mathsf{sym}}$. This representation is symmetric under inversion, hence Raman scattering does not result in a change of parity. Therefore, in molecules with inversion symmetry, IR (Rayleigh) and Raman scattering are complementary tools, since a mode can either be IR or Raman active, but not both. If there is no inversion symmetry, a mode can be both IR *and* Raman active. Of course, a mode can be inactive for both IR and Raman. Modes which are inactive for reasons other than parity are called *silent*.

As an example, consider our old friend C_{3v}, for which $\Gamma^{\mathsf{vec}} = A_1 \oplus E$, with $\chi^{\mathsf{vec}}(E) = 3$, $\chi^{\mathsf{vec}}(2C_3) = 0$, and $\chi^{\mathsf{vec}}(3\sigma_v) = 1$. From

$$\chi^{\mathsf{sym}}(g) = \tfrac{1}{2}\big[\chi^{\mathsf{vec}}(g)\big]^2 + \tfrac{1}{2}\chi^{\mathsf{vec}}(g^2) \quad , \tag{6.121}$$

we have $\chi^{\mathsf{sym}}(E) = 6$, $\chi^{\mathsf{sym}}(2C_3) = 0$, and $\chi^{\mathsf{sym}}(3\sigma_v) = 2$, whence the decomposition formula yields $\Gamma^{\mathsf{sym}} = 2A_1 \oplus 2E$. Thus, if the initial vibrational state is the ground state, the final state is Raman active if $\Gamma_{\rm f}$ is either A_1 or E but not A_2.

[36] See also the discussion in the appendix, §6.8.

[37] Stokes' law says that the frequency of fluorescent light is always less than or equal to that of the incident light. Hence Stokes lines are those which correspond to Stokes' law, and anti-Stokes lines are those which violate it.

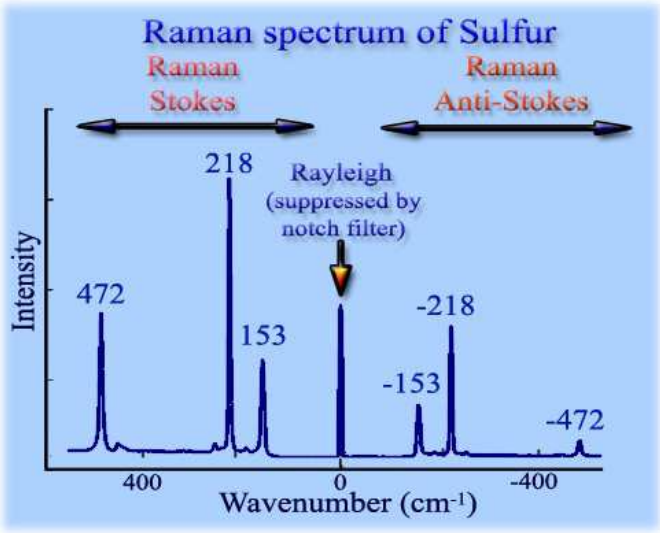


Figure 6.14: Rayleigh and Raman spectral lines in crystalline sulfur. Image credit: spectrometry316.blogspot.com.

For H_2O, with point group C_{2v}, we found $\Gamma^{\rm vib} = 2A_1 \oplus B_1$. We next need $\Gamma^{\rm sym}$, which we obtain by computing the characters $\chi^{\rm sym}(g)$ using Eqn. 6.121. Note that C_2, σ_v, and σ_v' are all of order two, and we obtain

$$\chi^{\rm sym}(E) = 6 \quad , \quad \chi^{\rm sym}(C_2) = \chi^{\rm sym}(\sigma_v) = \chi^{\rm sym}(\sigma_v') = 2 \quad . \tag{6.122}$$

Decomposing into C_{2v} IRREPs, we find

$$\Gamma^{\rm sym} = 3A_1 \oplus A_2 \oplus B_1 \oplus B_2 \quad , \tag{6.123}$$

the total dimension of which is six, corresponding to the degrees of freedom in a real 3×3 symmetric matrix. Thus, all IRREPs are present in $\Gamma^{\rm sym}$ and all modes are Raman active.

For the buckyball, $\Gamma^{\rm vec} = T_{1u}$, and one finds

$$I_h \ : \ \Gamma^{\rm vec} \times \Gamma^{\rm vec} = A_g \oplus T_{1g} \oplus H_g \quad . \tag{6.124}$$

The sum of the dimensions is nine, corresponding to a 3×3 real matrix. To obtain $\Gamma^{\rm sym}$, we must subtract out the antisymmetric tensor representation $\Gamma^{\rm ASY}$. Since this is of dimension three, we immediately know it must be T_{1g} and that $\Gamma^{\rm sym} = A_g \oplus H_g$, which is properly of total dimension six. Comparing with Fig. 6.13, we see that in addition to the Raman inactive parity-odd multiplets, all parity even multiplets other than A_g and H_g are Raman silent. A quick check of the character tables shows that the representation functions for T_{1g} are the angular momentum operators, which indeed correspond to an antisymmetric rank three tensor. But if this casual elimination of T_{1g} strikes one as too glib – even though it is obviously correct! – we can grind through a direct calculation using Eqn. 6.121 and Tab. 6.18. All we need to keep in mind is that $(C_5)^2 = C_5^2$, $(C_5^2)^2 = C_5^{-1}$ (class C_5), $(C_3)^2 = C_3^{-1}$ (class C_3), $I^2 = E$, $(S_{10}^3)^2 = C_5^3$ (class C_5^2), $(S_{10})^2 = C_5$, $(S_6)^2 = C_3$, and $\sigma^2 = 1$. It is then straightforward to derive

$$\chi^{\rm sym}(E) = \chi^{\rm sym}(I) = 6 \quad , \quad \chi^{\rm sym}(C_5) = \chi^{\rm sym}(S_{10}) = 1 \quad , \quad \chi^{\rm sym}(C_5^2) = \chi^{\rm sym}(S_{10}^3) = 1 \tag{6.125}$$

and

$$\chi^{\text{sym}}(C_3) = \chi^{\text{sym}}(S_6^3) = 0 \quad , \quad \chi^{\text{sym}}(C_2) = \chi^{\text{sym}}(\sigma) = 2 \quad . \tag{6.126}$$

One then derives the decomposition

$$n_\Gamma(\Gamma^{\text{sym}}) = \frac{1}{10}\Big(\chi^\Gamma(E) + 2\,\chi^\Gamma(C_5) + 2\,\chi^\Gamma(C_5^2) + 5\,\chi^\Gamma(C_2)\Big) \quad , \tag{6.127}$$

from which one readily recovers $\Gamma^{\text{sym}} = A_g \oplus H_g$.

6.4.4 Electronic spectra of molecules

The decomposition of electronic eigenstates follows the same general rubric as in §6.4.2, except rather than decomposing $\Gamma^{\text{vec}} \times \Gamma^{\text{per}}$, we must decompose $\Gamma^{\text{orb}} \times \Gamma^{\text{per}}$, where Γ^{orb} is the representation for the atomic orbitals. There are no translational or rotational zero modes to subtract.

Consider, for example, a benzene molecule, $\mathrm{C_6H_6}$. The symmetry group is C_{6v}. Each carbon atom has a $1\mathrm{s}^2\,2\mathrm{s}^2$ core plus two electrons in the 2p orbital, one of which forms a bond with its neighboring hydrogen atom. The remaining six electrons are associated with the carbon p_z (π) orbitals. A p_z orbital is invariant under all C_{6v} operations, since it is oriented perpendicular to the symmetry plane. Thus, $\Gamma^{\text{orb}} = A_1$ for benzene, and we are left with the task of decomposing Γ^{per}. The only symmetry operations which leave sites invariant are the identity, for which $\chi^{\text{per}}(E) = 6$, and the diagonal mirrors, for which $\chi^{\text{per}}(\sigma_d) = 2$. Consulting the character table for C_{6v}, one readily finds

$$\Gamma^{\text{per}} = A_1 \oplus B_2 \oplus E_1 \oplus E_2 \quad . \tag{6.128}$$

A simple tight-binding model for the π orbitals is given by

$$\hat{H} = -t \sum_{n=1}^{6} \sum_{\sigma} \Big(\big|\, n,\sigma \,\big\rangle\big\langle\, n{+}1,\sigma \,\big| + \big|\, n{+}1,\sigma \,\big\rangle\big\langle\, n,\sigma \,\big| \Big) \quad , \tag{6.129}$$

which is instantly diagonalized in the crystal momentum basis as

$$\hat{H} = -2t \sum_{k,\sigma} \cos(nk)\, \big|\, k,\sigma \,\big\rangle\big\langle\, k,\sigma \,\big| \quad , \tag{6.130}$$

where $k = 0, \pm\frac{1}{3}\,\pi, \pm\frac{2}{3}\,\pi$, and π. Note that without spin-orbit coupling, the spin just comes along for the ride, and we needn't bother with the trouble of the double group. The eigenfunctions are

$$\big|\, k,\sigma \,\big\rangle = \frac{1}{\sqrt{6}} \sum_{n=1}^{6} e^{ikn} \,\big|\, n,\sigma \,\big\rangle \quad . \tag{6.131}$$

We see that the $k = 0$ and $k = \pi$ states are singly degenerate, hence one must transform as A_1 and one as B_2. Obviously $k = 0$ transforms as A_1, so $k = \pi$ must transform as B_2. Just to check, note that the mirrors σ_v which run perpendicular to the hexagonal faces, exchange odd and even numbered sites, while the diagonal mirrors preserve the oddness or evenness of the site index n. Since $\chi^{B_2}(\sigma_v) = -1$ and $\chi^{B_2}(\sigma_d) = +1$, we can be sure there was no mistake, and the $k = \pi$ state indeed transforms as

B_2. The remaining eigenstates are organized into two doublets: $k = \pm\frac{1}{3}\pi$ and $k = \pm\frac{2}{3}\pi$. A check of the C_{3v} character table tells us that $\chi^{E_{1,2}}(C_2) = \pm 2$, so we can use this as a test. Under C_2, we have $n \to n + 3$. Since $\exp(3ik) = -1$ for $k = \pm\frac{1}{3}\pi$, we conclude that this doublet transforms as E_1 and $k = \pm\frac{2}{3}\pi$ transforms as E_2.

Next, consider a cubic molecule. If we construct a tight-binding model consisting of s-orbitals on each site, there will be a total of eight orbitals for each spin polarization. How are they arranged in IRREPs of O_h? Simple. We first note that the only operations $g \in O_h$ which leave sites are invariant are the identity, which preserves all eight sites, the threefold rotations $8C_3$ about the four axes running diagonally through the cube, which preserve the two sites along each axis, and the diagonal mirrors $6IC_2'$, which preserve the four sites lying in each mirror plane. For every other class, $\chi^{\mathsf{per}}(\mathcal{C}) = 0$. Since the orbitals are all s-states, we have $\Gamma^{\mathsf{orb}} = A_{1g}$, the trivial representation. After consulting the character table for O_h, we find

$$\Gamma^{\mathsf{orb}} \times \Gamma^{\mathsf{per}} = A_{1g} \oplus T_{1g} \oplus A_{2u} \oplus T_{2u} \quad . \tag{6.132}$$

Suppose instead each site contained p-orbitals rather than an s-orbital. In this case, $\Gamma^{\mathsf{orb}} = \Gamma^{\mathsf{vec}}$, and the decomposition formula yields

$$\Gamma^{\mathsf{orb}} \times \Gamma^{\mathsf{per}} = A_{1g} \oplus E_g \oplus T_{1g} \oplus 2T_{2g} \oplus A_{2u} \oplus E_u \oplus 2T_{1u} \oplus T_{2u} \quad . \tag{6.133}$$

Adding up all the dimensions yields 24, which corresponds to the total number of orbitals, as required.

O_h	E	$8C_3$	$6IC_2'$	decomposition
Γ^{vec}	3	0	1	T_{1u}
Γ^{per}	8	2	4	$A_{1g} \oplus T_{1g} \oplus A_{2u} \oplus T_{2u}$
$\Gamma^{\mathsf{vec}} \times \Gamma^{\mathsf{per}}$	24	0	4	see text

Table 6.19: Partial character table for O_h. Classes shown are those for which $\chi^{\mathsf{per}}(\mathcal{C}) \neq 0$ for the cube.

6.5 Phonons in Crystals

Consider next the vibrations of a crystalline solid, which are called *phonons*. We define $\boldsymbol{R}$ to be a Bravais lattice vector, *i.e.* a label for a unit cell, and $\boldsymbol{u}_i(\boldsymbol{R})$ to be the displacement of the ith basis ion in the $\boldsymbol{R}$ unit cell. The Hamiltonian is

$$H = \sum_{\boldsymbol{R},i} \frac{\boldsymbol{p}_i^2(\boldsymbol{R})}{2m_i} + \frac{1}{2} \sum_{\boldsymbol{R},\boldsymbol{R}'} \sum_{i,j} \sum_{\alpha,\beta} u_i^\alpha(\boldsymbol{R})\, \Phi_{ij}^{\alpha\beta}(\boldsymbol{R} - \boldsymbol{R}')\, u_j^\beta(\boldsymbol{R}') + \mathcal{O}(u^3) \quad , \tag{6.134}$$

where

$$\Phi_{ij}^{\alpha\beta}(\boldsymbol{R} - \boldsymbol{R}') = \frac{\partial^2 U}{\partial u_i^\alpha(\boldsymbol{R})\, \partial u_j^\beta(\boldsymbol{R}')} \quad . \tag{6.135}$$

Remember that the indices i and j run over the set $\{1, \ldots, r\}$, where r is the number of basis vectors, while α and β are Cartesian vector indices taken from $\{1, 2, \ldots, d\}$, where d is the dimension of space.

In the case of molecules, the dynamical matrix is of rank dN. For a molecule with no point group symmetries, this is the dimension of the eigenvalue problem to be solved. In crystals, by contrast, we may take advantage of translational invariance to reduce the dimension of the eigenvalue problem to dr, *i.e.* to the number of degrees of freedom within a unit cell. This is so even in the case of a triclinic system with no symmetries (*i.e.* point group C_1). Each vibrational state is labeled by a wavevector $\boldsymbol{k}$, and at certain high symmetry points $\boldsymbol{k}$ in the Brillouin zone, crystallographic point group symmetries may be used to group these dr states into multiplets transforming according to point group IRREPs.

Upon Fourier transform,

$$\begin{aligned} u_i^\alpha(\boldsymbol{R}) &= \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \hat{u}_i^\alpha(\boldsymbol{k})\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_i} \\ p_i^\alpha(\boldsymbol{R}) &= \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \hat{p}_i^\alpha(\boldsymbol{k})\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_i} \quad , \end{aligned} \tag{6.136}$$

where the sum is over all $\boldsymbol{k}$ within the first Brillouin zone. The Fourier space dynamical matrix is then

$$\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} \Phi_{ij}^{\alpha\beta}(\boldsymbol{R})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{\delta}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_j} \quad . \tag{6.137}$$

The Hamiltonian, to quadratic order, takes the form

$$H = \sum_{\boldsymbol{k},i} \frac{\hat{p}_i^\alpha(\boldsymbol{k})\,\hat{p}_i^\alpha(-\boldsymbol{k})}{2m_i} + \frac{1}{2}\sum_{\boldsymbol{k}}\sum_{i,j}\sum_{\alpha,\beta} \hat{u}_i^\alpha(-\boldsymbol{k})\,\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})\,\hat{u}_j^\beta(\boldsymbol{k}) \quad , \tag{6.138}$$

Note that $\hat{u}_i^\alpha(-\boldsymbol{k}) = \big[\hat{u}_i^\alpha(\boldsymbol{k})\big]^*$ because the displacements $u_i^\alpha(\boldsymbol{R})$ are real; a corresponding relation holds for the momenta. Note also the Poisson bracket relation in crystal momentum space becomes

$$\Big\{u_i^\alpha(\boldsymbol{R})\,,\, p_j^\beta(\boldsymbol{R}')\Big\}_{\text{PB}} = \delta_{\boldsymbol{R}\boldsymbol{R}'}\,\delta_{ij}\,\delta_{\alpha\beta} \quad \Rightarrow \quad \Big\{\hat{u}_i^\alpha(\boldsymbol{k})\,,\,\hat{p}_j^\beta(\boldsymbol{k}')\Big\}_{\text{PB}} = \delta^{\text{P}}_{\boldsymbol{k}+\boldsymbol{k}',\boldsymbol{0}}\,\delta_{ij}\,\delta_{\alpha\beta} \quad , \tag{6.139}$$

where $\delta^{\text{P}}_{\boldsymbol{k}+\boldsymbol{k}',\boldsymbol{0}} = \sum_{\boldsymbol{G}} \delta_{\boldsymbol{k}+\boldsymbol{k}',\boldsymbol{G}}$ requires $\boldsymbol{k}+\boldsymbol{k}' = \boldsymbol{0}$ modulo any reciprocal lattice vector. Note also that

$$\Phi_{ij}^{\alpha\beta}(\boldsymbol{R}) = \Phi_{ji}^{\beta\alpha}(-\boldsymbol{R}) \quad \Rightarrow \quad \hat{\Phi}_{ji}^{\beta\alpha}(\boldsymbol{k}) = \hat{\Phi}_{ij}^{\alpha\beta}(-\boldsymbol{k}) = \big[\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})\big]^* \quad . \tag{6.140}$$

The system is diagonalized by writing

$$\hat{u}_i^\alpha(\boldsymbol{k}) = \sum_{\lambda=1}^{dr} \hat{\mathrm{e}}_{i\lambda}^\alpha(\boldsymbol{k})\,\hat{q}_\lambda(\boldsymbol{k}) \qquad , \qquad \hat{p}_i^\alpha(\boldsymbol{k}) = m_i \sum_{\lambda=1}^{dr} \hat{\mathrm{e}}_{i\lambda}^{\alpha *}(-\boldsymbol{k})\,\hat{\pi}_\lambda(\boldsymbol{k}) \tag{6.141}$$

where $\big\{\hat{q}_\lambda(\boldsymbol{k}), \hat{\pi}_{\lambda'}(\boldsymbol{k})\big\}_{\text{PB}} = \delta_{\boldsymbol{k}+\boldsymbol{k}',\boldsymbol{0}}\,\delta_{\lambda\lambda'}$ and $S_{i\alpha,\lambda}(\boldsymbol{k}) \equiv \hat{\mathrm{e}}_{i\lambda}^\alpha(\boldsymbol{k}) \equiv m_i^{-1/2}\, U_{i\alpha,\lambda}(\boldsymbol{k})$ diagonalizes the dynamical matrix, with $U_{i\alpha,\lambda}(\boldsymbol{k})$ unitary. Thus,

$$\sum_{\beta,j} \hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})\,\hat{\mathrm{e}}_{j\lambda}^\beta(\boldsymbol{k}) = m_i\,\omega_\lambda^2(\boldsymbol{k})\,\hat{\mathrm{e}}_{i\lambda}^\alpha(\boldsymbol{k}) \tag{6.142}$$

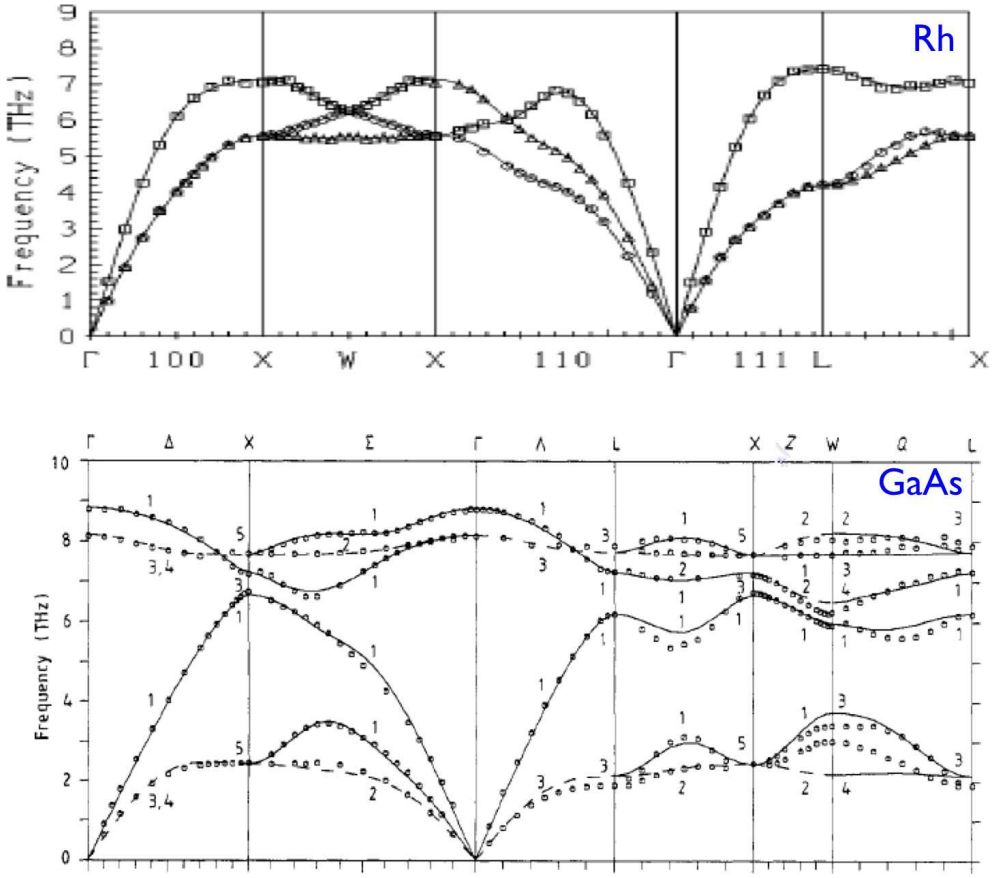


Figure 6.15: Upper panel: phonon spectrum in fcc elemental rhodium (Rh) at $T = 297\,\mathrm{K}$ measured by high precision inelastic neutron scattering (INS) by A. Eichler *et al.*, *Phys. Rev. B* **57**, 324 (1998). Note the three acoustic branches and no optical branches, corresponding to $d = 3$ and $r = 1$. Lower panel: phonon spectrum in gallium arsenide (GaAs) at $T = 12\,\mathrm{K}$, comparing theoretical lattice-dynamical calculations with INS results of D. Strauch and B. Dorner, *J. Phys.: Condens. Matter* **2**, 1457 (1990). Note the three acoustic branches and three optical branches, corresponding to $d = 3$ and $r = 2$. The Greek letters along the x-axis indicate points of high symmetry in the Brillouin zone.

with the completeness relation,

$$\sum_{\lambda=1}^{dr} \hat{\mathrm{e}}_{i\lambda}^{\alpha *}(\boldsymbol{k})\,\hat{\mathrm{e}}_{j\lambda}^{\beta}(\boldsymbol{k}) = \frac{1}{m_i}\,\delta_{ij}\,\delta_{\alpha\beta} \tag{6.143}$$

and the orthogonality relation,

$$\sum_{i=1}^{r}\sum_{\alpha=1}^{d} m_i\,\hat{\mathrm{e}}_{i\lambda}^{\alpha *}(\boldsymbol{k})\,\hat{\mathrm{e}}_{i\lambda'}^{\alpha}(\boldsymbol{k}) = \delta_{\lambda\lambda'} \quad , \tag{6.144}$$

which are the completeness and orthogonality relations, respectively. Since $\hat{\mathrm{e}}_{i\lambda}^{\alpha *}(-\boldsymbol{k})$ and $\hat{\mathrm{e}}_{i\lambda}^{\alpha}(\boldsymbol{k})$ obey the same equation, we have that $\omega_\lambda(-\boldsymbol{k}) = \omega_\lambda(\boldsymbol{k})$. If the phonon eigenmode $|\,\boldsymbol{k},\lambda\,\rangle$ is nondegenerate, we may choose $\hat{\mathrm{e}}_{i\lambda}^{\alpha}(-\boldsymbol{k}) = \hat{\mathrm{e}}_{i\lambda}^{\alpha *}(\boldsymbol{k})$. Else at best we can conclude $\hat{\mathrm{e}}_{i\lambda}^{\alpha}(-\boldsymbol{k}) = \hat{\mathrm{e}}_{i\lambda'}^{\alpha *}(\boldsymbol{k})\,e^{i\eta}$ where $|\,\boldsymbol{k},\lambda'\,\rangle$ is another state from the degenerate manifold of phonon states at this wavevector, and $e^{i\eta}$ is a phase.

The Hamiltonian takes the diagonalized form

$$H = \sum_{\boldsymbol{k}} \sum_{\lambda=1}^{dr} \left\{ \tfrac{1}{2}\,\hat{\pi}_\lambda(-\boldsymbol{k})\,\hat{\pi}_\lambda(\boldsymbol{k}) + \tfrac{1}{2}\,\omega_\lambda^2(\boldsymbol{k})\,\hat{q}_\lambda(-\boldsymbol{k})\,\hat{q}_\lambda(\boldsymbol{k}) \right\} \quad , \tag{6.145}$$

with $\big\{\hat{q}_\lambda(\boldsymbol{k})\,,\,\hat{\pi}_{\lambda'}(\boldsymbol{k}')\big\}_{\text{PB}} = \delta_{\lambda\lambda'}\,\delta^{\text{P}}_{\boldsymbol{k}+\boldsymbol{k}',\boldsymbol{0}}$. To quantize, promote the Poisson brackets to commutators: $\big\{A\,,\,B\big\}_{\text{PB}} \to -i\hbar^{-1}\,\big[A\,,\,B\big]$. Then define the ladder operators,

$$A_\lambda(\boldsymbol{k}) = \left(\frac{\omega_\lambda(\boldsymbol{k})}{2\hbar}\right)^{1/2} \hat{q}_\lambda(\boldsymbol{k}) + i\left(\frac{1}{2\hbar\omega_\lambda(\boldsymbol{k})}\right)^{1/2} \hat{\pi}_\lambda(\boldsymbol{k}) \quad , \tag{6.146}$$

which satisfy $\big[A_\lambda(\boldsymbol{k})\,,\,A^\dagger_{\lambda'}(\boldsymbol{k}')\big] = \delta^{\text{P}}_{\boldsymbol{k}\boldsymbol{k}'}\,\delta_{\lambda\lambda'}$. The quantum phonon Hamiltonian is then

$$\hat{H} = \sum_{\boldsymbol{k}} \sum_{\lambda=1}^{dr} \hbar\omega_\lambda(\boldsymbol{k}) \left(A^\dagger_\lambda(\boldsymbol{k})\,A_\lambda(\boldsymbol{k}) + \tfrac{1}{2} \right) \quad . \tag{6.147}$$

Of the dr phonon branches, d are *acoustic*, and behave as $\omega_a(\boldsymbol{k}) = c(\hat{\boldsymbol{k}})\,k$ as $\boldsymbol{k} \to 0$, which is the Γ point in the Brillouin zone. These gapless phonons are the Goldstone bosons of the spontaneously broken translational symmetry which gave rise to the crystalline phase. To each broken generator of translation, there corresponds a Goldstone mode. The remaining $d(r-1)$ modes are called *optical phonons*. Whereas for acoustic modes, all the ions in a given unit cell are moving in phase, for optical modes they are moving out of phase. Hence optical modes are always finite frequency modes. Fig. 6.15 shows the phonon spectra in elemental rhodium (space group $Fm\overline{3}m$, point group O_h), and in gallium arsenide (space group $F\overline{4}3m$, point group T_d). Since Rh forms an fcc Bravais lattice, there are no optical phonon modes. GaAs forms a zincblende structure, *i.e.* two interpenetrating fcc lattices, one for the gallium, the other for the arsenic. Thus $r = 2$ and we expect three acoustic and three optical branches of phonons.

Nota bene: One may choose to define the Fourier transforms above taking the additional phases for the basis elements to all be unity, *viz.*

$$u^\alpha_i(\boldsymbol{R}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \hat{u}^\alpha_i(\boldsymbol{k})\,e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \quad , \quad p^\alpha_i(\boldsymbol{R}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \hat{p}^\alpha_i(\boldsymbol{k})\,e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \quad , \quad \hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} \Phi^{\alpha\beta}_{ij}(\boldsymbol{R})\,e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \quad . \tag{6.148}$$

All the equations starting with Eqn. 6.138 remain the same. Setting the basis phases to unity amounts to a choice of *gauge*. It is somewhat simpler in certain contexts, but it may obscure essential space group symmetries. On the other hand, it should also be noted that the Fourier transforms $\hat{u}^\alpha_i(\boldsymbol{k})$, $\hat{p}^\alpha_i(\boldsymbol{k})$, and $\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{k})$ are not periodic in the Brillouin zone, but instead satisfy generalized periodic boundary conditions,

$$\begin{aligned} \hat{u}^\alpha_i(\boldsymbol{K}+\boldsymbol{k}) &= e^{-i\boldsymbol{K}\cdot\boldsymbol{\delta}_i}\,\hat{u}^\alpha_i(\boldsymbol{k}) \\ \hat{p}^\alpha_i(\boldsymbol{K}+\boldsymbol{k}) &= e^{-i\boldsymbol{K}\cdot\boldsymbol{\delta}_i}\,\hat{p}^\alpha_i(\boldsymbol{k}) \\ \hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{K}+\boldsymbol{k}) &= e^{-i\boldsymbol{K}\cdot(\boldsymbol{\delta}_i-\boldsymbol{\delta}_j)}\,\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{k}) \quad , \end{aligned} \tag{6.149}$$

where $\boldsymbol{K} \in \hat{\mathcal{L}}$ is any reciprocal lattice vector.

6.5.1 Translation and rotation invariance

The potential energy $U\big(\{u_i^\alpha(\boldsymbol{R})\}\big)$ must remain invariant under the operations

$$\begin{aligned} u_i^\alpha(\boldsymbol{R}) &\to u_i^\alpha(\boldsymbol{R}) + d^\alpha \\ u_i^\alpha(\boldsymbol{R}) &\to u_i^\alpha(\boldsymbol{R}) + \epsilon_{\alpha\mu\nu}\,(R^\mu + \delta_i^\mu - \delta_j^\mu)\,d^\nu \end{aligned} \tag{6.150}$$

for an infinitesimal vector $\boldsymbol{d}$. The first equation represents a uniform translation of all lattice sites by $\boldsymbol{d}$. The second represents an infinitesimal rotation about the $j^{\rm th}$ basis ion in the $\boldsymbol{R} = 0$ unit cell. We are free to choose any j.

Writing $U(u + \Delta u) = U(u)$, we must have that the linear terms in Δu vanish, hence

$$\begin{aligned} \sum_{\boldsymbol{R},i} \Phi_{ij}^{\alpha\beta}(\boldsymbol{R}) &= \sum_i \hat\Phi_{ij}^{\alpha\beta}(\boldsymbol{0}) = 0 \\ \epsilon_{\alpha\mu\nu} \sum_{\boldsymbol{R},i} (R^\mu + \delta_i^\mu - \delta_j^\mu)\,\Phi_{ij}^{\nu\beta}(\boldsymbol{R}) &= i\,\epsilon_{\alpha\mu\nu} \sum_i \frac{\partial \hat\Phi_{ij}^{\nu\beta}(\boldsymbol{k})}{\partial k^\mu}\bigg|_{\boldsymbol{k}=0} = 0 \quad . \end{aligned} \tag{6.151}$$

Note that (α, β, j) are free indices in both equations. The first of these equations says that any vector d^β is an eigenvector of the dynamical matrix at $\boldsymbol{k} = 0$, with zero eigenvalue. Thus, at $\boldsymbol{k} = 0$, there is a three-dimensional space of zero energy modes. These are the Goldstone modes associated with the three broken generators of translation in the crystal.

6.5.2 Phonons in an fcc lattice

When the crystal is a Bravais lattice, there are no basis indices, and the dynamical matrix becomes

$$\hat\Phi^{\alpha\beta}(\boldsymbol{k}) = {\sum_{\boldsymbol{R}}}'(1 - \cos\boldsymbol{k}\cdot\boldsymbol{R})\,\frac{\partial^2 v(\boldsymbol{R})}{\partial R^\alpha\,\partial R^\beta} \quad , \tag{6.152}$$

where $v(\boldsymbol{r})$ is the inter-ionic potential, and the prime on the sum indicates that $\boldsymbol{R} = 0$ is to be excluded. For central potentials $v(\boldsymbol{R}) = v(R)$,

$$\frac{\partial^2 v(\boldsymbol{R})}{\partial R^\alpha\,\partial R^\beta} = \big(\delta^{\alpha\beta} - \hat R^\alpha\,\hat R^\beta\big)\,\frac{v'(R)}{R} + \hat R^\alpha\,\hat R^\beta\,v''(R) \quad . \tag{6.153}$$

For simplicity, we assume $v(R)$ is negligible beyond the first neighbor. On the fcc lattice, there are twelve first neighbors, lying at $\boldsymbol{\Delta} = \frac{1}{2}a\,(\pm\hat{\boldsymbol{y}} \pm \hat{\boldsymbol{z}})$, $\boldsymbol{\Delta} = \frac{1}{2}a\,(\pm\hat{\boldsymbol{x}} \pm \hat{\boldsymbol{z}})$, and $\boldsymbol{\Delta} = \frac{1}{2}a\,(\pm\hat{\boldsymbol{x}} \pm \hat{\boldsymbol{y}})$. Here a is the side length of the underlying simple cubic lattice, so the fcc lattice constant is $a/\sqrt{2}$. We define

$$A = \frac{\sqrt{2}}{a}\,v'\big(a/\sqrt{2}\big) \quad , \quad B = v''\big(a/\sqrt{2}\big) \quad . \tag{6.154}$$

Along (100), we have $\boldsymbol{k} = k\hat{\boldsymbol{x}}$ and

$$\hat\Phi^{\alpha\beta}(\boldsymbol{k}) = 4\sin^2(\tfrac{1}{4}ka) \begin{pmatrix} 2A+2B & 0 & 0 \\ 0 & 3A+B & 0 \\ 0 & 0 & 3A+B \end{pmatrix} \quad , \tag{6.155}$$

which is already diagonal. Thus, the eigenvectors lie along the cubic axes and

$$\omega_{\rm L} = 2\sqrt{\tfrac{2(A+B)}{m}}\,\big|\sin(ka/4)\big| \quad , \quad \omega_{\rm T1} = \omega_{\rm T2} = 2\sqrt{\tfrac{3A+B}{m}}\,\big|\sin(ka/4)\big| \quad . \tag{6.156}$$

Along (111), we have $\boldsymbol{k} = \frac{1}{\sqrt{3}}\,k\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$. One finds

$$\hat{\Phi}^{\alpha\beta}(\boldsymbol{k}) = 4\sin^2\!\big(ka/\sqrt{12}\big)\begin{pmatrix} 4A+2B & B-A & B-A \\ B-A & 4A+2B & B-A \\ B-A & B-A & 4A+2B \end{pmatrix} \quad . \tag{6.157}$$

$$\omega_{\rm L} = 2\sqrt{\tfrac{A+2B}{m}}\,\big|\sin\!\big(ka/\sqrt{12}\big)\big| \quad , \quad \omega_{\rm T1} = \omega_{\rm T2} = 2\sqrt{\tfrac{5A+B}{2m}}\,\big|\sin\!\big(ka/\sqrt{12}\big)\big| \quad . \tag{6.158}$$

6.5.3 Elasticity theory redux : Bravais lattices

In a Bravais lattice, we have $\hat{\Phi}^{\alpha\beta}(\boldsymbol{0}) = 0$ from translational invariance. The potential energy may then be written in the form

$$U = U_0 - \frac{1}{4}\sum_{\boldsymbol{R},\boldsymbol{R}'}\sum_{\alpha,\beta}\big[u^\alpha(\boldsymbol{R}) - u^\alpha(\boldsymbol{R}')\big]\,\Phi^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}')\,\big[u^\beta(\boldsymbol{R}) - u^\beta(\boldsymbol{R}')\big] \quad . \tag{6.159}$$

We now assume a very long wavelength disturbance, and write

$$u^\alpha(\boldsymbol{R}) - u^\alpha(\boldsymbol{R}') = (R^\mu - R'^\mu)\,\frac{\partial u^\alpha}{\partial x^\mu}\bigg|_{\boldsymbol{R}} + \ldots \quad . \tag{6.160}$$

Thus,

$$U = U_0 - \frac{1}{4}\sum_{\boldsymbol{R},\boldsymbol{R}'}\sum_{\alpha,\beta}\sum_{\mu,\nu}\frac{\partial u^\alpha}{\partial x^\mu}\bigg|_{\boldsymbol{R}}\frac{\partial u^\beta}{\partial x^\nu}\bigg|_{\boldsymbol{R}}(R^\mu - R'^\mu)\,(R^\nu - R'^\nu)\,\Phi^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}') \quad . \tag{6.161}$$

We may symmetrize with respect to Cartesian indices[38] to obtain the elastic tensor

$$C_{\alpha\beta\mu\nu} \equiv -\frac{1}{8\Omega}\sum_{\boldsymbol{R}}\Big(R^\mu R^\nu\,\Phi^{\alpha\beta}(\boldsymbol{R}) + R^\mu R^\beta\,\Phi^{\alpha\nu}(\boldsymbol{R}) + R^\alpha R^\nu\,\Phi^{\mu\beta}(\boldsymbol{R}) + R^\alpha R^\beta\,\Phi^{\mu\nu}(\boldsymbol{R})\Big) \quad . \tag{6.162}$$

Note that

$$C_{\alpha\beta\mu\nu} = C_{\beta\alpha\mu\nu} = C_{\alpha\beta\nu\mu} = C_{\mu\nu\alpha\beta} \quad , \tag{6.163}$$

where Ω is the Wigner-Seitz cell volume.

Elasticity in solids

Recall from §6.3.6 that we may regard the rank four tensor $C_{\alpha\beta\mu\nu}$ as a symmetric 6×6 matrix C_{ab}, where we replace $(\alpha\beta) \to a$ and $(\mu\nu) \to b$ according to the scheme which we repeat from Tab. 6.15: In cubic

[38] Symmetrization is valid because the antisymmetric combination $\big(\frac{\partial u^\alpha}{\partial x^\beta} - \frac{\partial u^\beta}{\partial x^\alpha}\big)$ corresponds to a rotation.

$(\alpha\beta)$:	(11)	(22)	(33)	(23)	(31)	(12)
a :	1	2	3	4	5	6

Table 6.20: Abbreviation for symmetric compound indices $(\alpha\beta)$.

crystals, for example, we have

$$\begin{aligned} C_{11} &= C_{xxxx} = C_{yyyy} = C_{zzzz} \\ C_{12} &= C_{xxyy} = C_{xxzz} = C_{yyzz} \\ C_{44} &= C_{xyxy} = C_{xzxz} = C_{yzyz} \quad . \end{aligned} \tag{6.164}$$

Typical values of C_{ab} in solids are on the order of gigapascals, *i.e.* 10^9 Pa:

element	C_{11}	C_{12}	C_{44}
^{4}He	0.031	0.028	0.022
Cu	16	8	12
Al	108	62	28.3
Pb	48.8	41.4	14.8
C (diamond)	1040	170	550

Table 6.21: Elastic moduli for various solids (in GPa).

The *bulk modulus* of a solid is defined as $\mathcal{B} = V\,\partial^2 F/\partial V^2$. We consider a uniform dilation, which is described by $\boldsymbol{R} \to (1+\zeta)\boldsymbol{R}$ at each lattice site. Thus the displacement field is $\boldsymbol{u}(\boldsymbol{r}) = \zeta \boldsymbol{r}$. This leads to a volume change of $\delta V = 3\zeta V$, hence $\zeta = \delta V/3V$. The strain tensor is $\varepsilon_{\alpha\beta} = \zeta\,\delta_{\alpha\beta}$, hence

$$\delta F = \frac{(\delta V)^2}{18V} \sum_{\alpha,\beta} C_{\alpha\alpha\beta\beta} = \tfrac{1}{9} \sum_{a,b=1}^{3} C_{ab} \quad . \tag{6.165}$$

Thus, for cubic materials, $\mathcal{B} = \frac{1}{3}C_{11} + \frac{2}{3}C_{12}$.

Elastic waves

The Lagrangian of an elastic medium is be written as

$$L = \int d^d r\, \mathcal{L} = \int d^d r \left\{ \tfrac{1}{2}\,\rho \left(\frac{\partial u^\alpha}{\partial t} \right)^2 - \tfrac{1}{2}\, C_{\alpha\beta\mu\nu}\, \frac{\partial u^\alpha}{\partial x^\beta}\, \frac{\partial u^\mu}{\partial x^\nu} \right\} \quad , \tag{6.166}$$

where ρ is the overall mass density of the crystal, *i.e.* $\rho = m/\Omega$. The Euler-Lagrange equations of motion are then

$$\begin{aligned} 0 &= \frac{\partial}{\partial t}\,\frac{\partial \mathcal{L}}{\partial(\partial_t u^\alpha)} + \frac{\partial}{\partial x^\beta}\,\frac{\partial \mathcal{L}}{\partial(\partial_\beta u^\alpha)} \\ &= \rho\,\frac{\partial^2 u^\alpha}{\partial t^2} - C_{\alpha\beta\mu\nu}\,\frac{\partial^2 u^\nu}{\partial x^\beta\,\partial x^\mu} \quad . \end{aligned} \tag{6.167}$$

The solutions are *elastic waves*, with $\boldsymbol{u}(\boldsymbol{x},t) = \hat{\mathbf{e}}(\boldsymbol{k})\,e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)}$ where

$$\rho\omega^2\,\mathrm{e}^\alpha(\boldsymbol{k}) = C_{\alpha\beta\mu\nu}\,k^\beta\,k^\mu\,\mathrm{e}^\nu(\boldsymbol{k}) \quad . \tag{6.168}$$

Thus, the dispersion is $\omega_a(\boldsymbol{k}) = c_a(\hat{\boldsymbol{k}})\,k$, where

$$\det\Big[\rho\,c^2(\hat{\boldsymbol{k}})\,\delta_{\alpha\nu} - C_{\alpha\beta\mu\nu}\,\hat{k}^\beta\,\hat{k}^\mu\Big] = 0 \tag{6.169}$$

is the equation to be solved for the speeds of sound $c_a(\hat{\boldsymbol{k}})$ in each elastic wave branch a.

For isotropic solids, $C_{12} \equiv \lambda$, $C_{44} \equiv \mu$, and $C_{11} = C_{12} + 2C_{14} = \lambda + 2\mu$, where λ and μ are the Lamé coefficients. The free energy density is discussed in §6.3.6 and is given by

$$f = \tfrac{1}{2}\lambda\,(\partial_i u_i)^2 + \tfrac{1}{2}\mu\,(\partial_i u_j)\,(\partial_i u_j) + \tfrac{1}{2}\mu\,(\partial_i u_j)\,(\partial_j u_i) \quad , \tag{6.170}$$

which results in the Euler-Lagrange equations of motion

$$\rho\,\ddot{\boldsymbol{u}} = (\lambda+\mu)\,\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u}) + \mu\,\nabla^2\boldsymbol{u} \quad . \tag{6.171}$$

Writing $\boldsymbol{u}(\boldsymbol{r},t) = u_0\,\hat{\mathbf{e}}(\boldsymbol{k})\,e^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}$, where $\hat{\mathbf{e}}$ is a polarization unit vector, we obtain a longitudinal mode when $\hat{\mathbf{e}}(\boldsymbol{k})\cdot\hat{\boldsymbol{k}} = 1$ with $\omega_{\mathrm{L}}(\boldsymbol{k}) = c_{\mathrm{L}}\,|\boldsymbol{k}|$ and $c_{\mathrm{L}} = \sqrt{(\lambda+2\mu)/\rho}$, and two transverse modes when $\hat{\mathbf{e}}(\boldsymbol{k})\cdot\hat{\boldsymbol{k}} = 0$ with $\omega_{\mathrm{T}}(\boldsymbol{k}) = c_{\mathrm{T}}\,|\boldsymbol{k}|$ and $c_{\mathrm{T}} = \sqrt{\mu/\rho}$.

In cubic crystals, there are three independent elastic moduli, C_{11}, C_{12}, and C_{14}. We then have

$$\begin{aligned} \rho\,c^2(\hat{\boldsymbol{k}})\,\mathrm{e}^x &= \Big[C_{11}\,\hat{k}_x^2 + C_{44}\big(\hat{k}_y^2+\hat{k}_z^2\big)\Big]\hat{\mathrm{e}}^x + (C_{12}+C_{44})\big(\hat{k}_x\,\hat{k}_y\,\hat{\mathrm{e}}^y + \hat{k}_x\,\hat{k}_z\,\hat{\mathrm{e}}^z\big) \\ \rho\,c^2(\hat{\boldsymbol{k}})\,\mathrm{e}^y &= \Big[C_{11}\,\hat{k}_y^2 + C_{44}\big(\hat{k}_x^2+\hat{k}_z^2\big)\Big]\hat{\mathrm{e}}^y + (C_{12}+C_{44})\big(\hat{k}_x\,\hat{k}_y\,\hat{\mathrm{e}}^x + \hat{k}_y\,\hat{k}_z\,\hat{\mathrm{e}}^z\big) \\ \rho\,c^2(\hat{\boldsymbol{k}})\,\mathrm{e}^z &= \Big[C_{11}\,\hat{k}_z^2 + C_{44}\big(\hat{k}_x^2+\hat{k}_y^2\big)\Big]\hat{\mathrm{e}}^z + (C_{12}+C_{44})\big(\hat{k}_x\,\hat{k}_z\,\hat{\mathrm{e}}^x + \hat{k}_y\,\hat{k}_z\,\hat{\mathrm{e}}^y\big) \quad . \end{aligned} \tag{6.172}$$

This still yields a cubic equation, but it can be simplified by looking along a high symmetry direction in the Brillouin zone.

Along the (100) direction $\boldsymbol{k} = k\,\hat{\boldsymbol{x}}$, we have

$$\hat{\mathbf{e}}_{\mathrm{L}} = \hat{\boldsymbol{x}} \qquad c_{\mathrm{L}} = \sqrt{C_{11}/\rho} \tag{6.173}$$

$$\hat{\mathbf{e}}_{\mathrm{T}1} = \hat{\boldsymbol{y}} \qquad c_{\mathrm{T}1} = \sqrt{C_{44}/\rho} \tag{6.174}$$

$$\hat{\mathbf{e}}_{\mathrm{T}2} = \hat{\boldsymbol{z}} \qquad c_{\mathrm{T}2} = \sqrt{C_{44}/\rho} \quad . \tag{6.175}$$

Along the (110) direction, we have $\boldsymbol{k} = \frac{1}{\sqrt{2}}\,k\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})$. In this case

$$\hat{\mathbf{e}}_{\rm L} = \tfrac{1}{\sqrt{2}}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \qquad c_{\rm L} = \sqrt{(C_{11} + 2C_{12} + 4C_{44})/3\rho} \tag{6.176}$$

$$\hat{\mathbf{e}}_{\rm T1} = \tfrac{1}{\sqrt{2}}(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}) \qquad c_{\rm T1} = \sqrt{(C_{11} - C_{12})/2\rho} \tag{6.177}$$

$$\hat{\mathbf{e}}_{\rm T2} = \hat{\boldsymbol{z}} \qquad c_{\rm T2} = \sqrt{C_{44}/\rho} \quad . \tag{6.178}$$

Along the (111) direction, we have $\boldsymbol{k} = \frac{1}{\sqrt{3}}\,k\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$. In this case

$$\hat{\mathbf{e}}_{\rm L} = \tfrac{1}{\sqrt{3}}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) \qquad c_{\rm L} = \sqrt{(C_{11} + C_{12} + 2C_{44})/2\rho} \tag{6.179}$$

$$\hat{\mathbf{e}}_{\rm T1} = \tfrac{1}{\sqrt{6}}(2\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}}) \qquad c_{\rm T1} = \sqrt{(C_{11} - C_{12})/3\rho} \tag{6.180}$$

$$\hat{\mathbf{e}}_{\rm T2} = \tfrac{1}{\sqrt{2}}(\hat{\boldsymbol{y}} - \hat{\boldsymbol{z}}) \qquad c_{\rm T2} = \sqrt{(C_{11} - C_{12})/3\rho} \quad . \tag{6.181}$$

6.5.4 Elasticity theory in cases with bases

The derivation of the elastic tensor $C_{\alpha\beta\mu\nu}$ is significantly complicated by the presence of a basis. Sadly, translational invariance if of no direct avail because

$$U \neq U_0 - \frac{1}{4}\sum_{\boldsymbol{R},\boldsymbol{R}'}\sum_{\alpha,\beta}\sum_{i,j}\left[u_i^\alpha(\boldsymbol{R}) - u_i^\alpha(\boldsymbol{R}')\right]\Phi_{ij}^{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}')\left[u_j^\beta(\boldsymbol{R}) - u_j^\beta(\boldsymbol{R}')\right] \quad . \tag{6.182}$$

The student should understand why the above relation is not an equality.

Rather than work with the energy, we will work with the eigenvalue equation 6.142,

$$\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})\,\hat{\mathrm{e}}_{j\lambda}^{\beta}(\boldsymbol{k}) = m_i\,\omega_\lambda^2(\boldsymbol{k})\,\hat{\mathrm{e}}_{i\lambda}^{\alpha}(\boldsymbol{k}) \quad ,$$

and expand in powers of $\boldsymbol{k}$. Accordingly, we write

$$\begin{aligned}\hat{\mathrm{e}}_{i\lambda}^{\alpha}(\boldsymbol{k}) &= d_i^\alpha + k^\sigma f_{i\sigma}^\alpha + \tfrac{1}{2}\,k^\sigma k^\tau g_{i\sigma\tau}^\beta + \mathcal{O}(k^3) \\ \hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k}) &= \hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{0}) + k^\mu\,\frac{\partial\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})}{\partial k^\mu}\bigg|_{\boldsymbol{0}} + \tfrac{1}{2}\,k^\mu\,k^\nu\,\frac{\partial^2\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})}{\partial k^\mu\,\partial k^\nu}\bigg|_{\boldsymbol{0}} + \mathcal{O}(k^3) \quad .\end{aligned} \tag{6.183}$$

We retain the basis index i on d_i^α *even though it is independent of* i because we will use it to make clear certain necessary sums on the basis index within the Einstein convention. We then have

$$\begin{aligned}m_i\,\omega^2\left\{d_i^\alpha + k^\sigma f_{i\sigma}^\alpha + \ldots\right\} = \\ \left\{\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{0}) + k^\mu\,\frac{\partial\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})}{\partial k^\mu}\bigg|_{\boldsymbol{0}} + \tfrac{1}{2}\,k^\mu\,k^\nu\,\frac{\partial^2\hat{\Phi}_{ij}^{\alpha\beta}(\boldsymbol{k})}{\partial k^\mu\,\partial k^\nu}\bigg|_{\boldsymbol{0}} + \ldots\right\}\left\{d_j^\beta + k^\tau f_{j\tau}^\beta + \ldots\right\} \quad ,\end{aligned} \tag{6.184}$$

where there is no implied sum on i on the LHS. We now work order by order in $\boldsymbol{k}$. To start, note that $\omega^2(\boldsymbol{k}) = c^2(\hat{\boldsymbol{k}})\,k^2$ is already second order. On the RHS, we have $\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{0})\,d^\beta_j = 0$ to zeroth order in k. At first order, we must have

$$\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{0})\,f^\beta_{j\sigma} + \left.\frac{\partial\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{k})}{\partial k^\sigma}\right|_{\boldsymbol{0}} d^\beta_j = 0 \quad , \tag{6.185}$$

and defining the matrix inverse $\hat{\Upsilon}^{\gamma\alpha}_{li}(\boldsymbol{k})$ by the relation

$$\hat{\Upsilon}^{\gamma\alpha}_{li}(\boldsymbol{k})\,\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{k}) = \delta^{\gamma\beta}\,\delta_{lj} \quad , \tag{6.186}$$

we have

$$f^\gamma_{l\sigma} = -\hat{\Upsilon}^{\gamma\alpha}_{li}(\boldsymbol{0})\left.\frac{\partial\hat{\Phi}^{\alpha\beta}_{ij}(\boldsymbol{k})}{\partial k^\sigma}\right|_{\boldsymbol{0}} d^\beta_j \tag{6.187}$$

Finally, we obtain the eigenvalue equation for the elastic waves,

$$m_i\,\omega^2\,d^\alpha_i = \left[\frac{1}{2}\left.\frac{\partial^2\hat{\Phi}^{\alpha\beta}_{il}(\boldsymbol{k})}{\partial k^\mu\,\partial k^\nu}\right|_{\boldsymbol{0}} - \left.\frac{\partial\hat{\Phi}^{\alpha\sigma}_{ij}(\boldsymbol{k})}{\partial k^\mu}\right|_{\boldsymbol{0}}\hat{\Upsilon}^{\sigma\gamma}_{jm}(\boldsymbol{0})\left.\frac{\partial\hat{\Phi}^{\gamma\beta}_{ml}(\boldsymbol{k})}{\partial k^\nu}\right|_{\boldsymbol{0}}\right]k^\mu\,k^\nu\,d^\beta_l \quad . \tag{6.188}$$

Remember that d^α_i is independent of the basis index i. We have dropped the mode index λ here for notational convenience. Note that the quadratic coefficient $g^\beta_{i\sigma\tau}$ never entered our calculation because it leads to an inhomogeneous term in the eigenvalue equation, and therefore must be dropped. We do not report here the explicit form for the elastic tensor, which may be derived from the above eigenvalue equation.

6.6 Appendix : O(3) Characters of Point Group Operations

In tables Tab. 6.22 and 6.23 we present the characters of all crystallographic point group operations for several integer and half-odd-integer representations of SO(3).

6.7 Appendix : Construction of Group Invariants

6.7.1 Polar and axial vectors

We follow the discussion in §4.5 of Lax. Let $\boldsymbol{r}_j$ denote a polar vector and $\boldsymbol{m}_k$ an axial vector, where j and k are labels. Let's first recall how axial vectors transform. If we write $m_\mu = \epsilon_{\mu\nu\lambda}\,r^\nu_1\,r^\lambda_2$, where $\boldsymbol{r}_{1,2}$ are polar vectors, then under the action of a group element g, we have $\boldsymbol{m} \to \boldsymbol{m}'$, where

$$m'_\mu = \epsilon_{\mu\nu\lambda}\,D_{\nu'\nu}(g)\,D_{\lambda'\lambda}(g)\,r^{\nu'}_1\,r^{\lambda'}_2 \quad . \tag{6.189}$$

Now if R is any 3×3 matrix, then $R_{\mu'\mu}\,R_{\nu'\nu}\,R_{\lambda'\lambda}\,\epsilon^{\mu\nu\lambda} = \mathsf{det}(R)\,\epsilon^{\mu'\nu'\lambda'}$, and therefore $m'_\mu = m_{\mu'}\,\widetilde{D}_{\mu'\mu}(g)$, where $\widetilde{D}_{\alpha\beta}(g) = \mathsf{det}\,D(g)\cdot D_{\alpha\beta}(g)$. In other words,

$$\epsilon_{\mu\nu\lambda}\,D_{\nu'\nu}(g)\,D_{\lambda'\lambda}(g) = \mathsf{det}\,D(g)\cdot\epsilon_{\mu'\nu'\lambda'}D_{\mu'\mu}(g) \quad . \tag{6.190}$$

J	E	C_2	C_3	C_4	C_6	$\overline{E}$	$\overline{C}_3$	$\overline{C}_4$	$\overline{C}_6$
$1/2$	2	0	1	$\sqrt{2}$	$\sqrt{3}$	-2	-1	$-\sqrt{2}$	$-\sqrt{3}$
1	3	-1	0	1	2	3	0	1	2
$3/2$	4	0	-1	0	$\sqrt{3}$	-4	1	0	$-\sqrt{3}$
2	5	1	-1	-1	1	5	-1	-1	1
$5/2$	6	0	0	$-\sqrt{2}$	0	-6	0	$\sqrt{2}$	0
3	7	-1	1	-1	-1	7	1	-1	-1
$7/2$	8	0	1	0	$-\sqrt{3}$	-8	-1	0	$\sqrt{3}$
4	9	1	0	1	-2	9	0	1	-2
$9/2$	10	0	-1	$\sqrt{2}$	$-\sqrt{3}$	-10	1	$-\sqrt{2}$	$\sqrt{3}$
5	11	-1	-1	1	-1	11	-1	1	-1
$11/2$	12	0	0	0	0	-12	0	0	0
6	13	1	1	-1	1	13	1	-1	1

Table 6.22: $\mathsf{O}(3)$ characters of crystallographic point group operations. Note $\chi(\overline{C}_2) = \chi(C_2)$.

$\chi(\sigma)$	$\chi(\overline{\sigma})$	$\chi(I)$	$\chi(\overline{I})$	$\chi(S_3)$	$\chi(S_4)$	$\chi(S_6)$	$\chi(\overline{S}_3)$	$\chi(\overline{S}_4)$	$\chi(\overline{S}_6)$
$\eta\,\chi(C_2)$	$\eta\,\chi(C_2)$	$\eta\,\chi(E)$	$\eta\,\chi(\overline{E})$	$\eta\,\chi(C_6)$	$\eta\,\chi(C_4)$	$\eta\,\chi(C_3)$	$\eta\,\chi(\overline{C}_6)$	$\eta\,\chi(\overline{C}_4)$	$\eta\,\chi(\overline{C}_3)$

Table 6.23: Characters for improper $\mathsf{O}(3)$ operations. Here $\eta = \pm$ is the parity.

Thus for proper rotations, $\boldsymbol{m}$ transforms in the same way as a polar vector. But for improper operations, it incurs an extra minus sign. From these results, we can also determine that

- For polar vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, the cross product $\boldsymbol{r}_1 \times \boldsymbol{r}_2$ transforms as an axial vector (proven above).
- For axial vectors $\boldsymbol{m}_1$ and $\boldsymbol{m}_2$, the cross product $\boldsymbol{m}_1 \times \boldsymbol{m}_2$ also transforms as an axial vector.
- The cross product $\boldsymbol{r} \times \boldsymbol{m}$ of a polar vector with an axial vector transforms as a polar vector.

6.7.2 Invariant tensors

Suppose $T_{\alpha_1 \cdots \alpha_N \mu_1 \cdots \mu_M}$ transforms as a polar vector (*i.e.* 1^-) with respect to the indices $\{\alpha_j\}$ and as an axial vector (*i.e.* 1^+) with respect to indices $\{\mu_k\}$. Then the function

$$T\big(\{\boldsymbol{r}_j\}, \{\boldsymbol{m}_k\}\big) = T_{\alpha_1 \cdots \alpha_N \mu_1 \cdots \mu_M} \prod_{j=1}^{N} r_j^{\alpha_j} \prod_{k=1}^{M} m_k^{\mu_k} \quad . \tag{6.191}$$

transforms as a scalar (*i.e.* the trivial representation) under $\mathsf{O}(3)$. For example, if $T_{\alpha\beta\mu}$ transforms as a (polar) vector under α and β, and as an (axial) pseudovector under μ, then $T(\boldsymbol{x},\boldsymbol{y},\boldsymbol{m}) = T_{\alpha\beta\mu}\,x^\alpha\,y^\beta\,m^\mu$ is an invariant if $\boldsymbol{x}$ and $\boldsymbol{y}$ are vectors and $\boldsymbol{m}$ a pseudovector. Basically, so long as one is always taking the "dot product" on indices transforming according to the same IRREP of $\mathsf{O}(3)$, either 1^- or 1^+, then the resulting expression is a group scalar if all available indices are contracted. This also holds true if one internally contracts tensor indices which transform in the same way, *e.g.*

$$\widetilde{T}\big(\{\boldsymbol{r}_j\},\{\boldsymbol{m}_k\}\big) = T_{\alpha_1\cdots\alpha_N\mu_1\cdots\mu_M}\,\delta^{\alpha_1\alpha_2}\,\delta^{\mu_1\mu_2}\,\delta^{\mu_3\mu_4}\prod_{j=3}^{N} r_j^{\alpha_j}\prod_{k=5}^{M} m_k^{\mu_k} \tag{6.192}$$

is also a scalar. Now, following Lax, to every invariant polynomial of homogeneous degree K in $\big(\{\boldsymbol{r}_j\,,\,\boldsymbol{m}_k\}\big)$ there corresponds an invariant tensor of rank K, which one reads off from the coefficients of the monomials. Recall that any polynomial for which

$$T(\lambda\boldsymbol{r}_1,\ldots,\lambda\boldsymbol{r}_N,\lambda\boldsymbol{m}_1,\ldots,\lambda\boldsymbol{m}_M) = \lambda^K\,T(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N,\boldsymbol{m}_1,\ldots,\boldsymbol{m}_M) \tag{6.193}$$

is homogeneous of degree K. Thus, $T(\boldsymbol{x},\boldsymbol{y},\boldsymbol{m}) = \boldsymbol{x}\times\boldsymbol{y}\cdot\boldsymbol{m} = \epsilon_{\alpha\beta\gamma}\,x^\alpha\,y^\beta\,m^\mu$ is invariant and homogeneous of degree $K=3$. Therefore $T_{\alpha\beta\mu} = c\,\epsilon_{\alpha\beta\mu}$, where c is any constant, is an invariant rank three tensor, inverting the logic of our previous example.

For the group $\mathsf{SO}(n)$ of proper rotations, a theorem which we shall not prove establishes that all polynomial invariants of the n vectors $\{\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n\}$ are of the form

$$P(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n) = P_1\big(\{\boldsymbol{r}_i\cdot\boldsymbol{r}_j\}\big) + P_2\big(\{\boldsymbol{r}_i\cdot\boldsymbol{r}_j\}\big)\,\mathsf{det}(r_i^\mu) \quad , \tag{6.194}$$

where $P_{1,2}$ are functions of the dot products $\boldsymbol{r}_i\cdot\boldsymbol{r}_j$. In fact, the determinant is also a function of the dot products, although not a polynomial function thereof: $\mathsf{det}\,M_{i\mu} \equiv \mathsf{det}(r_i^\mu) = \mathsf{det}^{1/2}(\boldsymbol{r}_i\cdot\boldsymbol{r}_j) \equiv \big(\mathsf{det}\,N_{ij}\big)^{1/2}$.

6.7.3 Shell theorem

Let $\big\{\phi_\mu^\Gamma(\boldsymbol{r})\big\}$ and $\big\{\psi_\nu^\Gamma(\boldsymbol{r})\big\}$ be two sets of orthonormal basis functions for an IRREP Γ of some finite discrete group G. Then the function

$$F^\Gamma(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu=1}^{d_\Gamma}\phi_\mu^{\Gamma^*}(\boldsymbol{r})\,\psi_\mu^\Gamma(\boldsymbol{r}') \tag{6.195}$$

is invariant under the operation of all $g\in G$. Explicitly, we have

$$g\,F^\Gamma(\boldsymbol{r},\boldsymbol{r}') = \sum_{\alpha,\beta}\phi_\alpha^{\Gamma^*}(\boldsymbol{r})\,\psi_\beta^\Gamma(\boldsymbol{r}')\,\overbrace{\sum_\mu D^*_{\alpha\mu}(g)\,D_{\beta\mu}(g)}^{=\,\delta_{\alpha\beta}} \quad . \tag{6.196}$$

Similarly, we have

$$\frac{1}{N_G}\sum_{g\in G} g\left[\phi_\mu^{\Gamma^*}(\boldsymbol{r})\,\psi_\mu^\Gamma(\boldsymbol{r}')\right] = \sum_{\alpha,\beta}\phi_\alpha^{\Gamma^*}(\boldsymbol{r})\,\psi_\beta^\Gamma(\boldsymbol{r}')\,\frac{1}{N_G}\sum_{g\in G}D^*_{\alpha\mu}(g)\,D_{\beta\mu}(g) = \frac{1}{d_\Gamma}\sum_\alpha\phi_\alpha^{\Gamma^*}(\boldsymbol{r})\,\psi_\alpha^\Gamma(\boldsymbol{r}') \quad , \tag{6.197}$$

where there is no implicit sum on μ. The LHS above is an average over all group operations, whereas the RHS is a "shell average" over all the labels in the representation Γ.

These results may be used to construct invariant tensors. Lax presents an example from C_{3v}, taking

$$\phi_1^E = yz' - zy' \quad , \quad \phi_2^E = zx' - xz' \quad , \quad \psi_1^E = m_x \quad , \quad \psi_2^E = m_y \quad , \tag{6.198}$$

and

$$\phi^{A_2} = xy' - yx' \quad , \quad \psi^{A_2} = m_z \quad . \tag{6.199}$$

The general invariant is expressed as $F = a\, E\cdot E + b\, A_2 \cdot A_2$, *i.e.*

$$F = a\,(yz' - zy')\, m_x + a\,(zx' - xz')\, m_y + b\,(xy' - yx')\, m_z \quad . \tag{6.200}$$

We read off the coefficients of $r_\mu\, r'_\nu\, m_\lambda$ to obtain the invariant tensor elements $\chi_{\mu\nu\lambda}$,

$$\begin{aligned} \chi_{123} &= -\chi_{213} = a \\ \chi_{231} = \chi_{312} &= -\chi_{321} = -\chi_{132} = b \quad . \end{aligned} \tag{6.201}$$

With spin, the invariant carries spatial and spin information, and is written

$$F^\Gamma(\boldsymbol{r}, \boldsymbol{r}', s, s') = \sum_{\mu=1}^{d_\Gamma} \phi_\mu^{\Gamma^*}(\boldsymbol{r}, s)\, \psi_\mu^\Gamma(\boldsymbol{r}', s') \quad , \tag{6.202}$$

where s and s' are spinor indices.

6.8 Appendix : Quasi-degenerate Perturbation Theory

Oftentimes, as in our discussion of Raman spectroscopy in §6.4.3, we would like to focus on a subset of Hilbert space and derive an effective Hamiltonian valid for a restricted group of states. This may be accomplished by decoupling the target group of states from the rest of Hilbert space perturbatively order by order in a canonical transformation[39].

6.8.1 Type A and type B operators

Consider a Hamiltonian $H = H^0 + V$, with $H^0 |\, j\,\rangle = E_j^0 |\, j\,\rangle$. Typically the Hilbert space in which H operates will be infinite-dimensional. Now consider some finite subset of levels $\{j_1, j_j, \ldots, j_K\}$ and define P to be be the projector onto this subspace, *i.e.* $P = \sum_{\alpha=1}^K |\, j_\alpha\,\rangle\langle\, j_\alpha\,|$. Let $Q = \mathbb{1} - P$ be the orthogonal projector onto the complementary subspace. Typically we will be interested in cases where P projects onto a small number of energy levels, such as the low-lying vibrational states of a molecule, or, in a solid, a group of levels in the vicinity of the Fermi energy, such as the valence band(s) plus conduction band(s) in a semiconductor.

[39] See, *e.g.* Appendix B of R. Winkler, *Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems* (Springer, 2003).

Let us write $V = V_{\rm A} + V_{\rm B}$, where

$$\begin{aligned} V_{\rm A} &= P\,V\,P + Q\,V\,Q \\ V_{\rm B} &= P\,V\,Q + Q\,V\,P \quad . \end{aligned} \tag{6.203}$$

The operator $V_{\rm A}$ has no matrix elements connecting the P and Q subspaces, while $V_{\rm B}$ *only* has matrix elements between those subspaces. Clearly H^0, which is diagonal, is a "type A" operator. Fig. 6.16 shows schematically the difference between type A and type B.

6.8.2 Unitary transformation for block diagonalization

Consider now a unitary transformation with

$$\begin{aligned} \widetilde{H} = e^{-S}\,H\,e^{S} &= H + [H,S] + \frac{1}{2!}\big[[H,S],S\big] + \frac{1}{3!}\Big[\big[[H,S],S\big],S\Big] + \ldots \\ &\equiv \sum_{k=0}^{\infty} \frac{1}{k!}\,\big[H,S\big]_{(k)}\,, \end{aligned} \tag{6.204}$$

where $S = -S^\dagger$ is antihermitian in order that e^S be unitary, and where

$$\big[H,S\big]_{(k)} = \overbrace{\big[\big[\big[H,S\big],S\big]\cdots,S\big]}^{k\ \text{times}}\,, \tag{6.205}$$

with $[H,S]_{(0)} \equiv H$. As we shall see, we may assume $S = S_{\rm B}$ is of type B., in which case $\widetilde{H} = \widetilde{H}_{\rm A} + \widetilde{H}_{\rm B}$, with

$$\begin{aligned} \widetilde{H}_{\rm A} &= \sum_{j=0}^{\infty} \frac{1}{(2j)!}\big[H^0 + V_{\rm A}, S\big]_{(2j)} + \sum_{j=0}^{\infty} \frac{1}{(2j+1)!}\big[V_{\rm B},S\big]_{(2j+1)} \\ \widetilde{H}_{\rm B} &= \sum_{j=0}^{\infty} \frac{1}{(2j+1)!}\big[H^0 + V_{\rm A}, S\big]_{(2j+1)} + \sum_{j=0}^{\infty} \frac{1}{(2j)!}\big[V_{\rm B},S\big]_{(2j)} \quad . \end{aligned} \tag{6.206}$$

We choose S such that $\widetilde{H}_{\rm B} = 0$. This is done perturbatively. We start by formally replacing $V_{\rm A} \to \lambda V_{\rm A}$ and $V_{\rm B} \to \lambda V_{\rm B}$, with $\lambda = 1$ at the end of the day. We then write S as a Taylor series in powers of λ:

$$S = \lambda\,S^{(1)} + \lambda^2\,S^{(2)} + \ldots \quad . \tag{6.207}$$

X	Y	$[X,Y]$
type A	type A	type A
type A	type B	type B
type B	type A	type B
type B	type B	type A

Table 6.24: Commutators and their types.

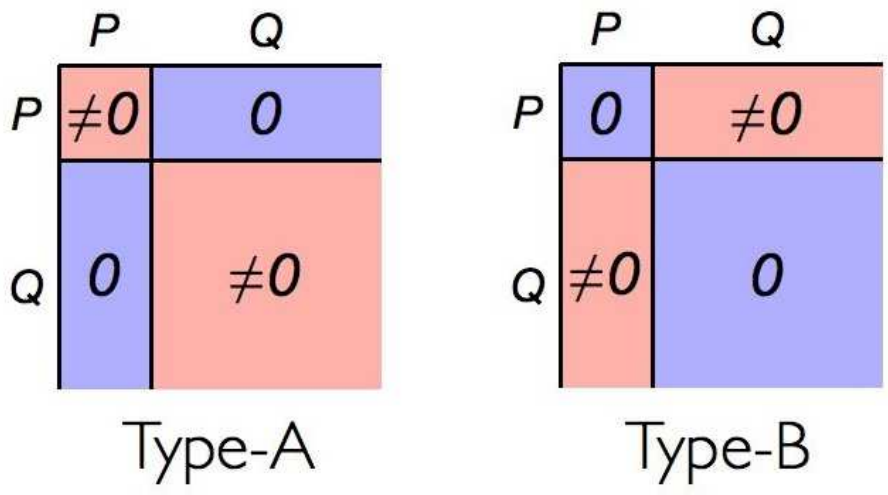


Figure 6.16: Type-A operators preserve the subspace; type B operators change the subspace.

To third order in λ, we will need the following expressions:

$$\begin{aligned}\big[H^0+\lambda V_{\rm A},S\big]_{(1)} &= \lambda\,\big[H^0,S^{(1)}\big]+\lambda^2\Big(\big[H^0,S^{(1)}\big]+\big[V_{\rm A},S^{(1)}\big]\Big)\\ &\qquad\qquad +\lambda^3\Big(\big[H^0,S^{(3)}\big]+\big[V_{\rm A},S^{(2)}\big]\Big)+\mathcal{O}(\lambda^4)\\ \big[H^0+\lambda V_{\rm A},S\big]_{(3)} &= \lambda^3\,\big[\big[\big[H^0,S^{(1)}\big],S^{(1)}\big],S^{(1)}\big]+\mathcal{O}(\lambda^4)\end{aligned}\tag{6.208}$$

and

$$\begin{aligned}\big[\lambda V_{\rm B},S\big]_{(0)} &= \lambda V_{\rm B}\\ \big[\lambda V_{\rm B},S\big]_{(2)} &= \lambda^3\,\big[\big[V_{\rm B},S^{(1)}\big],S^{(1)}\big]+\mathcal{O}(\lambda^4)\end{aligned}\tag{6.209}$$

To order λ^3, then, we make $\widetilde{H}_{\rm B}$ vanish by demanding

$$\begin{aligned}0&=\big[H^0,S^{(1)}\big]+V_{\rm B}\\ 0&=\big[H^0,S^{(2)}\big]+\big[V_{\rm A},S^{(1)}\big]\\ 0&=\big[H^0,S^{(3)}\big]+\big[V_{\rm A},S^{(2)}\big]+\tfrac{1}{6}\Big[\big[\big[H^0,S^{(1)}\big],S^{(1)}\big],S^{(1)}\Big]+\tfrac{1}{2}\big[\big[V_{\rm B},S^{(1)}\big],S^{(1)}\big]\quad .\end{aligned}\tag{6.210}$$

We solve the first equation for $S^{(1)}$, then plug this into the second to obtain an equation for $S^{(2)}$, the solution of which is used in the third equation to obtain $S^{(3)}$, *etc.* Setting $\lambda=1$, the Hamiltonian is then

$$\begin{aligned}\widetilde{H}=\widetilde{H}_{\rm A}&=H^0+V_{\rm A}+\big[V_{\rm B},S^{(1)}\big]+\tfrac{1}{2}\big[\big[H^0,S^{(1)}\big],S^{(1)}\big]+\ldots\\ &=H^0+V_{\rm A}+\tfrac{1}{2}\big[V_{\rm B},S^{(1)}\big]+\ldots\quad .\end{aligned}\tag{6.211}$$

Let a and b index states in P and let n and m index states in Q. The equation for $S^{(1)}$ then yields

$$0=V_{an}+H^0_{ab}\,S^{(1)}_{bn}-S^{(1)}_{am}\,H^0_{mn}=V_{an}+\big(E^0_a-E^0_n\big)\,S^{(1)}_{an}\quad .\tag{6.212}$$

X	$[X,S]_{(2j)}$	$[X,S]_{(2j+1)}$
type A	type A	type B
type B	type B	type A

Table 6.25: Multiple commutators and their types.

Therefore, we have

$$S^{(1)}_{an} = \frac{V_{an}}{E^0_n - E^0_a} \qquad , \qquad S^{(1)}_{na} = \frac{V_{na}}{E^0_a - E^0_n} \quad . \tag{6.213}$$

Note that V_{an} and V_{na} both come from the $V_{\rm B}$ part of V.

The equation for $S^{(2)}$ may be written in component form as

$$\begin{aligned} 0 &= H^0_{ab}\, S^{(2)}_{bn} - S^{(2)}_{am}\, H^0_{mn} + V_{ab}\, S^{(1)}_{bn} - S^{(1)}_{am}\, V_{mn} \\ &= \left(E^0_a - E^0_n\right) S^{(2)}_{an} + \frac{V_{ab}V_{ma}}{E^0_n - E^0_b} - \frac{V_{am}V_{mn}}{E^0_m - E^0_a} \quad . \end{aligned} \tag{6.214}$$

Restoring the summation symbols for added clarity, we then have

$$S^{(2)}_{an} = \frac{1}{E^0_a - E^0_n} \cdot \left(\sum_b \frac{V_{ab}V_{bn}}{E^0_n - E^0_b} - \sum_m \frac{V_{am}V_{mn}}{E^0_m - E^0_a} \right) , \tag{6.215}$$

with a corresponding expression for $S^{(2)}_{na}$. At this point, the student should write down the expression for $S^{(2)}_{an}$. The Hamiltonian in the P sector, to this order, is then

$$\begin{aligned} \widetilde{H}_{ab} &= E^0_a\, \delta_{ab} + V_{ab} + \tfrac{1}{2}\left(V_{an} S^{(1)}_{nb} - S^{(1)}_{an} V_{nb}\right) \\ &= E^0_a\, \delta_{ab} + V_{ab} + \tfrac{1}{2} \sum_n \left(\frac{1}{E^0_a - E^0_n} + \frac{1}{E^0_b - E^0_n} \right) V_{an} V_{nb} \quad . \end{aligned} \tag{6.216}$$

6.9 Jokes for Chapter Six

MATHEMATICS JOKE : Q: What does the "B" in Benoit B. Mandelbrot stand for? A: Benoit B. Mandelbrot.

GRAMMAR JOKE : A businessman is in Boston for only the second time in his life. On his first visit he had some delicious New England seafood, and he's looking forward to going back to the same restaurant. So he hails a cab, and asks the driver, "I was in Boston a few years ago. Can you take me to Angela's, where I had scrod before?" The driver replies, "You know, lots of people ask me that, but never in the pluperfect subjunctive."

LOGICIAN JOKE : A logician's husband tells his wife, "please go to the grocery store on your way home from work. We need a gallon of milk. And if they have eggs, get a dozen." She returns home with twelve gallons of milk. "What the hell happened?!" asks the husband. "They had eggs," she explained.

MUSICIAN JOKE : A conductor who is preparing for a performance is having trouble finding a good clarinet player. He calls a contractor who tells him, "The only guy I've got is a jazz clarinetist." "I can't stand working with jazz musicians!" says the conductor. "They dress like bums, they're always late, and every one of them has an attitude problem." "Hey, he's all I've got," says the contractor. The conductor is desperate, so he agrees.

The conductor arrives early for the first rehearsal and sees the jazz clarinetist wearing a suit and tie, a pencil resting on his stand, and practicing his part. During the rehearsal, he plays sensitively and writes down all of the conductor's suggestions. At the second rehearsal, the clarinetist plays even better. At the final dress rehearsal, he is absolutely flawless.

During the dress rehearsal break, the conductor tells the orchestra, "I've got an apology to make, and I wanted to do so publicly, because there is a lesson here for us all. I was really dreading having to work with a jazz musician, but I must say that our clarinetist has proven me wrong. He's always neatly dressed, comes early to rehearsal, and he really listened to me and learned his part very well indeed." Turning to the clarinet player the maestro says, "I just wanted to tell you that I truly appreciate your effort and dedication."

The clarinetist replies, "Hey man, it's the least I can do since I can't make the gig."

SPECIAL JOKE FOR CHAPTER SIX : A Mn^{4+} ion walks into a bar. The bartender asks, "would you like a point group?" The ion replies, "better make it a double."[40]

[40] I made this joke up all by myself. It is term-splitting, if not side-splitting. "They laughed when I said I wanted to be a comedian. Well, nobody is laughing now!"

Chapter 7

Time Reversal

7.1 The Poincaré Group

7.1.1 Space inversion and time-reversal

Recall that the Poincaré group $\mathsf{P}(1,n)$ in n space dimensions is the set of matrices

$$R(L,\boldsymbol{b}) = \left[\begin{array}{ccc|c} L_{00} & \cdots & L_{0n} & b_0 \\ \vdots & \ddots & \vdots & \vdots \\ L_{n0} & \cdots & L_{nn} & b_n \\ \hline 0 & \cdots & 0 & 1 \end{array}\right] \quad , \tag{7.1}$$

where $L \in \mathsf{O}(1,n)$ is a Lorentz transformation, meaning $L^{\mathsf{T}} g L = g$ with $g = \mathsf{diag}(1,-1,\ldots,-1)$ is a diagonal matrix of rank $(n+1)$, and b is an $(n+1)$-component column vector[1]. Note g is of rank $n+2$, and its action on a vector ξ whose transpose is $\xi^{\mathsf{T}} = (x_0\,,\,x_1\,,\,\ldots\,,\,x_n\,,\,1)$ is given by

$$R(L,\boldsymbol{b})\,\xi = \left[\begin{array}{ccc|c} L_{00} & \cdots & L_{0n} & b_0 \\ \vdots & \ddots & \vdots & \vdots \\ L_{n0} & \cdots & L_{nn} & b_n \\ \hline 0 & \cdots & 0 & 1 \end{array}\right] \begin{pmatrix} x_0 \\ \vdots \\ x_n \\ 1 \end{pmatrix} = \begin{pmatrix} x'_0 \\ \vdots \\ x'_n \\ 1 \end{pmatrix} \equiv \xi' \quad , \tag{7.2}$$

where $x'_\mu = L_{\mu\nu} x_\nu + b_\mu$. The space inversion and time-reversal operators, I and T, respectively, expressed as elements of $\mathsf{O}(1,n)$, are then

$$I = \left[\begin{array}{c|c} 1 & 0_{1\times n} \\ \hline 0_{n\times 1} & -1_{n\times n} \end{array}\right] \qquad , \qquad T = \left[\begin{array}{c|c} -1 & 0_{1\times n} \\ \hline 0_{n\times 1} & 1_{n\times n} \end{array}\right] \quad , \tag{7.3}$$

[1] In chapter 1, we called this group $\mathsf{P}(n,1)$, which is equivalent to $\mathsf{P}(1,n)$. In both cases, the metric tensor $g_{\mu\nu}$ is diagonal and the temporal entry g_{00} is of opposite sign to the spatial entries $g_{11} = g_{22} = \cdots = g_{nn}$.

and are both of rank $(n+1)$. Their corresponding rank matrices $\mathcal{I}$ and $\mathcal{T}$, which are elements of $\mathsf{P}(1,n)$ and therefore of rank $(n+2)$, are then given by

$$\mathcal{I} = \left[\begin{array}{c|c} I_{(n+1)\times(n+1)} & 0_{(n+1)\times 1} \\ \hline 0_{1\times(n+1)} & 1 \end{array}\right] \quad , \quad \mathcal{T} = \left[\begin{array}{c|c} T_{(n+1)\times(n+1)} & 0_{(n+1)\times 1} \\ \hline 0_{1\times(n+1)} & 1 \end{array}\right] \quad . \tag{7.4}$$

Note that $\mathcal{I}^{-1} = \mathcal{I}$ and $\mathcal{T}^{-1} = \mathcal{T}$, and furthermore that

$$\begin{aligned} \mathcal{I}\, R(L,b)\, \mathcal{I}^{-1} &= R(ILI^{-1}, Ib) \\ \mathcal{T}\, R(L,b)\, \mathcal{T}^{-1} &= R(TLT^{-1}, Tb) \quad . \end{aligned} \tag{7.5}$$

The product $\mathcal{I}\mathcal{T} = \mathcal{T}\mathcal{I}$ is

$$\mathcal{I}\mathcal{T} = \left[\begin{array}{c|c} -1_{(n+1)\times(n+1)} & 0_{(n+1)\times 1} \\ \hline 0_{1\times(n+1)} & 1 \end{array}\right] \quad , \tag{7.6}$$

which commutes with all pure Lorentz transformations, but fails to commute with space-time translations, since

$$\mathcal{I}\mathcal{T}\, R(E,b)\, (\mathcal{I}\mathcal{T})^{-1} = R(E,-b) \quad . \tag{7.7}$$

7.1.2 Representations of the Poincaré Lie algebra

We now restrict our attention to the case $n = 3$, where the Poincaré group consists of 5×5 matrices. The generators of the Poincaré Lie algebra $\mathsf{p}(1,3)$ are classified as being translations, rotations, or boosts. The lowest order variation of $R(L,b)$ about the identity $R(E,0)$ is

$$\delta R = \left[\begin{array}{c|ccc|c} 0 & \delta\omega_{01} & \delta\omega_{02} & \delta\omega_{03} & \delta b_0 \\ \hline \delta\omega_{01} & 0 & \delta\omega_{12} & -\delta\omega_{31} & \delta b_1 \\ \delta\omega_{02} & -\delta\omega_{12} & 0 & \delta\omega_{23} & \delta b_2 \\ \delta\omega_{03} & \delta\omega_{31} & -\delta\omega_{23} & 0 & \delta b_3 \\ \hline 0 & 0 & 0 & 0 & 0 \end{array}\right] \equiv -iP^\mu\, \delta b_\mu - iJ^{\mu\nu}\, \delta\omega_{\mu\nu} \quad . \tag{7.8}$$

More precisely,

$$\begin{aligned} R(E, \delta b) &= \exp\bigl(-iP^\mu\, \delta b_\mu\bigr) \\ R(E+\delta\omega, 0) &= \exp\bigl(-iJ^{\mu\nu}\, \delta\omega_{\mu\nu}\bigr) \quad , \end{aligned} \tag{7.9}$$

where $A^\mu B_\mu = g_{\mu\nu} A^\mu B^\nu$, and where $\delta\omega^{\mathsf{T}} = -g\, \delta\omega\, g$ and $J^{\mathsf{T}} = -gJg$. We stress that for each $\mu \in \{0,1,2,3\}$ the generator P^μ is a 5×5 matrix, as is each of the six independent elements of $J^{\mu\nu}$. The latter is further split into its rotation and boost components by writing

$$J_i = \tfrac{1}{2}\epsilon_{ijk}\, J^{jk} \quad , \quad K_i = J_{i0} \quad , \tag{7.10}$$

with $i \in \{1,2,3\}$. $\boldsymbol{J}$ are the generators of rotations, and $\boldsymbol{K}$ the generators of boosts. Thus, we have a total of ten generators of the Lie algebra $\mathsf{p}(1,3)$: P^0, $\boldsymbol{P}$, $\boldsymbol{J}$, and $\boldsymbol{K}$, the 5×5 matrices of which can be read off from Eqn. 7.8. Under space inversion and time-reversal,

$$\mathcal{I}\,P^0\,\mathcal{I}^{-1} = +P_0 \quad , \quad \mathcal{I}\,\boldsymbol{P}\,\mathcal{I}^{-1} = -\boldsymbol{P} \quad , \quad \mathcal{I}\,\boldsymbol{J}\,\mathcal{I}^{-1} = +\boldsymbol{J} \quad , \quad \mathcal{I}\,\boldsymbol{K}\,\mathcal{I}^{-1} = -\boldsymbol{K} \tag{7.11}$$

$$\mathcal{T}\,P^0\,\mathcal{T}^{-1} = -P_0 \quad , \quad \mathcal{T}\,\boldsymbol{P}\,\mathcal{T}^{-1} = +\boldsymbol{P} \quad , \quad \mathcal{T}\,\boldsymbol{J}\,\mathcal{T}^{-1} = +\boldsymbol{J} \quad , \quad \mathcal{T}\,\boldsymbol{K}\,\mathcal{T}^{-1} = -\boldsymbol{K} \quad . \tag{7.12}$$

7.1.3 Whither time-reversal?

The problem is that P^0 changes sign under $\mathcal{T}$, but $\boldsymbol{P}$ does not. In classical mechanics, the action of time-reversal is

$$\boldsymbol{r}^T = \boldsymbol{r} \quad , \quad \boldsymbol{p}^T = -\boldsymbol{p} \quad , \quad \boldsymbol{L}^T = -\boldsymbol{L} \quad , \quad \boldsymbol{E}^T = \boldsymbol{E} \quad , \quad \boldsymbol{B}^T = -\boldsymbol{B} \quad . \tag{7.13}$$

Thus, if $H(\boldsymbol{E},\boldsymbol{B})$ is the Hamiltonian for a charged particle in the presence of electric and magnetic fields, $\big[H(\boldsymbol{E},\boldsymbol{B})\big]^T = H(\boldsymbol{E},-\boldsymbol{B})$. Unlike space inversion, time-reversal in classical mechanics is *not* a canonical transformation, since it does not preserve the Poisson bracket $\big\{x^\mu\,,\,p^\nu\big\}_{\text{PB}} = \delta^{\mu\nu}$. This is our first clue that there is something special about time-reversal and that attempting to implement it in quantum mechanics via a unitary transformation is doomed to fail.

Indeed, if we use Eqn. 7.12 to define Hermitian generators of $\mathsf{p}(1,3)$, we run into problems quantizing because the generator of time translations, P^0, which is the Hamiltonian, is apparently odd under time-reversal, while the momentum $\boldsymbol{P}$, which is the generator of space translations, is even under time-reversal. This poses severe problems for the classical-quantum correspondence.

Indeed, suppose we define a time-reversal operator $\hat{T}$ whose action on wavefunctions $\psi(\boldsymbol{x},t)$ is

$$\psi'(\boldsymbol{x},t) = \hat{T}\psi(\boldsymbol{x},t) = \lambda\,\psi(\boldsymbol{x},-t) \quad , \tag{7.14}$$

where $\lambda \in \mathbb{C}$. Does $\psi'(\boldsymbol{x},t)$ satisfy the Schrödinger equation?

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\,\psi'(\boldsymbol{x},t) = i\hbar\lambda\,\frac{\partial}{\partial t}\,\psi(\boldsymbol{x},-t) &= -i\hbar\lambda\frac{\partial}{\partial(-t)}\,\psi(\boldsymbol{x},-t) \\ &= -\lambda\,\hat{H}\,\psi(\boldsymbol{x},-t) = -\hat{H}\,\psi'(\boldsymbol{x},t) \quad . \end{aligned} \tag{7.15}$$

No, it does not. In hindsight, this was obvious from the start. The Schrödinger equation is first order in time, hence it is not invariant under $t \to -t$. So at this point we are left with three possibilities:

(i) Quantum physics, unlike Newtonian physics, is not invariant under time-reversal. *[horrible!]*

(ii) $\hat{T}\hat{H}\hat{T}^{-1} = -\hat{H}$ and the correspondence principle fails. *[horrible!]*

(iii) $i\hbar\frac{\partial}{\partial t}$ does not change sign under time-reversal. *[hmmm...]*

7.2 Antilinearity : The Solution to All Our Problems

I don't know about you, but I'm putting my money on option (iii). How could we make that work out? Well, suppose that the action of time-reversal is not given by Eqn. 7.14, but rather by

$$\psi'(\boldsymbol{x},t) = \lambda\check{K}\psi(\boldsymbol{x},-t) = \lambda\,\psi^*(\boldsymbol{x},-t) \quad , \tag{7.16}$$

where $\check{K}$ is the scalar *complex conjugation operator*[2] which complex conjugates every scalar to its right. Now we have

$$i\hbar\frac{\partial}{\partial t}\,\psi'(\boldsymbol{x},t) = i\hbar\lambda\,\frac{\partial}{\partial t}\,\psi^*(\boldsymbol{x},-t) = \lambda\left[i\hbar\frac{\partial}{\partial(-t)}\,\psi(\boldsymbol{x},-t)\right]^* = \lambda\,\hat{H}^*\psi^*(\boldsymbol{x},-t) = \hat{H}^*\psi'(\boldsymbol{x},t) \quad , \tag{7.17}$$

and so long as $\hat{H} = \hat{H}^*$, the Schrödinger equation remains invariant under time-reversal. Now that was so fun, let's do it again:

$$\psi''(\boldsymbol{x},t) = \lambda\check{K}\,\lambda\check{K}\,\psi\big(\boldsymbol{x},-(-t)\big) = |\lambda|^2\,\psi(\boldsymbol{x},t) \quad , \tag{7.18}$$

and if time-reversal applied twice preserves the state $\psi(\boldsymbol{x},t)$ up to a phase, we conclude that phase $|\lambda|^2$ must be unity, *i.e.* $\check{T}^2 = 1$ and $\lambda = e^{i\theta}$ is a unimodular complex number. This result is applicable to scalar wavefunctions ψ. When there is a spinor component due to intrinsic angular momentum, then the most general form for $\check{T}$ is $\check{T} = \hat{U}\check{K}$, where $\hat{U}$ is a unitary operator. In this case the unitary $\hat{U}$ may act on the spinor coordinates of Ψ, but since two applications of $\check{T}$ must result in the same state, *i.e.* must preserve the *ray* in Hilbert space, we conclude $\check{T}^2\,\Psi = e^{i\alpha}\,\Psi$, *i.e.* $\check{T}^2 = e^{i\alpha}$ is at most a constant phase. But then

$$\begin{aligned}\check{T}^3\,\Psi &= \check{T}\,(\check{T}^2\,\Psi) = \check{T}\,e^{i\alpha}\,\Psi = e^{-i\alpha}\,\check{T}\,\Psi \\ &= (\check{T}^2)\,\check{T}\,\Psi = e^{i\alpha}\,\check{T}\,\Psi \quad ,\end{aligned} \tag{7.19}$$

and we conclude $e^{2i\alpha} = 1$, hence $\alpha = 0$ or $\alpha = \pi$. As we shall see below, the case $\alpha = 0$ applies when the intrinsic angular momentum is $j \in \mathbb{Z}$, while $\alpha = \pi$ applies when $j \in \mathbb{Z} + \frac{1}{2}$.

An operator $\check{A}$ for which

$$\check{A}\Big[\alpha\,\big|\,\phi\,\big\rangle + \beta\,\big|\,\psi\,\big\rangle\Big] = \alpha^*\check{A}\,\big|\,\phi\,\big\rangle + \beta^*\check{A}\,\big|\,\psi\,\big\rangle \tag{7.20}$$

is called *antilinear*. Thus, time-reversal operator for spinless particles, $\check{T} = e^{i\theta}\check{K}$, is antilinear. Note that we use the inverted hat symbol (ˇ) to denote an antilinear operator.

7.2.1 Properties of antilinear operators

The following are True Facts about antilinear operators:

- An antilinear operator does not commute with complex numbers. Rather

$$\check{A}\,c = c^*\check{A} \qquad \Rightarrow \qquad \check{A}\,c\,\check{A}^{-1} = c^* \quad . \tag{7.21}$$

[2] We shall see below in §7.2.4 how to define time-reversal for particles with $S = \frac{1}{2}$.

- Rather than $\langle\,\phi\,|\,\hat{A}\,\psi\,\rangle = \langle\,\hat{A}^\dagger\,\phi\,|\,\psi\,\rangle$ as for linear $\hat{A}$, for antilinear $\check{A}$ we have

$$\langle\,\phi\,\big|\,\check{A}\,\psi\,\rangle = \langle\,\check{A}^\dagger\phi\,\big|\,\psi\,\rangle^* \quad . \tag{7.22}$$

  Indeed, the familiar Dirac notation $\langle\,\phi\,|\,\hat{A}\,|\,\psi\,\rangle = \langle\,\phi\,|\,\hat{A}\,\psi\,\rangle = \langle\,\hat{A}^\dagger\phi\,|\,\psi\,\rangle$ is misleading and should be eschewed in the case of antilinear operators, for which we may write

$$\Big(\langle\,\phi\,|\check{A}\Big) = \langle\,\check{A}^\dagger\,\phi\,| \quad , \quad \Big(\check{A}\,\big|\,\psi\,\rangle\Big) = |\,\check{A}\,\psi\,\rangle \tag{7.23}$$

  and

$$\Big(\langle\,\phi\,|\check{A}\Big)|\,\psi\,\rangle = \Big[\langle\,\phi\,|\Big(\check{A}\,\big|\,\psi\,\rangle\Big)\Big]^* \tag{7.24}$$

  Thus, $\langle\,\check{A}^\dagger\,\phi\,|\,\psi\,\rangle = \langle\,\phi|\check{A}\,\psi\,\rangle^*$. It is very dangerous and often wrong to remove the parentheses in the above relations!

- Though this follows from the first bullet, it is worth emphasizing:

$$(c\,\check{A})^{-1} = \check{A}^{-1}\,c^{-1} = c^{*-1}\,\check{A}^{-1} \quad . \tag{7.25}$$

- The time-reversal operator is both unitary and antilinear, *i.e.* it is *antiunitary*. Because it is unitary, $\check{T}^\dagger\check{T} = \hat{E}$. Thus entails

$$\big\langle\,\check{T}\phi\,\big|\,\check{T}\psi\,\big\rangle = \big\langle\,\check{T}^\dagger\check{T}\,\phi\,\big|\,\psi\,\big\rangle^* = \big\langle\,\phi\,\big|\,\psi\,\big\rangle^* = \big\langle\,\psi\,\big|\,\phi\,\big\rangle \quad . \tag{7.26}$$

  Thus,

$$\big|\big\langle\,\check{T}\phi\,\big|\,\check{T}\psi\,\big\rangle\big|^2 = \big|\big\langle\,\phi\,\big|\,\psi\,\big\rangle\big|^2 \tag{7.27}$$

  for all $|\,\phi\,\rangle$ and $|\,\psi\,\rangle$. So time-reversal preserves probabilities.

- Let $\hat{U}$ and $\hat{V}$ be unitary, and let $\check{A}$ and $\check{B}$ be antiunitary. Then $\hat{U}\hat{V}$ and $\check{A}\check{B}$ are both unitary, while $\hat{U}\check{B}$ and $\hat{V}\check{A}$ are both antiunitary. These follow directly from Eqn. 7.20.

- Any symmetry operation which preserves probabilities can be represented as an operator acting on the Hilbert space of states that is either both linear and unitary, or antilinear and antiunitary.

The proof of the last bullet point is elementary[3]. Let $\widetilde{Q}$ be an operator which preserves probabilities. Then it must preserve the norm, *i.e.*

$$\big\langle\,\widetilde{Q}\,\Psi\,\big|\,\widetilde{Q}\,\Psi\,\big\rangle = \big\langle\,\Psi\,\big|\,\Psi\,\big\rangle \quad . \tag{7.28}$$

for all $|\,\Psi\,\rangle$. Now let $|\,\Psi\,\rangle = c\,|\,\phi\,\rangle + |\,\psi\,\rangle$. Then

$$\begin{aligned}
\big\langle\,\widetilde{Q}\,(c\,\phi+\psi)\,\big|\,\widetilde{Q}\,(c\,\phi+\psi)\,\big\rangle &= \big\langle\,c\,\phi+\psi\,\big|\,c\phi+\psi\,\big\rangle \\
&= |c|^2\,\big\langle\,\phi\,\big|\,\phi\,\big\rangle + \big\langle\,\psi\,\big|\,\psi\,\big\rangle + 2\,\mathsf{Re}\Big[c\,\big\langle\,\psi\,\big|\,\phi\,\big\rangle\Big] \\
&= \big\langle\,\tilde{c}\,\widetilde{Q}\,\phi + \widetilde{Q}\,\psi\,\big|\,\tilde{c}\,\widetilde{Q}\,\phi + \widetilde{Q}\,\psi\,\big\rangle \\
&= |\tilde{c}|^2\,\big\langle\,\phi\,\big|\,\phi\,\big\rangle + \big\langle\,\psi\,\big|\,\psi\,\big\rangle + 2\,\mathsf{Re}\Big[\tilde{c}\,\big\langle\,\psi\,\big|\,\phi\,\big\rangle\Big] \quad ,
\end{aligned} \tag{7.29}$$

[3]Wigner said it, so it must be true. See, *e.g.*, Appendix A of S. Weinberg, *The Quantum Theory of Fields* (vol. 1) or Theorem 10.4.2 of Lax. Here we follow Lax's proof.

where $\tilde{c} = c$ if $\widetilde{Q}$ is linear and $\tilde{c} = c^*$ if $\widetilde{Q}$ is antilinear. Note $|\tilde{c}|^2 = |c|^2$ in either case. Then setting $c = 1$ and $c = i$ gives

$$\begin{aligned} c = 1 \qquad &\Rightarrow \qquad \mathsf{Re}\,\big\langle\, \widetilde{Q}\,\psi \,\big|\, \widetilde{Q}\,\phi\,\big\rangle = \mathsf{Re}\,\big\langle\,\psi\,\big|\,\phi\,\big\rangle \\ c = i \qquad &\Rightarrow \qquad \mathsf{Im}\,\big\langle\, \widetilde{Q}\,\psi \,\big|\, \widetilde{Q}\,\phi\,\big\rangle = \pm\,\mathsf{Im}\,\big\langle\,\psi\,\big|\,\phi\,\big\rangle \quad , \end{aligned} \tag{7.30}$$

where the top sign holds for $\widetilde{Q}$ linear and the bottom sign for $\widetilde{Q}$ antilinear. For $\widetilde{Q}$ linear, we have $\langle\, \widetilde{Q}\,\psi \,|\, \widetilde{Q}\,\phi\,\rangle = \langle\,\psi\,|\,\phi\,\rangle$, which establishes that $\widetilde{Q}$ is unitary. For $\widetilde{Q}$ antilinear, $\langle\, \widetilde{Q}\,\psi \,|\, \widetilde{Q}\,\phi\,\rangle = \langle\,\phi\,|\,\psi\,\rangle$, which establishes that $\widetilde{Q}$ is antiunitary.

As a result of the complex conjugation, we now have an updated and more suitable version of Eqn. 7.12,

$$\hat{I}\,\hat{P}^0\,\hat{I}^{-1} = +P_0 \quad , \quad \hat{I}\,\hat{\boldsymbol{P}}\,\hat{I}^{-1} = -\hat{\boldsymbol{P}} \quad , \quad \hat{I}\,\hat{\boldsymbol{J}}\,\hat{I}^{-1} = +\hat{\boldsymbol{J}} \quad , \quad \hat{I}\,\hat{\boldsymbol{K}}\,\hat{I}^{-1} = -\hat{\boldsymbol{K}} \tag{7.31}$$

$$\check{T}\,\hat{P}^0\,\check{T}^{-1} = +P_0 \quad , \quad \check{T}\,\hat{\boldsymbol{P}}\,\check{T}^{-1} = -\hat{\boldsymbol{P}} \quad , \quad \check{T}\,\hat{\boldsymbol{J}}\,\check{T}^{-1} = -\hat{\boldsymbol{J}} \quad , \quad \check{T}\,\hat{\boldsymbol{K}}\,\check{T}^{-1} = +\hat{\boldsymbol{K}} \quad . \tag{7.32}$$

All is well!

7.2.2 Position and momentum eigenstates

We may now compute the action of $\check{T}$ on operators, but how does it act on basis states? We first consider the case in which the particles are spinless. With respect to time-reversal, one can define an orthonormal basis $|\,\psi_\mu\,\rangle$ which is defined to be real, *i.e.* for which $|\,\check{T}\,\psi_\mu\,\rangle = |\,\psi_\mu\,\rangle$. To see why this is so, consider an arbitrary basis vector $|\,\phi_\mu\,\rangle$ and form $|\,\widetilde{\psi}_\mu\,\rangle \equiv |\,\phi_\mu\,\rangle + |\,\check{T}\,\phi_\mu\,\rangle$. For spinless particles, $\check{T}^2 = 1$, hence $|\,\check{T}\,\widetilde{\psi}_\mu\,\rangle = |\,\widetilde{\psi}_\mu\,\rangle$ and $|\,\widetilde{\psi}_\mu\,\rangle$ is an eigenstate of $\check{T}$ with eigenvalue $+1$. Now consider any vector $|\,\phi_\nu\,\rangle$ satisfying $\langle\,\widetilde{\psi}_\mu\,|\,\phi_\nu\,\rangle = 0$ and form $|\,\widetilde{\psi}_\nu\,\rangle \equiv |\,\phi_\nu\,\rangle + |\,\check{T}\,\phi_\nu\,\rangle$. Then

$$\big\langle\,\widetilde{\psi}_\mu\,\big|\,\widetilde{\psi}_\nu\,\big\rangle = \big\langle\,\widetilde{\psi}_\mu\,\big|\,\check{T}\,\phi_\nu\,\big\rangle = \big\langle\,\check{T}\,\widetilde{\psi}_\mu\,\big|\,\check{T}^2\,\phi_\nu\,\big\rangle^* = \big\langle\,\widetilde{\psi}_\mu\,\big|\,\phi_\nu\,\big\rangle^* = 0 \tag{7.33}$$

because $\check{T}^2 = +1$ and $\langle\,\check{T}\,\widetilde{\psi}_\mu\,| = \langle\,\widetilde{\psi}_\mu\,|$. Followed to its conclusion (for a finite-dimensional Hilbert space), this procedure results in a complete set of mutually orthogonal vectors, which can further be normalized so as to be orthonormal, *viz.* $\langle\,\psi_\mu\,|\,\psi_\nu\,\rangle = \delta_{\mu\nu}$ with $|\,\check{T}\,\psi_\mu\,\rangle = |\,\psi_\mu\,\rangle$ for all μ. Furthermore, if $\check{T}\hat{H}\check{T} = \hat{H}$, then its matrix elements in this basis are

$$\begin{aligned} H_{\mu\nu} &= \big\langle\,\psi_\mu\,\big|\,\hat{H}\,\psi_\nu\,\big\rangle = \big\langle\,\check{T}\,\psi_\mu\,\big|\,\check{T}\hat{H}\,\psi_\nu\,\big\rangle^* \\ &= \big\langle\,\psi_\mu\,\big|\,\check{T}\hat{H}\check{T}^2\psi_\nu\,\big\rangle^* = \big\langle\,\psi_\mu\,\big|\,\check{T}\hat{H}\check{T}\,\psi_\nu\,\big\rangle^* = H^*_{\mu\nu} \quad , \end{aligned} \tag{7.34}$$

and therefore all the matrix elements $H_{\mu\nu}$ are real.

Typically this is taken to be the case for position eigenstates, $|\,\boldsymbol{r}\,\rangle$, *i.e.*

$$\big|\,\boldsymbol{r}\,\big\rangle = \big|\,\check{T}\boldsymbol{r}\,\big\rangle = \big|\,\check{T}^\dagger\boldsymbol{r}\,\big\rangle \quad , \tag{7.35}$$

and therefore

$$\begin{aligned} \big\langle\,\boldsymbol{r}\,\big|\,\check{T}\Big(\alpha\,\big|\,\phi\,\big\rangle + \beta\,\big|\,\psi\,\big\rangle\Big) &= \Big[\alpha\,\big\langle\,\check{T}^\dagger\boldsymbol{r}\,\big|\,\phi\,\big\rangle + \beta\,\big\langle\,\check{T}^\dagger\boldsymbol{r}\,\big|\,\psi\,\big\rangle\Big]^* \\ &= \alpha^*\big\langle\,\boldsymbol{r}\,\big|\,\phi\,\big\rangle^* + \beta^*\big\langle\,\boldsymbol{r}\,\big|\,\psi\,\big\rangle^* = \alpha^*\phi^*(\boldsymbol{r}) + \beta^*\psi^*(\boldsymbol{r}) \quad . \end{aligned} \tag{7.36}$$

Furthermore, if $|\,\psi\,\rangle = \int d^dr\,|\,\boldsymbol{r}\,\rangle\langle\,\boldsymbol{r}\,|\,\psi\,\rangle$, then

$$|\,\check{T}\psi\,\rangle = \check{T}\int d^dr\,\langle\,\boldsymbol{r}\,|\,\psi\,\rangle\,\check{T}^{-1}\,|\,\check{T}\boldsymbol{r}\,\rangle = \int d^dr\,|\,\boldsymbol{r}\,\rangle\,\langle\,\boldsymbol{r}\,|\,\psi\,\rangle^* \quad . \tag{7.37}$$

We also have $\check{T}\hat{H}\check{T}^{-1} = \hat{H}^*$, so if $\hat{H} = \hat{H}^*$, then $\hat{H}\,|\,\psi\,\rangle = E\,|\,\psi\,\rangle$ entails

$$\hat{H}\,\big|\,\check{T}\psi\,\big\rangle = \check{T}\hat{H}\check{T}^{-1}\,\big|\,\check{T}\psi\,\big\rangle = \check{T}\hat{H}\,\big|\,\psi\,\big\rangle = E\,\big|\,\check{T}\psi\,\big\rangle \quad , \tag{7.38}$$

and since

$$\big\langle\,\boldsymbol{r}\,\big|\,\check{T}\psi\,\big\rangle = \big\langle\,\check{T}^\dagger\boldsymbol{r}\,\big|\,\psi\,\big\rangle^* = \big\langle\,\boldsymbol{r}\,\big|\,\psi\,\big\rangle^* = \psi^*(\boldsymbol{r}) \quad , \tag{7.39}$$

if the eigenstate $|\,\psi\,\rangle$ is nondegenerate, $\psi(\boldsymbol{r})$ can be chosen to be real. This is very important, so let's say it again, this time with feeling:

- ⋆ *For spinless particles, if $\check{T}\hat{H} = \hat{H}\check{T}$, the non-degenerate eigenstates of $\hat{H}$ are real, possibly multiplied by a constant phase.*

For momentum eigenstates, we have

$$e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar} = \big\langle\,\boldsymbol{r}\,\big|\,\boldsymbol{p}\,\big\rangle = \big\langle\,\check{T}\boldsymbol{p}\,\big|\,\check{T}\boldsymbol{r}\,\big\rangle = \big\langle\,\boldsymbol{r}\,\big|\,\check{T}\boldsymbol{p}\,\big\rangle^* \quad , \tag{7.40}$$

and we conclude $|\,\check{T}\boldsymbol{p}\,\rangle = |\,\check{T}^\dagger\boldsymbol{p}\,\rangle = |\,-\boldsymbol{p}\,\rangle$. This can also be deduced from the operator transformation properties,

$$\check{T}\,\hat{\boldsymbol{r}}\,\check{T}^{-1} = +\hat{\boldsymbol{r}} \qquad , \qquad \check{T}\,\hat{\boldsymbol{p}}\,\check{T}^{-1} = -\hat{\boldsymbol{p}} \quad , \tag{7.41}$$

where the latter follows from the action of complex conjugation on $\hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla}$.

If $\hat{Q}$ is any operator with a definite signature under spinless time-reversal, *i.e.* if

$$\check{K}\,\hat{Q}\,\check{K}^{-1} = \eta_{\hat{Q}}\,\hat{Q} \tag{7.42}$$

with $\eta_{\hat{Q}} = \pm 1$, then if $\hat{H} = \hat{H}^*$ is time-reversal invariant,

$$\check{K}\,\hat{Q}(t)\,\check{K}^{-1} = \check{K}\,e^{i\hat{H}t/\hbar}\,\hat{Q}\,e^{-i\hat{H}t/\hbar}\,\check{K}^{-1} = e^{-i\hat{H}t/\hbar}\,\check{K}\,\hat{Q}\,\check{K}^{-1}\,e^{i\hat{H}t/\hbar} = \eta_{\hat{Q}}\,\hat{Q}(-t) \quad . \tag{7.43}$$

7.2.3 Change of basis for time-reversal

Recall $\check{T} = \lambda\check{K}$ with $|\lambda| = 1$. We are free to choose $\lambda = 1$, in which case $\check{T} = \check{K}$ is the complex conjugation operator. Thus far we have defined $\check{K}$ with respect to a particular $\check{T}$-invariant basis, *i.e.* the position basis[4] We could choose a different basis, $\big\{|\,n\,\rangle\big\}$, and define the action of a new time-reversal operator $\check{K}'$ as

$$\check{K}'\sum_n \psi_n\,\big|\,n\,\big\rangle = \sum_n \psi_n^*\,\big|\,n\,\big\rangle \quad . \tag{7.44}$$

[4]The "time-reversal basis" is one for which the basis states have time-reversal eigenvalue $+1$.

Since $\check{T} = \check{K}'$ and $\check{K}$ are both antilinear, they must be related by a unitary operator, *i.e.* $\check{T} = \hat{U}\check{K}$. Then

$$\check{T}^2 = \hat{U}\check{K}\hat{U}\check{K} = \hat{U}\hat{U}^* \equiv e^{i\alpha} \quad , \tag{7.45}$$

since a second time-reversal operation must restore the original state up to a phase. Thus, $e^{i\alpha}\,\hat{U}^\dagger = \hat{U}^*$, and taking the transpose we obtain $e^{i\alpha}\,\hat{U}^* = \hat{U}^\dagger$, whence $e^{2i\alpha} = 1$, which says that $\alpha = 0$ or $\alpha = \pi$. For spinless particles, as we have seen, $\check{T}^2 = +1$. In the next section, we consider the case of $S = \frac{1}{2}$.

7.2.4 Time reversal with spin

In order that the spin-orbit term in the electron Hamiltonian[5],

$$\hat{H}_{\rm SO} = \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}V\times\boldsymbol{p} \quad , \tag{7.46}$$

remain invariant under time-reversal, we must have $\check{T}\boldsymbol{\sigma}\check{T}^{-1} = -\boldsymbol{\sigma}$. With $\check{T} = \hat{U}\check{K}$,

$$\begin{aligned}\check{T}\boldsymbol{\sigma}\check{T}^{-1} &= \hat{U}\check{K}\boldsymbol{\sigma}\check{K}^{-1}\hat{U}^{-1} \\ &= \hat{U}\big(\sigma^x\,\hat{\boldsymbol{x}} - \sigma^y\,\hat{\boldsymbol{y}} + \sigma^z\,\hat{\boldsymbol{z}}\big)\,\hat{U}^\dagger = -\boldsymbol{\sigma} \quad .\end{aligned} \tag{7.47}$$

Thus, $\hat{U}\sigma^x\hat{U}^\dagger = -\sigma^x$, $\hat{U}\sigma^y\hat{U}^\dagger = +\sigma^y$, $\hat{U}\sigma^z\hat{U}^\dagger = -\sigma^z$, and $\hat{U} = e^{i\beta}\sigma^y$ is a solution, where $e^{i\beta}$ is an arbitrary phase, which we may take to be i, so that $U = i\sigma^y \in \mathsf{SU}(2)$ has unit determinant. We now have

$$\check{T}^2 = (i\sigma^y)\,\check{K}\,(i\sigma^y)\,\check{K} = (i\sigma^y)^2 = -1 \quad . \tag{7.48}$$

For N spins each with $S = \frac{1}{2}$,

$$\check{T} = (i\sigma_1^y)\cdots(i\sigma_N^y)\,\check{K} \tag{7.49}$$

and $\check{T}^2 = (-1)^N$. Note that $\prod_{n=1}^N (i\sigma_n^y) = \exp(i\pi S^y/\hbar)$ corresponds to a rotation by π of all the spins about the y-axis in internal space.

Now consider the case of general angular momentum $\hat{\boldsymbol{J}}$, with $\hat{\boldsymbol{J}}^2 = \hbar^2 j(j+1)$. We have $\check{T}\hat{\boldsymbol{J}}\check{T}^{-1} = -\hat{\boldsymbol{J}}$, which entails $\check{T}\hat{\boldsymbol{J}}^2\check{T}^{-1} = \hat{\boldsymbol{J}}^2$, hence $\check{T}$ preserves the j quantum number. We also have

$$\hat{J}^z\,\check{T}\,\big|\,j,m\,\big\rangle = \check{T}\,(\check{T}^{-1}\hat{J}^z\,\check{T})\,\big|\,j,m\,\big\rangle = -\hbar m\,\check{T}\,\big|\,j,m\,\big\rangle \quad , \tag{7.50}$$

from which we conclude $\check{T}\,|\,j,m\,\rangle = C_{j,m}\,|\,j,-m\,\rangle$, where $C_{j,m}$ is a complex scalar. We furthermore have

$$\begin{aligned}\hat{J}^\pm\,\check{T}\,\big|\,j,m\,\big\rangle &= -\check{T}\,\hat{J}^\mp\,\big|\,j,m\,\big\rangle = -A_\mp(j,m)\,\check{T}\,\big|\,j,m\mp1\,\big\rangle = -A_\mp(j,m)\,C_{j,m\mp1}\,\big|\,j,-m\pm1\,\big\rangle \\ &= C_{j,m}\,\hat{J}^\pm\,\big|\,j,-m\,\big\rangle = C_{j,m}\,A_\pm(j,-m)\,\big|\,j,-m\pm1\,\big\rangle \quad ,\end{aligned} \tag{7.51}$$

where $A_\pm(j,m) = A_\mp(j,-m) = \hbar\sqrt{j(j+1)-m(m\mp1)}$. Thus, we conclude $C_{j,m\mp1} = -C_{j,m}$, which we may choose to solve with the assignment $C_{j,m} = (-1)^{j+m}$. One more time, with great feeling:

$$\check{T}\,\big|\,j,m\,\big\rangle = (-1)^{j+m}\,\big|\,j,-m\,\big\rangle \quad . \tag{7.52}$$

[5]Our notation is somewhat inconsistent as we generally do not place hats on $\boldsymbol{r}$, $\boldsymbol{p}$, and $\boldsymbol{\sigma}$. That these entities function as operators on Hilbert space is taken for granted.

Thus, $\check{T} = \hat{U}\check{K}$ with $\check{K}\,\big|\,j,m\,\big\rangle = \big|\,j,m\,\big\rangle$ and

$$\hat{U} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & -1 & 0 \\ \vdots & \iddots & & \vdots & \vdots \\ (-1)^{2j} & 0 & \cdots & 0 & 0 \end{pmatrix} \tag{7.53}$$

so that

$$\check{T}^2 = \hat{U}\,\check{K}\,\hat{U}\,\check{K} = \hat{U}^2 = (-1)^{2j} \quad . \tag{7.54}$$

Therefore, in the case of a single j-quantum, we have $\check{T}^2 = +1$ or $j \in \mathbb{Z}$, and $\check{T}^2 = -1$ for $j \in \mathbb{Z} + \frac{1}{2}$. For the general case of N j-quanta, $\check{T}^2 = (-1)^{2jN}$.

7.2.5 Kramers degeneracy

When $\big[\check{T}, \hat{H}\big] = 0$ and $\check{T}^2 = -1$, all states in the eigenspectrum of $\hat{H}$ are evenfold degenerate. We prove this by showing that $|\,\psi\,\rangle$ and $|\,\check{T}\psi\,\rangle$ are degenerate and orthogonal. The proof of degeneracy is provided in Eqn. 7.38. As to orthogonality,

$$\big\langle\,\psi\,\big|\,\check{T}\psi\,\big\rangle = \big\langle\,\check{T}\psi\,\big|\,\check{T}^2\psi\,\big\rangle^* = -\big\langle\,\check{T}\psi\,\big|\,\psi\,\big\rangle^* = -\big\langle\,\psi\,\big|\,\check{T}\psi\,\big\rangle \quad , \tag{7.55}$$

and therefore $\langle\,\psi\,|\,\check{T}\psi\,\rangle = 0$. Thus, the dimension of Hilbert space must be even. For N spin-$\frac{1}{2}$ objects, this requires N odd, *i.e.* the total spin $S_{\rm tot}$ is a half odd integer.

In the absence of $\hat{H}_{\rm SO}$, we are free to define $\check{T} = \check{K}$ even though electrons have $S = \frac{1}{2}$. The reasoning is the same as that which permitted us to use the ordinary point group and not the double group in such circumstances. In the context of time-reversal, $\big[\check{K}, \hat{H}\big] = 0$ in the absence of $\hat{H}_{\rm SO}$, so we are free to classify states by their properties with respect to $\check{K}$ alone.

7.2.6 External fields

In the presence of external fields, the one electron Hamiltonian is given by

$$\begin{aligned} \hat{H} = \frac{1}{2m}\big(\boldsymbol{p} + \tfrac{e}{c}\boldsymbol{A}\big)^2 + V(\boldsymbol{r}) + \frac{e\hbar}{2mc}\,\boldsymbol{\sigma}\cdot\boldsymbol{B} \\ + \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}V\times\big(\boldsymbol{p} + \tfrac{e}{c}\boldsymbol{A}\big) + \frac{\hbar^2}{8m^2c^2}\,\nabla^2 V + \mathcal{O}(m^{-3}) \quad , \end{aligned} \tag{7.56}$$

where $V(\boldsymbol{r}) = -e\,\phi(\boldsymbol{r})$, $\boldsymbol{E} = -\boldsymbol{\nabla}\phi$, and $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$. Beyond the kinetic and potential energy terms in this expression, we have, respectively, the Zeeman and spin-orbit terms, both of which involve the electron's spin, and the Darwin term, which in the presence of a potential $V(\boldsymbol{r}) = -Ze^2/r$ is proportional to $\nabla^2(1/r) = -4\pi\,\delta(\boldsymbol{r})$. In general $\phi(\boldsymbol{r})$ is generated by an external charge density $\rho(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r})$ by an external current density $\boldsymbol{j}(\boldsymbol{r})$. Where do all these terms come from, by the way? From the Dirac equation, of course:

$$i\hbar\,\frac{\partial\Psi}{\partial t} = \begin{pmatrix} mc^2 + V & c\,\boldsymbol{\sigma}\cdot\big(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\big) \\ c\,\boldsymbol{\sigma}\cdot\big(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\big) & -mc^2 + V \end{pmatrix}\Psi \quad . \tag{7.57}$$

The wavefunction Ψ is a four-component Dirac spinor; each of the entries in the above Hamiltonian matrix is a 2×2 subblock. Since mc^2 is the largest energy scale in town, the coupling between the upper two "positive energy" components and the lower two "negative energy" components is relatively weak, and can be eliminated order by order in $(mc^2)^{-1}$ by successive canonical transformations of the type discussed in §6.7. This procedure is known as the *Foldy-Wouthuysen transformation* and is described in standard texts of yore such as Bjorken and Drell (see the Appendix §7.6 for a derivation). The Dirac equation is of course wrong[6], and the real theory of electrons interacting with photons is given by quantum electrodynamics. Thus the g-factor multiplying $(e/2mc)\,\boldsymbol{B}\cdot\boldsymbol{S}$, where $\boldsymbol{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$, is $g = 2$, which is the "tree level" value. Radiative corrections, calculable within QED, lead to $g = 2 + \frac{\alpha}{\pi} + \mathcal{O}(\alpha^2)$, where $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant. But I digress.

The Hamiltonian $\hat{H}^T = \check{T}\hat{H}\check{T}^{-1}$ is invariant under time-reversal provided

$$\rho^T(\boldsymbol{r},t) = \rho(\boldsymbol{r},-t) \quad , \quad \boldsymbol{j}^T(\boldsymbol{r},t) = -\boldsymbol{j}(\boldsymbol{r},-t) \tag{7.58}$$

$$\phi^T(\boldsymbol{r},t) = \phi(\boldsymbol{r},-t) \quad , \quad \boldsymbol{A}^T(\boldsymbol{r},t) = -\boldsymbol{A}(\boldsymbol{r},-t) \tag{7.59}$$

$$\boldsymbol{E}^T(\boldsymbol{r},t) = \boldsymbol{E}(\boldsymbol{r},-t) \quad , \quad \boldsymbol{B}^T(\boldsymbol{r},t) = -\boldsymbol{B}(\boldsymbol{r},-t) \quad , \tag{7.60}$$

where the conditions on ϕ and $\boldsymbol{A}$ are of course true up to a gauge transformation. We then have $\hat{H}^T(\boldsymbol{E},\boldsymbol{B}) = \hat{H}(\boldsymbol{E}^T,\boldsymbol{B}^T)$ and $\psi^T(t\,;\,\boldsymbol{E},\boldsymbol{B}) = \hat{U}\check{K}\psi(-t\,;\,\boldsymbol{E}^T,\boldsymbol{B}^T)$.

7.3 Time Reversal and Point Group Symmetries

All point group operations $\hat{g} \equiv \hat{U}(g)$ commute with time-reversal: $\big[\check{T},\hat{g}\big] = 0$. The reason is that proper point group operations are rotations, hence $\hat{g} = \exp\big(-i\xi\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{J}}/\hbar\big)$, and $\check{T}\,i\hat{\boldsymbol{J}}\,\check{T}^{-1} = i\hat{\boldsymbol{J}}$. The improper operations include spatial inversion $\hat{I}$, which also commutes with $\check{T}$.

Consider the case of a particle of total spin j subjected to point group operations. We have

(i) $\check{T}^2 = +1$, $j = 0$: The time-reversal operator is then simply complex conjugation, *i.e.* $\check{T} = \check{K}$. Consider any complex scalar basis function $\psi(\boldsymbol{r})$. Then

$$\check{T}\,\hat{g}\,\psi(\boldsymbol{r}) = \hat{g}\,\check{T}\,\psi(\boldsymbol{r}) = \psi^*(\boldsymbol{r}g) \quad . \tag{7.61}$$

(ii) $\check{T}^2 = -1$, $j = \frac{1}{2}$: The time-reversal operator is $\hat{T} = i\sigma^y\check{K}$, and we write the wavefunction as a two-component column vector, with $\psi^{\mathsf{T}}(\boldsymbol{r}) = \big(\psi_\uparrow(\boldsymbol{r})\,,\,\psi_\downarrow(\boldsymbol{r})\big)$. Then it can be shown that

$$\check{T}\,\hat{g}\,\psi(\boldsymbol{r}) = \hat{g}\,\check{T}\,\psi(\boldsymbol{r}) = i\sigma^y\left[D^{1/2}(g)\right]^*\begin{pmatrix}\psi^*_\uparrow(\boldsymbol{r}g)\\ \psi^*_\downarrow(\boldsymbol{r}g)\end{pmatrix} \quad . \tag{7.62}$$

The essential step in establishing the above result is to show $\sigma^y D^{1/2}(g)\,\sigma^y = \big[D^{1/2}(g)\big]^*$, which is left as an exercise for the student.

[6] With respect to QED, the Dirac equation is correct "at tree level".

(iii) For general j, one has $\psi^{\mathsf{T}}(\boldsymbol{r}) = \big(\psi_m(\boldsymbol{r})\ ,\ \ldots\ ,\ \psi_{-m}(\boldsymbol{r})\big)$, and

$$\check{T}\,\hat{g}\,\psi(\boldsymbol{r}) = \hat{g}\,\check{T}\,\psi(\boldsymbol{r}) = \psi^{T}(\boldsymbol{r}g) \tag{7.63}$$

whose components are given by

$$\psi^{T}_{m}(\boldsymbol{r}g) = (-1)^{j-m}\left[D^{j}_{-m,m'}(g)\right]^{*}\psi^{*}_{m'}(\boldsymbol{r}g) \quad . \tag{7.64}$$

This is readily derived using the definition and properties of rotation matrices, discussed in §4.3.2.

7.3.1 Complex conjugate representations

Suppose $|\,\psi^{\Gamma}_{\mu}\,\rangle$ for $\mu \in \{1,\ldots,d_{\Gamma}\}$ are basis vectors for an invariant subspace $\mathcal{V}^{\Gamma}$ transforming according to a representation Γ of the point group G. Then combining point group and time-reversal operations yields

$$\hat{g}\,\big|\,\check{T}\,\psi^{\Gamma}_{\nu}\,\big\rangle = \check{T}\,\hat{g}\,\big|\,\psi^{\Gamma}_{\nu}\,\big\rangle = \check{T}\,\Big[\,\big|\,\psi^{\Gamma}_{\mu}\,\big\rangle\,D^{\Gamma}_{\mu\nu}(g)\Big] = \big|\,\check{T}\,\psi^{\Gamma}_{\mu}\,\big\rangle\,D^{\Gamma^*}_{\mu\nu}(g) \quad . \tag{7.65}$$

This tells us that the basis vectors $|\,\check{T}\psi^{\Gamma}_{\mu}\,\rangle$ transform as the complex conjugate representation Γ^*. In §2.5, we discussed the significance of the Frobenius-Schur indicator,

$$\varepsilon_{\Gamma} = \frac{1}{N_G}\sum_{g\in G}\chi^{\Gamma}(g^2) \quad , \tag{7.66}$$

which takes the values $\varepsilon_{\Gamma} \in \{-1,0,+1\}$, in determining whether a given IRREP can be made real, *i.e.* whether it is equivalent to one whose representation matrices are all real. We found

(i) $\varepsilon_{\Gamma} = +1$: The representation matrices $D^{\Gamma}(G)$ may be brought to real form by a similarity transformation $S\,D^{\Gamma}(G)\,S^{-1}$. All characters $\chi^{\Gamma}(g)$ are real. In such cases, Γ is said to be *real*.

(ii) $\varepsilon_{\Gamma} = -1$: $D^{\Gamma}(G)$ and D^{Γ^*} are equivalent, meaning they are related by a similarity transformation, but they cannot be brought to real form. All characters $\chi^{\Gamma}(g)$ are real. In such cases, Γ is said to be *pseudoreal*.

(iii) $\varepsilon_{\Gamma} = 0$: $D^{\Gamma}(G)$ and D^{Γ^*} are inequivalent, and $\chi^{\Gamma}(g) \notin \mathbb{R}$ for some group elements g. In such cases, Γ is said to be *complex*.

The single crystallographic point groups have no pseudoreal IRREPs. The following crystallographic groups have complex IRREPs: C_3 , C_{3h} , C_4 , C_{4h} , C_6 , C_{6h} , T, T_h. The spin IRREPs of the double point groups all have dimensions $d_{\Gamma} = 1$, 2, or 4. They are real only for the case $d_{\Gamma} = 1$. For $d_{\Gamma} = 2$ and 4, they are pseudoreal. For $\mathsf{SO}(3)$, we use the invariant measure to compute the Frobenius-Schur indicator. The invariant measure is given by

$$d\mu(\xi,\hat{\boldsymbol{n}}) = (1-\cos\xi)\,\frac{d\xi}{2\pi}\,\frac{d\hat{\boldsymbol{n}}}{4\pi} \quad , \tag{7.67}$$

hence

$$\begin{aligned}\varepsilon_j &= \frac{1}{2\pi}\int\limits_0^{2\pi} d\xi\,(1-\cos\xi)\,\chi^{(j)}(2\xi) \\ &= \frac{1}{2\pi}\int\limits_0^{2\pi} d\xi\,(1-\cos\xi)\,\frac{\sin(2j+1)\xi}{\sin\xi} = \begin{cases} +1 & \text{if } j\in\mathbb{Z} \\ -1 & \text{if } j\in\mathbb{Z}+\frac{1}{2} \end{cases} \quad .\end{aligned} \tag{7.68}$$

Does the presence of time-reversal symmetry lead to additional degeneracies in the eigenspectrum? We state the following results without proof:[7]

(i) If $\varepsilon_\Gamma\check{T}^2 = +1$, then there are no additional degeneracies. This is the case for real IRREPs when $\check{T}=+1$, and for pseudoreal IRREPs when $\check{T}^2=-1$. In the latter case, one can redefine the states so that $|\,\psi_\mu^{\Gamma^*}\,\rangle = |\,\check{T}\psi_\mu^\Gamma\,\rangle$.

(ii) If $\varepsilon_\Gamma\check{T}^2 = -1$, then there is a doubling, and $|\,\check{T}\psi_\mu^\Gamma\,\rangle$ is orthogonal to $|\,\psi_\nu^\Gamma\,\rangle$ for all μ and ν. This is the case for real IRREPs when $\check{T}^2=-1$ and for pseudoreal IRREPs when $\check{T}^2=+1$. Doubling means that a given representation appears twice, with degenerate energies.

(iii) If $\varepsilon_\Gamma\check{T}^2 = 0$, the IRREPs Γ and Γ^* are inequivalent and degenerate. Such degenerate IRREPs are called *paired*.

7.3.2 Generalized time-reversal

In cases where $\big[\check{T},\hat{H}\big]\neq 0$, but $\big[\hat{r}\,\check{T},\hat{H}\big]=0$ for some point group operation $r\in G$, the following result is useful:

$$\hat{g}\,|\,\check{\Theta}\,\psi_\nu^\Gamma\,\rangle = \Big(\hat{r}\,|\,\check{\Theta}\,\psi_\mu^\Gamma\,\rangle\Big)\,D^{\Gamma^*}_{\mu\nu}(h^{-1}gh) \quad , \tag{7.69}$$

where $\check{\Theta}=\hat{r}\,\check{T}$ is an antiunitary operator which effectively stands in for time-reversal $\check{T}$. This state of affairs persists, for example, when a magnetic field $\boldsymbol{H}$ is present, which by itself breaks time-reversal symmetry, but there is a point group operation $\hat{r}$, such as a twofold axis perpendicular to $\boldsymbol{H}$ or a mirror plane containing $\boldsymbol{H}$[8], both of which reverse $\boldsymbol{H}$. Thus $\check{\Theta}$ preserves $\boldsymbol{H}$ and is a symmetry, assuming time-reversal is otherwise unbroken. Above we considered the time-reverse representation $\Gamma^T=\Gamma^*$. We denote the generalized time-reverse representation by Γ^Θ. The details are worked out in §10.6 of Lax, and we present the results in Tab. 7.1. We define

$$\widetilde{\varepsilon}_\Gamma = \frac{1}{N_G}\sum_{g\in G}\chi^\Gamma\big((rg)^2\big) \tag{7.70}$$

as well as

$$D^{\Gamma^\Theta}(g) = \big[D^\Gamma(r^{-1}gr)\big]^* \quad , \qquad \chi^{\Gamma^\Theta}(g) = \mathsf{Tr}\,D^{\Gamma^\Theta}(g) = \big[\chi^\Gamma(r^{-1}gr)\big]^* \quad . \tag{7.71}$$

[7] For a proof, see Lax §10.7.

[8] Since $\boldsymbol{H}$ is a pseudovector, it is reversed by a mirror containing $\boldsymbol{H}$ and preserved by a mirror orthogonal to $\boldsymbol{H}$.

		equivalence of representations				degeneracies	
type	$\widetilde{\varepsilon}_\Gamma$	$\chi^{\Gamma^\Theta} = \chi^\Gamma$?	$D^{\Gamma^\Theta} = S^{-1} D^\Gamma S$?	S symmetry	$D^{\Gamma^\Theta} = D^\Gamma$?	$\check{T}^2 = +1$	$\check{T}^2 = -1$
1	$+1$	yes	yes	$S = D^\Gamma(r^2)\, S^{\mathsf{T}}$	if $S^{\mathsf{T}} = S$	none	doubling
2	-1	yes	yes	$S = -D^\Gamma(r^2)\, S^{\mathsf{T}}$	if $S^{\mathsf{T}} = S$	doubling	none
3	0	no	no	none	no	pairing	pairing

Table 7.1: Representations and degeneracies for generalized time reversal $\check{\Theta} = \hat{r}\,\check{T}$.

The issue is whether a given IRREP Γ is equivalent to its generalized time-reverse Γ^Θ, as well as whether the generalized time-reversal symmetry entails any extra degeneracies in the spectrum of $\hat{H}$. Equivalence of IRREPs means that there exists a fixed matrix S with $D^{\Gamma^\Theta}(g) = S^{-1} D^\Gamma(g)\, S$ for all $g \in G$. Since we presume our representations to be unitary, S is also unitary. The analysis hinges on the value of the generalized Frobenius-Schur indicator, $\widetilde{\varepsilon}_\Gamma$, defined above in eqn. 7.70. When $r = E$, the results in Tab. 7.1 recapitulate those already stated. For the cases $\widetilde{\varepsilon}_\Gamma = \pm 1$ (types 1 and 2), the representation matrices may be made to be identical, *i.e.* $D^{\Gamma^\Theta}(g) = D^\Gamma(g)$, provided $S = S^{\mathsf{T}}$, *i.e.* if $D^\Gamma(r^2) = \widetilde{\varepsilon}_\Gamma\, D^\Gamma(E)$.

7.4 Consequences of Time-Reversal

7.4.1 Selection rules and time-reversal

Selection rules in quantum mechanics refer to symmetries which result in the vanishing of certain matrix elements of the form $V_{\alpha\beta}^{\Gamma_a\Gamma_b} = \langle\, \Psi_\alpha^{\Gamma_a} \,|\, \hat{V} \,|\, \Psi_\beta^{\Gamma_b} \,\rangle$. From the point of view of the Wigner-Eckart theorem, we may always decompose the potential $\hat{V}$ into components which transform according to IRREPs of our symmetry group, *viz.*

$$\hat{V} = \sum_{\Gamma_c,\gamma} v_{\Gamma_c,\gamma}\, \hat{Q}_\gamma^{\Gamma_c} \quad , \tag{7.72}$$

in which the various matrix elements are subject to the considerations underlying the Wigner-Eckart theorem of §3.2.5. Here we are interested in the consequences of time-reversal symmetry.

Consider a matrix element

$$\big\langle\, \Psi \,\big|\, \hat{V} \,\big|\, \Psi' \,\big\rangle = \big\langle\, \hat{V}^\dagger\, \Psi \,\big|\, \Psi' \,\big\rangle = \big\langle\, \check{T}\Psi' \,\big|\, \check{T}\hat{V}^\dagger \check{T}^{-1}\, \check{T}\Psi \,\big\rangle = \eta_V \big\langle\, \check{T}\Psi' \,\big|\, \hat{V}\, \check{T}\Psi \,\big\rangle \quad , \tag{7.73}$$

where we assume $\check{T}\, \hat{V}^\dagger\, \check{T}^{-1} = \eta_V\, \hat{V}$. Typically $\hat{V}$ will be Hermitian, *i.e.* $\hat{V} = \hat{V}^\dagger$. Suppose further that $\Psi' = \check{T}\,\Psi$ is the time-reverse mate of Ψ. If $\check{T}^2 = \varepsilon_T$ then we have

$$\big\langle\, \Psi \,\big|\, \hat{V} \,\big|\, \Psi' \,\big\rangle = \eta_V\, \varepsilon_T \big\langle\, \Psi \,\big|\, \hat{V} \,\big|\, \Psi' \,\big\rangle \quad , \tag{7.74}$$

which means $\langle\, \Psi \,|\, \hat{V} \,|\, \Psi' \,\rangle = 0$ if $\eta_V\, \varepsilon_T = -1$. This is of course to be expected.

Now consider the thermal average of some Hermitian operator, $\langle \hat{V}(t) \rangle = \mathsf{Tr}\left(\hat{\varrho}\,\hat{V}(t)\right) = \sum_n P_n \langle\, n \,|\, \hat{V}(t) \,|\, n \,\rangle$, where $\hat{\varrho}$ is the equilibrium density matrix $Z^{-1}\exp(-\beta\hat{H})$ and $P_n = Z^{-1}\exp(-\beta E_n)$. Assuming $\check{T}\,\hat{H}\,\check{T}^{-1} = \hat{H}$, we can equally well take the trace over the states $|\,\hat{T}n\,\rangle$, which are each energetically degenerate with the corresponding $|\,n\,\rangle$. Then

$$\langle\, \hat{V}(t)\,\rangle = \sum_n P_n \left\langle\, \check{T}n \,\middle|\, \hat{V}(t)\,\check{T}n \,\right\rangle = \sum_n P_n\,\eta_V \left\langle\, n \,\middle|\, \hat{V}^\dagger(-t) \,\middle|\, n \,\right\rangle = \langle\, \hat{V}(-t)\,\rangle \quad , \tag{7.75}$$

where we have used

$$\left\langle\, \check{T}n \,\middle|\, \hat{V}(t)\,\check{T}n \,\right\rangle = \left\langle\, \check{T}n \,\middle|\, \check{T}\,\overbrace{\check{T}^{-1}\,\hat{V}(t)\,\check{T}}^{\eta_V \hat{V}(-t)}\, n \,\right\rangle = \eta_V \left\langle\, \hat{V}(-t)\,n \,\middle|\, n \,\right\rangle = \left\langle\, n \,\middle|\, \hat{V}^\dagger(-t) \,\middle|\, n \,\right\rangle \quad . \tag{7.76}$$

More generally, time-reversal symmetry has the following consequences,

$$\langle\, \hat{A}(t)\,\hat{B}(0)\,\rangle = \eta_A\,\eta_B\,\langle\, \hat{B}(0)\,\hat{A}(-t)\,\rangle \quad , \tag{7.77}$$

which leads us to the following discussion.

7.4.2 Onsager reciprocity

Now consider a general quantum mechanical system with a Hamiltonian $\hat{H}_0$ subjected to a time-dependent perturbation, $\hat{H}_1(t)$, where

$$\hat{H}_1(t) = -\sum_i \hat{Q}_i\,\phi_i(t)\ . \tag{7.78}$$

Here, the $\{\hat{Q}_i\}$ are a set of Hermitian operators, and the $\{\phi_i(t)\}$ are fields or potentials. Some examples:

$$\hat{H}_1(t) = \begin{cases} -\hat{\boldsymbol{M}}\cdot\boldsymbol{B}(t) & \text{magnetic moment – magnetic field} \\ \int d^3r\,\hat{\varrho}(\boldsymbol{r})\,\phi(\boldsymbol{r},t) & \text{density – scalar potential} \\ -\frac{1}{c}\int d^3r\,\hat{\boldsymbol{j}}(\boldsymbol{r})\cdot\boldsymbol{A}(\boldsymbol{r},t) & \text{electromagnetic current – vector potential} \end{cases}$$

We now ask, what is $\langle \hat{Q}_i(t)\rangle$? We assume that the lowest order response is linear, *i.e.*

$$\langle \hat{Q}_i(t)\rangle = \int\limits_{-\infty}^{\infty} \chi_{ij}(t-t')\,\phi_j(t') + \mathcal{O}(\phi_k\,\phi_l)\ . \tag{7.79}$$

Note that we assume that the $\mathcal{O}(\phi^0)$ term vanishes, which can be assured with a judicious choice of the $\{Q_i\}$[9]. We also assume that the responses are all causal, *i.e.* $\chi_{ij}(t-t') = 0$ for $t < t'$. To compute $\chi_{ij}(t-t')$, we will use first order perturbation theory to obtain $\langle \hat{Q}_i(t)\rangle$ and then functionally differentiate with respect to $\phi_j(t')$:

$$\chi_{ij}(t-t') = \frac{\delta\left\langle \hat{Q}_i(t)\right\rangle}{\delta\phi_j(t')}\ . \tag{7.80}$$

[9]If not, define $\delta\hat{Q}_i \equiv \hat{Q}_i - \langle\hat{Q}_i\rangle_0$ and consider $\langle\delta\hat{Q}_i(t)\rangle$.

The first step is to establish the result,

$$\big|\,\Psi(t)\,\big\rangle = \mathcal{T}\,\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\Big[\hat{H}_0 + \hat{H}_1(t')\Big]\right\}\big|\,\Psi(t_0)\,\big\rangle\,, \tag{7.81}$$

where $\mathcal{T}$ is the *time ordering operator*, which places earlier times to the right. This is easily derived starting with the Schrödinger equation,

$$i\hbar\frac{d}{dt}\big|\,\Psi(t)\,\big\rangle = \hat{H}(t)\big|\,\Psi(t)\,\big\rangle\,, \tag{7.82}$$

where $\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$. Integrating this equation from t to $t + dt$ gives

$$\begin{aligned}\big|\,\Psi(t+dt)\,\big\rangle &= \left(1 - \frac{i}{\hbar}\hat{H}(t)\,dt\right)\big|\,\Psi(t)\,\big\rangle \\ \big|\,\Psi(t_0 + N\,dt)\,\big\rangle &= \left(1 - \frac{i}{\hbar}\hat{H}\big(t_0 + (N-1)\,dt\big)\right)\cdots\left(1 - \frac{i}{\hbar}\hat{H}(t_0)\right)\big|\,\Psi(t_0)\,\big\rangle\,,\end{aligned} \tag{7.83}$$

hence

$$\big|\,\Psi(t_2)\,\big\rangle = U(t_2,t_1)\,\big|\,\Psi(t_1)\,\big\rangle \tag{7.84}$$

where

$$\hat{U}(t_2,t_1) = \mathcal{T}\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt\,\hat{H}(t)\right\} \tag{7.85}$$

is a unitary linear operator, known as the *time evolution operator* between times t_1 and t_2. It satisfies a composition law, $U(t_3,t_1) = U(t_3,t_2)\,U(t_2,t_1)$.

If $t_1 < t < t_2$, then differentiating $\hat{U}(t_2,t_1)$ with respect to $\phi_i(t)$ yields

$$\frac{\delta\hat{U}(t_2,t_1)}{\delta\phi_j(t)} = \frac{i}{\hbar}\,\hat{U}(t_2,t)\,\hat{Q}_j\,\hat{U}(t,t_1)\,, \tag{7.86}$$

since $\partial\hat{H}(t)/\partial\phi_j(t) = -\hat{Q}_j$. We may therefore write (assuming $t_0 < t, t'$)

$$\begin{aligned}\left.\frac{\delta\,|\,\Psi(t)\,\rangle}{\delta\phi_j(t')}\right|_{\{\phi_i=0\}} &= \frac{i}{\hbar}\,e^{-i\hat{H}_0(t-t')/\hbar}\,\hat{Q}_j\,e^{-i\hat{H}_0(t'-t_0)/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\,\Theta(t-t') \\ &= \frac{i}{\hbar}\,e^{-i\hat{H}_0 t/\hbar}\,\hat{Q}_j(t')\,e^{+i\hat{H}_0\,t_0/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\,\Theta(t-t')\,,\end{aligned} \tag{7.87}$$

where

$$\hat{Q}_j(t) \equiv e^{i\hat{H}_0 t/\hbar}\,\hat{Q}_j\,e^{-i\hat{H}_0 t/\hbar} \tag{7.88}$$

is the operator $\hat{Q}_j$ in the time-dependent *interaction representation*. Finally, we have

$$\begin{aligned}\chi_{ij}(t-t') &= \frac{\delta}{\delta\phi_j(t')}\big\langle\,\Psi(t)\,\big|\,\hat{Q}_i\,\big|\,\Psi(t)\,\big\rangle = \frac{\delta\,\langle\,\Psi(t)\,|}{\delta\phi_j(t')}\,\hat{Q}_i\,\big|\,\Psi(t)\,\big\rangle + \big\langle\,\Psi(t)\,\big|\,\hat{Q}_i\,\frac{\delta\,|\,\Psi(t)\,\rangle}{\delta\phi_j(t')} \\ &= \left\{-\frac{i}{\hbar}\big\langle\,\Psi(t_0)\,\big|\,e^{-i\hat{H}_0 t_0/\hbar}\,\hat{Q}_j(t')\,e^{+i\hat{H}_0 t/\hbar}\,\hat{Q}_i\,\big|\,\Psi(t)\,\big\rangle\right. \\ &\qquad\left. + \frac{i}{\hbar}\,\big\langle\,\Psi(t)\,\big|\,\hat{Q}_i\,e^{-i\hat{H}_0 t/\hbar}\,\hat{Q}_j(t')\,e^{+i\hat{H}_0 t_0/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\right\}\Theta(t-t') \\ &= \frac{i}{\hbar}\,\big\langle\big[\hat{Q}_i(t),\hat{Q}_j(t')\big]\big\rangle\,\Theta(t-t')\,,\end{aligned} \tag{7.89}$$

were averages are with respect to the wavefunction $|\,\Psi\,\rangle \equiv \exp(-i\hat{H}_0\,t_0/\hbar)\,|\,\Psi(t_0)\,\rangle$, with $t_0 \to -\infty$. This is sometimes known as the *retarded* response function. This result is valid at finite temperature if we take the bracket $\langle\cdots\rangle$ to denote thermal averaging, *viz.*

$$\begin{aligned}\chi_{ij}(t-t') &= \frac{i}{\hbar}\sum_m P_m \,\langle\, m \,|\, \big[\hat{Q}_i(t), \hat{Q}_j(t')\big] \,|\, m\,\rangle\,\Theta(t-t') \\ &= \frac{i}{\hbar}\sum_{m,n} P_m \Big\{ \langle\, m \,|\, \hat{Q}_i(t) \,|\, n\,\rangle\langle\, n \,|\, \hat{Q}_j(t') \,|\, m\,\rangle - \langle\, m \,|\, \hat{Q}_j(t') \,|\, n\,\rangle\langle\, n \,|\, \hat{Q}_i(t) \,|\, m\,\rangle \Big\}\,\Theta(t-t') \quad .\end{aligned} \tag{7.90}$$

Now the sums over states $|\,m\,\rangle$ and $|\,n\,\rangle$ can equally well be performed over their time-reverses $|\,\check{T}m\,\rangle$ and $|\,\check{T}n\,\rangle$. Assuming $\mathcal{H}_0$ is time-reversal invariant, the energy spectrum is identical. Note then that

$$\begin{aligned}\langle\, \check{T}m \,|\, \hat{Q}_i(t)\,\check{T}n\,\rangle\langle\, \check{T}n \,|\, \hat{Q}_j(t')\,\check{T}m\,\rangle &= \langle\, \check{T}^{-1}\hat{Q}_i(t)\check{T}\,n \,|\, m\,\rangle\langle\, \check{T}^{-1}\hat{Q}_j(t')\check{T}\,m \,|\, n\,\rangle \\ &= \eta_i\,\eta_j\,\langle\, \hat{Q}_i(-t)\,n \,|\, m\,\rangle\langle\, \hat{Q}_j(-t')\,m \,|\, n\,\rangle \\ &= \eta_i\,\eta_j\,\langle\, m \,|\, Q_j^\dagger(-t') \,|\, n\,\rangle\langle\, n \,|\, \hat{Q}_i^\dagger(-t) \,|\, m\,\rangle \quad ,\end{aligned} \tag{7.91}$$

where

$$\check{T}^{-1}\,\hat{Q}_i(t)\,\check{T} = \check{T}^{-1}\,e^{i\hat{H}_0 t/\hbar}\,\hat{Q}_i\,e^{-i\hat{H}_0 t/\hbar}\,\check{T} = e^{-i\hat{H}_0 t/\hbar}\,\check{T}^{-1}\,\hat{Q}_i\,\check{T}\,e^{+i\hat{H}_0 t/\hbar} = \eta_i\,\hat{Q}_i(-t) \quad . \tag{7.92}$$

Here, $\eta_i = \pm 1$ is the signature of the operator $\hat{Q}_i$ under time-reversal. Appealing now to hermiticity of $\hat{Q}_i$, we have

$$\chi_{ij}(t-t') = \frac{i}{\hbar}\,\eta_i\,\eta_j\,\langle\big[\hat{Q}_j(-t'), \hat{Q}_i(-t)\big]\rangle\,\Theta(t-t') = \eta_i\,\eta_j\,\chi_{ji}(t-t') \quad , \tag{7.93}$$

where we have also appealed to time translation invariance. The above relation is a consequence of time-reversal invariance, and is known as *Onsager reciprocity*. In the frequency domain, the linear response of a system to a finite frequency perturbations $\phi_j(\omega)$ is given by $\langle\hat{Q}_i(\omega)\rangle = \chi_{ij}(\omega)\,\phi_j(\omega)$.

We have assumed here that $\check{T}\hat{H}_0\check{T}^{-1} = \hat{H}_0$. Suppose though that $\hat{H}_0 = \hat{H}_0(\boldsymbol{H})$ where $\boldsymbol{H}$ is a magnetic field, which reverses under time-reversal. Then the derivation goes through as before, with the important *caveat* that $\hat{H}_0(\boldsymbol{H})$ must be replaced by $\hat{H}_0(-\boldsymbol{H})$ after time-reversal. The statement of Onsager reciprocity is then

$$\chi_{ij}(t-t') = \eta_i\,\eta_j\,\chi^T_{ji}(t-t') \quad , \tag{7.94}$$

where $\chi_{ij}(t-t')$ is the response function for a system with Hamiltonian $\hat{H}_0(\boldsymbol{H})$, and $\chi^T_{ji}(t-t')$ is the response function for a system with Hamiltonian $\hat{H}_0(-\boldsymbol{H})$.

7.5 Color groups

Cesium chloride is a cubic structure in which the Cs and Cl ions lie on interpenetrating simple cubic lattices. Its space group is $Pm\overline{3}m$, and consists of operations $\{\, g \,|\, \boldsymbol{R}\,\}$ where $g \in O_h$ and $\boldsymbol{R}$ is a simple cubic direct lattice vector. We could also describe the symmetries of CsCl by including another space

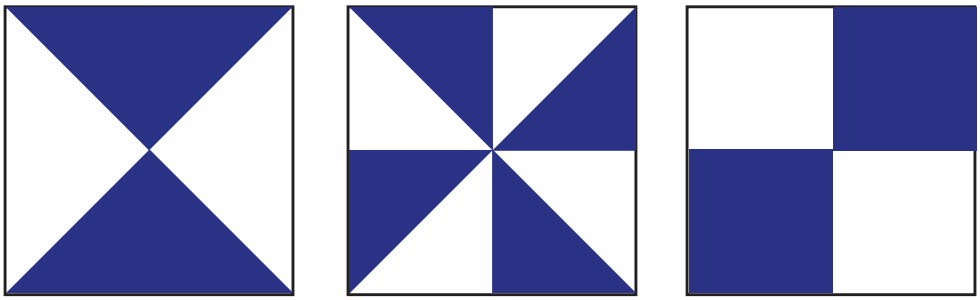


Figure 7.1: Colored squares and their magnetic point group symmetries.

group generator $\{\,\theta\,|\,\boldsymbol{\tau}\,\}$, where $\boldsymbol{\tau} = \frac{1}{2}(\boldsymbol{a}_1 + \boldsymbol{a}_2 + \boldsymbol{a}_3)$ translates from a corner to a center of any cubic cell, and θ is an alchemy operation which converts Cs to Cl and vice versa. Thus $\theta^2 = E$.

Consider the symmetries of the three colored squares in Fig. 7.1. The symmetry of an uncolored square is C_{4v}, which has eight elements: $\{E, C_2, 2C_4, 2\sigma_v, 2\sigma_d\}$. In the figure, the square on the left is symmetric under the subgroup $\{E, C_2, 2\sigma_v\}$, but any of the operations $\{2C_4, 2\sigma_d\}$ is a symmetry only if they are accompanied by an operation θ which exchanges blue and white; again $\theta^2 = E$. Thus, it is symmetric under the operations of the *magnetic point group*[10]

$$4'm'm = \{E, C_2, 2\sigma_v, 2\theta C_4, 2\theta\sigma_d\} \quad . \tag{7.95}$$

The square in the center is symmetric under the subgroup $\{E, C_2, 2C_4\}$ and under $\{2\theta\sigma_v, 2\theta\sigma_d\}$, which altogether constitute the magnetic point group $4m'm'$:

$$4m'm' = \{E, C_2, 2C_4, 2\theta\sigma_v, 2\theta\sigma_d\} \quad . \tag{7.96}$$

Finally, the square on the right is symmetric under the subgroup $\{E, C_2, 2\sigma_d\}$ and under $\{2\theta C_4, 2\theta\sigma_v\}$, which altogether constitute the magnetic point group $4mm'$:

$$4'mm' = \{E, C_2, 2\sigma_v, 2\theta C_4, 2\theta\sigma_d\} \quad . \tag{7.97}$$

Since $4'mm'$ and $4m'm$ differ only by swapping the mirrors, they are equivalent, as can be seen by redefining their respective unit cells after a 45° rotation. We shall comment on the significance of the primes presently (astute students should be able to infer their meaning!).

Let $\mathcal{P}$ be an ordinary point group which we wish to extend to a magnetic point group $\mathcal{P}_{\rm M}$. It is easy to see that there are only the following three possibilities:

(i) No group operations involve color changes and $\mathcal{P}_{\rm M} = \mathcal{P}$. Such magnetic point groups are *uncolored*. Uncolored point groups describe nonmagnetic structures, or ferromagnets where all the local moments are of the same polarization ("color").

[10] See Mirman [1999], Joshua [1991], V. Kopský, *Symmetry* **7**, 135 (2015) and R. Lifshitz, *Magnetic Point Groups and Space Groups* in *Encyclopedia of Condensed Matter* **3**, 219 (Elsevier, 2005).

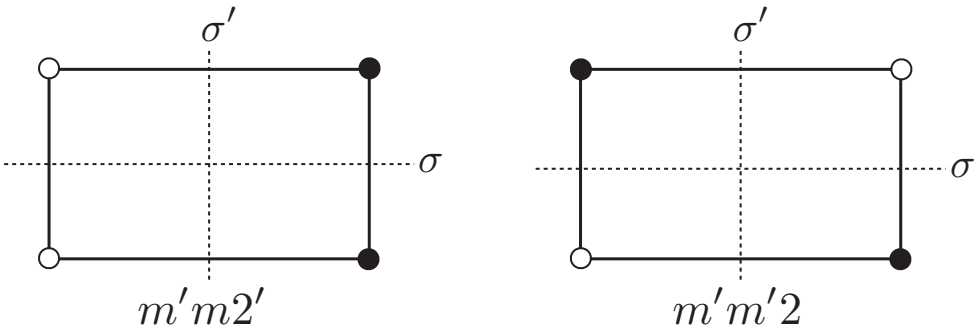


Figure 7.2: The two magnetic point groups deriving from $C_{2v} = mm2$. A black dot indicates spin polarization $m = +j$ and a white dot indicates a spin polarization $m = -j$, with $j \in \mathbb{Z}$.

(ii) To every element $g \in \mathcal{P}$ corresponds an element $\theta\, g \in \mathcal{P}_{\rm M}$. Thus $\mathcal{P}_{\rm M} = \mathcal{P} \times 1'$ where $1' = \{E, \theta\}$ is a $\mathbb{Z}_2$ clone. Such magnetic point groups are called *grey*. Note that $\theta \in \mathcal{P}_{\rm M}$ for all grey groups, which cannot be a symmetry element for any site group $\mathcal{P}_{\rm M}(\boldsymbol{r})$, because it changes the color on each site. However, coupled with lattice translations, the θ operation does appear in space group elements. For example, consider the one-dimensional antiferromagnet consisting of identical atoms whose local moments are arranged as $\big|\, \cdots \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow \cdots \,\big\rangle$. Then if τ is half the wavelength of the spin pattern, *i.e.* the distance between consecutive $\uparrow$ and $\downarrow$ sites, $\big\{\, \theta \,\big|\, \tau \,\big\} \in \mathcal{S}_{\rm M}$ is an element of the magnetic space group and then by definition $\theta \in \mathcal{P}_{\rm M}$ is in the magnetic point group. The situation is roughly analogous to the status of the inversion operation I in diamond. The maximally symmetric site group for diamond is T_d, which does not contain I. But diamond is nonsymmorphic and $\big\{\, I \,\big|\, \boldsymbol{\tau}_I \,\big\} \in \mathcal{S}$ is in diamond's space group $Fd\overline{3}m$. Clearly this state of affairs requires translational symmetries and thus grey groups do not occur in finite systems such as molecules. Grey groups have twice the number of elements as their corresponding ordinary point groups.

(iii) Suppose $\mathcal{P}$ has a normal subgroup $\mathcal{B}$ of index two, which means that $\mathcal{P} = \mathcal{B} \cup (\mathcal{P} - \mathcal{B})$ and furthermore that $\mathcal{P} - \mathcal{B} = u\mathcal{B}$ for any $u \notin \mathcal{B}$. Thus the order $N_{\mathcal{P}}$ is even, and both $\mathcal{B}$ and $\mathcal{P} - \mathcal{B}$ contain $\frac{1}{2}N_{\mathcal{P}}$ elements. Now form the group $\mathcal{P}_{\rm M} = \mathcal{B} \cup \theta(\mathcal{P} - \mathcal{B})$, whose order is also $N_{\mathcal{P}}$ This is the familiar coset construction via Lagrange's theorem which we discussed in the dim and distant past (see §1.3.1). How do we find which point groups have normal subgroups of order two? Check the character tables for their one-dimensional representations other than the trivial IRREP. Such one-dimensional IRREPs will necessarily have $\chi^{\Gamma}(g) = -1$ for half the group elements, and the classes for which $\chi^{\Gamma}(\mathcal{C}) = +1$ contain the elements of an index two normal subgroup $\mathcal{B}$. Such groups $\mathcal{P}_{\rm M}$ are called *black and white groups*.

For example, C_{4v} has three nontrivial one-dimensional IRREPs: A_2, B_1, and B_2. In A_2, the classes with $\chi^{A_2}(\mathcal{C}) = 1$ are $\{E, C_2, 2C_4\}$, whose elements form an index two normal subgroup $\boldsymbol{B}$, whence the construction of $\mathcal{P}_{\rm M} = 4m'm'$ in Eqn. 7.96. Choosing the B_1 IRREP, we find $\mathcal{B} = \{E, C_2, 2\sigma_v\}$, whence the construction of $\mathcal{P}_{\rm M} = 4'm'm$ in Eqn. 7.95. Choosing B_2 just swaps the mirrors and yields a group equivalent to $4'm'm$. Another example is shown in Fig. 7.2, which depicts the two magnetic point groups deriving from $C_{2v} = mm2$.

The notation for magnetic space groups is to place a prime on elements of the Hermann-Maugin symbol which are paired with the θ operation in order to produce a symmetry. In other words, the primed

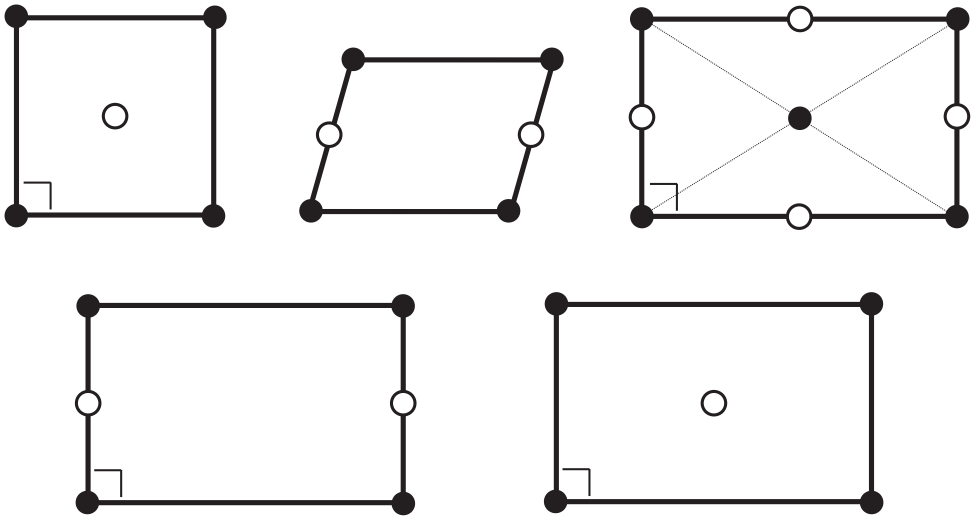


Figure 7.3: The five new black and white Bravais lattices in two dimensions. Clockwise from upper left, they derive from the square (1), oblique (1), centered rectangular (1), and rectangular (2) uncolored lattices. When the colors both fade to grey, each of these figures becomes a Bravais lattice (45° rotated square, oblique, rectangular, centered rectangular, and rectangular, respectively).

elements are those *not* in the subgroup $\mathcal{B}$.

7.5.1 Magnetic Bravais lattices and magnetic space groups

In constructing magnetic space groups, we must include translations. For ordinary space groups $\mathcal{S}$, the elements $\{ E \,|\, \boldsymbol{R} \}$ represent translations by a Bravais lattice vector $\boldsymbol{R}$. But for magnetic space groups $\mathcal{S}_{\rm M}$ we can have operations such as $\{ \theta \,|\, \boldsymbol{R} \}$, where $\boldsymbol{R}$ is a translation vector in the direct *magnetic Bravais lattice*. A magnetic Bravais lattice (or *colored lattice*) is one in which there are two sublattices, one black and one white. An important restriction is that a colored lattice must turn into a regular lattice if the colors fade, *i.e.* if the distinction between the black and white sites is removed. In two dimensions, there are five uncolored lattices (oblique, hexagonal, rectangular, centered rectangular, and square), and it turns out there are five black and white (BW) lattices, for a total of ten. In three dimensions, there are 14 uncolored lattices and 22 BW ones for a total of 36. Why are there almost double the number of BW as compared to uncolored lattices in $d = 3$? The reason is that the BW lattices have an additional primitive lattice vector $\boldsymbol{\tau}_{\rm BW}$, *i.e.* that which connects the B and W sublattices. There can be more than one possible such $\boldsymbol{\tau}_{\rm BW}$, however. The situation is roughly analogous to the different centering possibilities for cubic, tetragonal, orthorhombic, and monoclinic Bravais lattices. In Fig. 7.3 we show the additional five BW lattices which arise in two dimensions. Recall in $d = 2$ there are five lattices: oblique, hexagonal, rectangular, centered rectangular, and square. From the all-black oblique lattice, we can imagine adding white sites in the center of each plaquette or in the middle of one set of parallel edges. However these options are equivalent, as one can simply redefine the original direct lattice vectors such that one of them extends diagonally across the cell, *i.e.* replace $\boldsymbol{a}_2$ by $\boldsymbol{a}_2' = \boldsymbol{a}_1 + \boldsymbol{a}_2$. The center of the original oblique plaquette now lies at the midpoint of the side $\boldsymbol{a}_2'$. When faded, this BW lattice becomes an

oblique uncolored lattice. So we can only conjure up one additional BW lattice from the black oblique. The hexagonal case adds nothing new to what we have just derived, since the addition of a sublattice breaks the hexagonal symmetry anyway. With rectangular, we may place white sites in the center of each cell, or at the midpoint of a parallel pair of sides. When faded, the former yields a centered rectangular lattice and the latter another rectangular lattice. Attempting to place white sites at the midpoints of all sides of the rectangle does not produce a Bravais lattice when faded and is therefore not a permitted extension of the rectangular case, but it is a permitted extension of the centered rectangular case, and when faded produces a rectangular lattice. Finally, placing white sites at the centers of a pair of parallel sides of a square is equivalent to the same extension of the rectangular cell, hence yields nothing new. But placing a white site at the center of each square is permitted and leads to a θC_4 symmetry not present in any of the rectangular extensions. So there are a total of five additional BW lattices in two dimensoins. In three dimensions, to the 14 all black Bravais lattices, we get unique BW extensions from triclinic (1), monoclinic (5), orthorhombic (8), tetragonal (4), trigonal (0), hexagonal (2), and cubic (2), for a total of 22 BW extensions, and 36 colored Bravais lattices in all.

When it comes to point groups, we follow the recipe in §7.5 above. In any dimension, there is a grey (G) point group $\mathcal{P}' = \mathcal{P} \times \{E, \theta\}$ for each uncolored (U) point group $\mathcal{P}$. To create a black and white (BW) point group $\mathcal{P}_{\rm M}$, we must identify uncolored point groups $\mathcal{P}$ with normal subgroups $\mathcal{B}$ of index 2, and then construct $\mathcal{P}_{\rm M} = \mathcal{B} \cup \theta(\mathcal{P} - \mathcal{B})$. Since a given $\mathcal{P}$ may have several such maximal proper subgroups, the number of BW point groups is greater than then number of U or G point groups. In three dimensions, for example, there are 32 U and 32 G point groups, and 58 BW point groups. The latter are listed in Tab. 7.2. A summary of the numbers of U, G, and BW point groups in $d = 2$ and $d = 3$ dimensions is given in Tab. 7.3.

Next, we come to space groups. These may be build upon either uncolored or black and white Bravais lattices. For example, in $d = 3$ we have learned that there are a total of 230 uncolored space groups. For each space group $\mathcal{S}$ we can add the color changing element θ as a generator of the point group to create a grey space group $\mathcal{S}'$ with twice the number of elements of $\mathcal{S}$. There is a one-to-one correspondence between uncolored and grey groups, hence there are 230 grey space groups as well. When it comes to building the black and white space groups, if the underlying Bravais lattice is uncolored, the recipe is the same as for the point groups. That is, we start with a space group $\mathcal{S}$ generated by $\{ E \,|\, \boldsymbol{R} \}$ and $\{ g \,|\, \boldsymbol{\tau}_g \}$, where $g \in \mathcal{P} - \mathcal{B}$, and $\{ \theta\, h \,|\, \boldsymbol{\tau}_h \}$, where $h \in \mathcal{B}$. Thus results in 674 new black and white space groups. But we are not quite done! We could have started with a black and white Bravais lattice, in which case the black and white space group generators are $\{ E \,|\, \boldsymbol{R} \}$, $\{ g \,|\, \boldsymbol{\tau}_g \}$ where $g \in \mathcal{P} - \mathcal{B}$, and $\{ \theta\, h \,|\, \boldsymbol{\tau}_h + \boldsymbol{\tau}_{\rm BW} \}$ where $h \in \mathcal{B}$. This adds another 517 lattices, for a total of 1191 BW space groups. Adding this to the 230 uncolored and 230 grey space groups, we arrive at a total of 1,651 colored three-dimensional space groups, the properties of which are tabulated in a riveting 11,976 page text by D. B. Litvin, entitled *Magnetic Group Tables, Part 2* (International Union of Crystallography, 2013).

system	$\mathcal{P}^{(\mathrm{Sch})}$	$\mathcal{P}^{\mathrm{HM}}$	$N_{\mathcal{P}}$	colored point groups $\mathcal{P}_{\mathrm{M}}$
triclinic	C_1	1	1	none
	C_i	$\overline{1}$	2	$\overline{1}'$
monoclinic	C_2	2	2	$2'$
	C_s	m	2	m'
	C_{2h}	$2/m$	4	$2/m'$, $2'/m$, $2'/m'$
orthorhombic	D_2	222	4	$2'2'2$
	C_{2v}	$mm2$	4	$m'm2$, $m'm'2$
	D_{2h}	mmm	8	$m'mm$, $m'm'm$, $m'm'm'$
tetragonal	C_4	4	4	$4'$
	S_4	$\overline{4}$	4	$\overline{4}'$
	C_{4h}	$4/m$	8	$4/m'$, $4'/m$, $4'/m'$
	D_4	422	8	$4'22'$, $4'2'2'$
	C_{4v}	$4mm$	8	$4'm'm$, $4m'm'$
	D_{2d}	$\overline{4}2m$	8	$\overline{4}'2'm$, $\overline{4}'2m'$, $\overline{4}'2'm'$
	D_{4h}	$4/mmm$	16	$4/m'mm$, $4/mm'm'$, $4/m'm'm'$, $4'/mm'm$, $4'/m'm'm$
trigonal	C_3	3	3	none
	S_6	$\overline{3}$	3	$\overline{3}'$
	D_3	32	6	$32'$
	C_{3v}	$3m$	6	$3m'$
	D_{3d}	$\overline{3}m$	12	$\overline{3}'m$, $\overline{3}m'$, $\overline{3}'m'$
hexagonal	C_6	6	6	$6'$
	C_{3h}	$\overline{6}$	6	$\overline{6}'$
	C_{6h}	$6/m$	12	$6'/m$, $6/m'$, $6'/m'$
	D_6	622	12	$6'2'2$, $62'2'$
	C_{6v}	$6mm$	12	$6'm'm$, $6m'm'$
	D_{3h}	$\overline{6}m2$	12	$\overline{6}'m'2$, $\overline{6}'m2'$, $\overline{6}m'2'$
	D_{6h}	$6/mmm$	24	$6/m'mm$, $6/mm'm'$, $6/m'm'm'$, $6'/mm'm$, $6'/m'm'm$
cubic	T	23	12	none
	T_h	$m\overline{3}$	24	$m'\overline{3}$
	O	432	24	$4'32'$
	T_d	$\overline{4}3m$	24	$\overline{4}'3m'$
	O_h	$m\overline{3}m$	48	$m'\overline{3}m$, $m\overline{3}m'$, $m'\overline{3}m'$

Table 7.2: The 58 colored three-dimensional magnetic point groups.

	Bravais lattices			point groups				space groups			
	U	BW	total	U	G	BW	total	U	G	BW	total
$d = 2$	5	5	10	10	10	11	31	17	17	46	80
$d = 3$	14	22	36	32	32	58	122	230	230	1191	1651

Table 7.3: True Facts about magnetic lattices, point groups, and space groups. Notation: U (uncolored), G (grey), and BW (black and white).

7.5.2 Corepresentations of color groups

7.6 Appendix : The Foldy-Wouthuysen Transformation

The Dirac Hamiltonian is

$$H = mc^2\,\gamma^0 + c\gamma^0\,\boldsymbol{\gamma}\cdot\boldsymbol{\pi} + V \quad , \tag{7.98}$$

where $\boldsymbol{\pi} = \boldsymbol{p} + \frac{e}{c}\boldsymbol{A}$ is the dynamical momentum and where the γ^μ are the Dirac matrices,

$$\gamma^0 = \begin{pmatrix} 1_{2\times2} & 0_{2\times2} \\ 0_{2\times2} & -1_{2\times2} \end{pmatrix} \qquad , \qquad \boldsymbol{\gamma} = \begin{pmatrix} 0_{2\times2} & \boldsymbol{\sigma}_{2\times2} \\ -\boldsymbol{\sigma}_{2\times2} & 0_{2\times2} \end{pmatrix} \quad . \tag{7.99}$$

Here $\boldsymbol{\sigma}$ is the vector of Pauli matrices. The Dirac equation is

$$i\hbar\frac{d\Psi}{dt} = H\Psi \quad , \tag{7.100}$$

where Ψ is a four-component Dirac spinor.

The idea behind the FW transformation is to unitarily transform to a different Hilbert space basis such that the coupling in H between the upper and lower components of the Dirac spinor vanishes. This may be done systematically as an expansion in inverse powers of the electron mass m. We begin by defining $K \equiv c\gamma^0\boldsymbol{\gamma}\cdot\boldsymbol{\pi} + V$ so that $H = mc^2\,\gamma^0 + K$. Note that K is of order m^0. We then write

$$\widetilde{H} = e^{iS}\,H\,e^{-iS} = H + i\big[S,H\big] + \frac{(i)^2}{2!}\,\big[S,[S,H]\big] + \ldots \quad , \tag{7.101}$$

where S itself is written as a power series in $(mc^2)^{-1}$:

$$S = \frac{S_0}{mc^2} + \frac{S_1}{(mc^2)^2} + \ldots \ . \tag{7.102}$$

The job now is to write $\widetilde{H}$ as a power series in m^{-1}. The first few terms are easy to find:

$$\widetilde{H} = mc^2\,\gamma^0 + K + i\big[S_0,\gamma^0\big] + \frac{1}{mc^2}\bigg(i\big[S_0,K\big] + i\big[S_1,\gamma^0\big] - \tfrac{1}{2}\big[S_0,[S_0,\gamma^0]\big]\bigg) + \ldots \tag{7.103}$$

We choose the operators S_n so as to cancel, at each order in m^{-1}, the off-diagonal terms in $\widetilde{H}$ that couple the upper two components of Ψ to the lower two components of Ψ. To order m^0, we then demand

$$c\gamma^0\boldsymbol{\gamma}\cdot\boldsymbol{\pi} + i\big[S_0,\gamma^0\big] = 0\,. \tag{7.104}$$

Note that we do not demand that $i\big[S_0,\gamma^0\big]$ completely cancel K – indeed it is impossible to find such an S_0, and one way to see this is to take the trace. The trace of any commutator must vanish, but $\mathrm{Tr}\,K = 4V$, which is in general nonzero. But this is of no concern to us, since we only need cancel the (traceless) *off-diagonal* part of K, which is to say $c\gamma^0\boldsymbol{\gamma}\cdot\boldsymbol{\pi}$.

To solve for S_0, one can write it in terms of its four 2×2 subblocks, compute the commutator with γ^0, and then impose eqn. 7.104. One then finds $S_0 = -\frac{i}{2} c \boldsymbol{\gamma} \cdot \boldsymbol{\pi}$, the derivation of which is left as an exercise.

At the next level, we have to deal with the term in the round brackets in eqn. 7.103. Since we know S_0, we can compute the first and the third terms therein. In general, this will leave us with an off-diagonal term coupling upper and lower components of Ψ. We then choose S_1 so as to cancel this term. This calculation already is tedious, and we haven't even gotten to the spin-orbit interaction term yet, since it is of order m^{-2}.

7.6.1 Derivation of the Spin-Orbit Interaction

Here's a simpler way to proceed to order m^{-2}. Let a, b be block indices and i, j be indices within each block. Thus, the component Ψ_{ai} is the $i^{\rm th}$ component of the $a^{\rm th}$ block; $\Psi_{a=1,i=2}$ is the lower component of the upper block, *i.e.* the second component of the four-vector Ψ.

Write the Hamiltonian as

$$H = mc^2\,\tau^z + c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\,\tau^x + V(\boldsymbol{r}) \quad , \tag{7.105}$$

where τ^μ are Pauli matrices with indices a, b and σ^ν are Pauli matrices with indices i, j. The σ and τ matrices commute because they act on different indices.

A very important result regarding Pauli matrices:

$$e^{i\theta\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\tau}/2}\,\tau^\alpha\,e^{-i\theta\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\tau}/2} = n^\alpha n^\beta\,\tau^\beta + \cos\theta\,(\delta^{\alpha\beta} - n^\alpha n^\beta)\,\tau^\beta + \sin\theta\,\epsilon^{\alpha\beta\gamma}\,n^\beta\,\tau^\gamma \quad . \tag{7.106}$$

STUDENT EXERCISE: Verify and interpret the above result.

Using this result, we can write

$$A\,\tau^z + B\,\tau^x = \sqrt{A^2+B^2}\cdot e^{-i\tan^{-1}(B/A)\,\tau^y/2}\,\tau^z\,e^{i\tan^{-1}(B/A)\,\tau^y/2}\,, \tag{7.107}$$

and, for our specific purposes,

$$mc^2\,\tau^z + \boldsymbol{\sigma}\cdot\boldsymbol{\pi}\,\tau^x = \sqrt{(mc^2)^2 + (c\,\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2}\cdot U\,\tau^z\,U^\dagger \quad , \tag{7.108}$$

where $U = \exp\big(-i\tan^{-1}(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{mc})\,\tau^y/2\big)$. The fact that $\boldsymbol{\sigma}\cdot\boldsymbol{\pi}$ is an operator is no obstacle here, since it commutes with the τ^μ matrices. We can give meaning to expressions like $\tan^{-1}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}/mc)$ in terms of their Taylor series expansions.

We therefore have the result,

$$U^\dagger\,H\,U = \sqrt{(mc^2)^2 + (c\,\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2}\,\tau^z + U^\dagger\,V(\boldsymbol{r})\,U \quad . \tag{7.109}$$

The first term is diagonal in the block indices. Expanding the square root, we have

$$\begin{aligned} mc^2\sqrt{1+\Big(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{mc}\Big)^2} &= mc^2 + \frac{(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2}{2m} + \mathcal{O}(m^{-3}) \\ &= mc^2 + \frac{\boldsymbol{\pi}^2}{2m} + \frac{e\hbar}{2mc}\,\boldsymbol{B}\cdot\boldsymbol{\sigma} + \mathcal{O}(m^{-3}) \quad , \end{aligned} \tag{7.110}$$

since

$$\begin{aligned}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2 &= \sigma^\mu\sigma^\nu\,\pi^\mu\pi^\nu = (\delta^{\mu\nu} + i\epsilon^{\mu\nu\lambda}\sigma^\lambda)\,\pi^\mu\pi^\nu \\ &= \boldsymbol{\pi}^2 + \tfrac{i}{2}\epsilon^{\mu\nu\lambda}\left[p^\mu + \tfrac{e}{c}A^\mu, p^\nu + \tfrac{e}{c}A^\nu\right] \\ &= \boldsymbol{\pi}^2 + \frac{e\hbar}{c}\,\boldsymbol{B}\cdot\boldsymbol{\sigma} \quad .\end{aligned} \tag{7.111}$$

We next need to compute $U^\dagger\,V(\boldsymbol{r})\,U$ to order m^{-2}. To do this, first note that

$$U = 1 - \frac{i}{2}\,\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{mc}\,\tau^y - \frac{1}{8}\Big(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{mc}\Big)^2 + \ldots \quad , \tag{7.112}$$

Thus,

$$U^\dagger\,V\,U = V + \frac{i}{2mc}\big[\boldsymbol{\sigma}\cdot\boldsymbol{\pi}, V\big]\,\tau^y - \frac{1}{8m^2c^2}\big[\boldsymbol{\sigma}\cdot\boldsymbol{\pi}, [\boldsymbol{\sigma}\cdot\boldsymbol{\pi}, V]\big] + \ldots \quad . \tag{7.113}$$

Upon reflection, one realizes that, to this order, it suffices to take the first term in the Taylor expansion of $\tan^{-1}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}/mc)$ in the expression for U, in which case one can then invoke eqn. 7.101 to obtain the above result. The second term on the RHS of eqn. 7.113 is simply $\frac{\hbar}{2mc}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V\,\tau^y$. The third term is

$$\begin{aligned}\frac{i\hbar}{8m^2c^2}\big[\sigma^\mu\pi^\mu, \sigma^\nu\partial^\nu V\big] &= \frac{i\hbar}{8m^2c^2}\Big\{\sigma^\mu\,\big[\pi^\mu, \sigma^\nu\partial^\nu V\big] + \big[\sigma^\mu, \sigma^\nu\partial^\nu V\big]\,\pi^\mu\Big\} \\ &= \frac{i\hbar}{8m^2c^2}\Big\{\frac{\hbar}{i}\partial^\mu\partial^\nu V\,\sigma^\mu\sigma^\nu + 2i\epsilon^{\mu\nu\lambda}\sigma^\lambda\partial^\nu V\,\pi^\mu\Big\} \\ &= \frac{\hbar^2}{8m^2c^2}\,\boldsymbol{\nabla}^2 V + \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V\times\boldsymbol{\pi} \quad .\end{aligned} \tag{7.114}$$

Therefore,

$$\begin{aligned}U^\dagger\,H\,U = \left(mc^2 + \frac{\boldsymbol{\pi}^2}{2m} + \frac{e\hbar}{2mc}\,\boldsymbol{B}\cdot\boldsymbol{\sigma}\right)\tau^z + V + \frac{\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V\,\tau^y \\ + \frac{\hbar^2}{8m^2c^2}\,\boldsymbol{\nabla}^2 V + \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V\times\boldsymbol{\pi} + \mathcal{O}(m^{-3}) \quad .\end{aligned} \tag{7.115}$$

This is not block-diagonal, owing to the last term on the RHS of the top line. We can eliminate this term by effecting yet another unitary transformation. However, this will result in a contribution to the energy of order m^{-3}, so we can neglect it. To substantiate this last claim, drop all the block-diagonal terms except for the leading order one, $mc^2\,\tau^z$, and consider the Hamiltonian

$$K = mc^2\,\tau^z + \frac{\hbar}{2mc}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V\,\tau^y\,. \tag{7.116}$$

We now know how to bring this to block-diagonal form. The result is

$$\widetilde{K} = mc^2\sqrt{1 + \left(\frac{\hbar\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V}{2m^2c^3}\right)^2}\,\tau^z = \left(mc^2 + \frac{\hbar^2(\boldsymbol{\nabla}\,V)^2}{8m^3c^4} + \ldots\right)\tau^z \quad , \tag{7.117}$$

and the correction is of order m^{-3}, as promised.

We now assume all the negative energy ($\tau^z = -1$) states are filled. The Hamiltonian for the electrons, valid to $\mathcal{O}(m^{-3})$, is then

$$\widetilde{H} = mc^2 + V + \frac{\boldsymbol{\pi}^2}{2m} + \frac{e\hbar}{2mc}\,\boldsymbol{B}\cdot\boldsymbol{\sigma} + \frac{\hbar^2}{8m^2c^2}\,\boldsymbol{\nabla}^2 V + \frac{\hbar}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,V\times\boldsymbol{\pi} + \mathcal{O}(m^{-3}) \quad . \tag{7.118}$$

Chapter 8

Lie Groups and Lie Algebras, and their Representations

8.1 Mathematical Preliminaries

A *Lie group* G is a smooth manifold endowed with a group structure, such that the product $\mu : G \times G \to G$, with $\mu(g,h) = gh$, and and the inverse $\nu : G \to G$, with $\nu(g) = g^{-1}$, are also smooth. To briefly unpack some of the mathematical language, an n-dimensional *topological manifold* M is a Hausdorff topological space[1] that is everywhere locally homeomorphic to $\mathbb{R}^n$, the n-dimensional Euclidean space[2]. An *atlas* $\mathcal{A}$ is a collection of charts $\{(U_\alpha, \varphi_\alpha) \,|\, \alpha \in A\}$[3] which cover M. That is to say $M = \bigcup_\alpha U_\alpha$. An atlas is *smooth* if the functions $\varphi_\beta \circ \varphi_\alpha^{-1}$, which map $\mathbb{R}^n$ to itself, are all C^∞ (infinitely differentiable) on the overlaps $\varphi_\alpha(U_\alpha \cap U_\beta) \in \mathbb{R}^n$. Finally, a *smooth manifold* is a topological manifold with a smooth atlas[4].

The upshot of all this is that a Lie group is an n-dimensional space on which there are local coordinates $\boldsymbol{x} = \{x^1, \ldots, x^n\}$, so we can write $g = g(\boldsymbol{x})$ as a unique relation, at least within some coordinate patch (*i.e.* chart) on G. We write the inverse of this as $\boldsymbol{x}_g$, *i.e.* $g(\boldsymbol{x}_g) = g$. The identity e plays a special role, and the coordinates $\boldsymbol{x}_e$ of the identity are conventionally set to $\boldsymbol{x}_e = \boldsymbol{0}$. Note that G may not be connected, in which case its connected components are cosets. For example, $\mathsf{O}(3) = \mathsf{SO}(3) \cup I\,\mathsf{SO}(3)$, where I is inversion. In such cases each coset is described by its own coordinate system(s).

[1] A Hausdoff space M is a topological space such that for any $p, q \in M$ with $p \neq q$, there exist neighborhoods (*i.e.* open sets) U and V with $p \in U$ and $q \in V$ such that $U \cap V = \emptyset$. The collocation *topological space* M basically means a set of points $p \in M$, and, for each such p, a set of neighborhoods $\mathcal{N}(p)$ satisfying some pretty obvious axioms, such as: (i) if $N \in \mathcal{N}(p)$ then $p \in N$, (ii) if $N, N' \in \mathcal{N}(p)$, then $N \cap N' \in \mathcal{N}(p)$, *etc.*

[2] A homeomorphism is a bicontinuous bijection between topological spaces, *i.e.* a continuous function with a continuous inverse. A homeomorphism is thus a *topological* notion. A *homomorphism*, by contrast, is an *algebraic* notion, and is a map which preserves some algebraic structure, such as group multiplication. *E.g.* $\phi(A * B) = \phi(A) * \phi(B)$. A smooth homeomorphism between manifolds is called a *diffeomorphism*. To explicitly indicate the dimension of a manifold, it is conventional to add a superscript. Thus, M^m denotes an m-dimensional manifold.

[3] The set A consists of the labels α for the individual charts.

[4] More precisely, a smooth manifold is a topological manifold together with an equivalence class of smooth atlases. Two atlases $\mathcal{A}_1$ and $\mathcal{A}_2$ are said to be equivalent if their union $\mathcal{A}_1 \cup \mathcal{A}_2$ is smooth. A continuous map $F : M^m \to N^n$ is *smooth* if $\psi_\beta \circ F \circ \varphi_\alpha^{-1}$ is C^∞ wherever it is defined, where φ_α and ψ_β are coordinate systems on $U_\alpha \subset M$ and $V_\beta \subset N$, respectively.

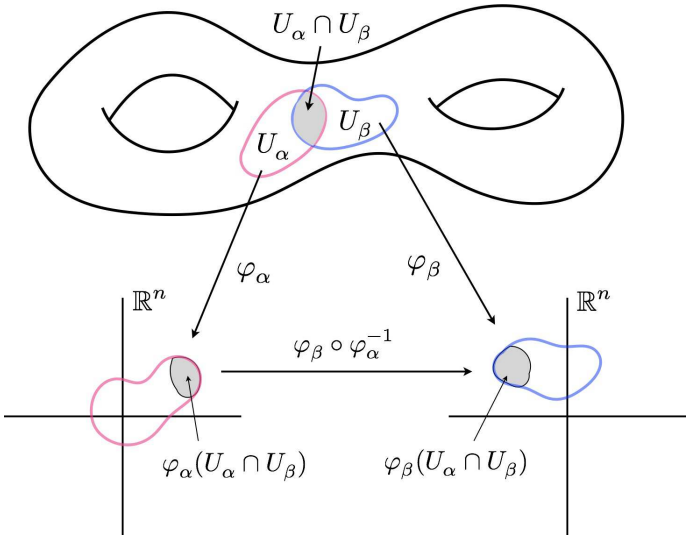


Figure 8.1: A manifold and two overlapping charts. The composition $\varphi_\beta \circ \varphi_\alpha^{-1}$ is smooth.

8.1.1 Why Lie groups are special smooth manifolds

What is special about Lie groups, as opposed to generic smooth manifolds, is of course the existence of group multiplication and group inverse operations, which relate the local properties of G in the vicinity of any $g \in G$ to those in the vicinity of the identity e. A *Lie group homomorphism* $F : G \to K$ preserves these operations, *i.e.* $F(g)\,F(h) = F(gh)$ and $F(g^{-1}) = \big(F(g)\big)^{-1}$. For all $g, h \in G$, the coordinates of their product gh are given by $\boldsymbol{x}_{gh}$. This must be depend uniquely on the coordinates $\boldsymbol{x}_g$ and $\boldsymbol{x}_h$ of g and h, respectively, *i.e.*

$$\boldsymbol{x}_{gh} = \boldsymbol{f}(\boldsymbol{x}_g, \boldsymbol{x}_h) \quad . \tag{8.1}$$

$\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y})$ is the *group composition function*[5], which we met previously in §4.3.4, where we noted its consistency conditions

$$\begin{aligned} \boldsymbol{f}\big(\boldsymbol{f}(\boldsymbol{x},\boldsymbol{y})\,,\boldsymbol{z}\big) &= \boldsymbol{f}\big(\boldsymbol{x}\,,\boldsymbol{f}(\boldsymbol{y},\boldsymbol{z})\big) \\ \boldsymbol{f}(\boldsymbol{x}_e,\boldsymbol{y}) &= \boldsymbol{f}(\boldsymbol{y},\boldsymbol{x}_e) = \boldsymbol{y} \\ \boldsymbol{f}(\boldsymbol{x},\boldsymbol{x}^{-1}) &= \boldsymbol{f}(\boldsymbol{x}^{-1},\boldsymbol{x}) = \boldsymbol{x}_e \quad . \end{aligned} \tag{8.2}$$

Here, $\boldsymbol{x}^{-1} \equiv \boldsymbol{x}_{[g(\boldsymbol{x})]^{-1}}$ are the coordinates of the group element $\big[g(\boldsymbol{x})\big]^{-1}$. Consider now a *representation* of G, which is to say a map $D : G \to \mathsf{End}(\mathcal{V})$ from G to the space of endomorphisms of a vector space $\mathcal{V}$. We will write $D(g(\boldsymbol{x})) \equiv D(\boldsymbol{x})$. Whenever we multiply a group element g, close to some g_0, by g_0^{-1}, the

[5]We have very casually assumed here the existence of global coordinates for our Lie group, *i.e.* that G is covered by a single chart. In general this may not be the case, in which case the group composition function should be appended with labels denoting the patches corresponding to g, h, and gh. The *transition functions* relating the coordinates of a given $g \in G$ in one patch to those in an overlapping patch are smooth. We should stress, though, that the Lie algebra $\mathfrak{g}$ is dependent only on the properties of G in the vicinity of the identity e, and the transition functions, derived below in eqn.8.14, can be computed within a single patch containing e.

result must lie close to e. In other words,

$$D(\boldsymbol{x}+d\boldsymbol{x})\,D(\boldsymbol{x}^{-1}) = D(\boldsymbol{x}_e + d\boldsymbol{y}) \quad , \tag{8.3}$$

where the differentials $d\boldsymbol{y}$ and $d\boldsymbol{x}$ are related by

$$\boldsymbol{x}_e + d\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}+d\boldsymbol{x}, \boldsymbol{x}^{-1}) \quad . \tag{8.4}$$

In component notation,

$$dy^b = \left.\frac{\partial f^b(\boldsymbol{x},\boldsymbol{u})}{\partial x^a}\right|_{\boldsymbol{u}=\boldsymbol{x}^{-1}} dx^a = \sum_b S_a{}^b(\boldsymbol{x})\,dx^a \quad . \tag{8.5}$$

$$S_a{}^b(\boldsymbol{x}) = \left.\frac{\partial f^b(\boldsymbol{x},\boldsymbol{u})}{\partial x^a}\right|_{\boldsymbol{u}=\boldsymbol{x}^{-1}} \quad . \tag{8.6}$$

Note that the functions $S_a{}^b(\boldsymbol{x})$ are real and representation-independent. They are, however, dependent on the choice of local coordinates of G. We then have

$$\sum_a \frac{\partial D(\boldsymbol{x})}{\partial x^a}\,D(\boldsymbol{x}^{-1})\,dx^a = \sum_b \left.\frac{\partial D(\boldsymbol{y})}{\partial y^b}\right|_{\boldsymbol{y}=\boldsymbol{x}_e} dy^b \tag{8.7}$$

We define the *generators* of the *Lie algebra* $\mathfrak{g}$ in the representation D as[6]

$$X_a = -i\,T_a \equiv \left.\frac{\partial D(\boldsymbol{x})}{\partial x^a}\right|_{\boldsymbol{x}_e} \quad . \tag{8.8}$$

Note that the number of generators is thus $n = \dim(G)$, independent of the representation D. We then have

$$\frac{\partial D(\boldsymbol{x})}{\partial x^a} = \sum_b S_a{}^b(\boldsymbol{x})\,X_b\,D(\boldsymbol{x}) \quad . \tag{8.9}$$

This establishes that the representation for a connected Lie group is completely determined by the generators of its corresponding Lie algebra. Under a change of coordinates $\boldsymbol{x} \to \tilde{\boldsymbol{x}}$, there is a linear relation between the old and new generators, *viz.*

$$\widetilde{X}_a = \frac{\partial D}{\partial \tilde{x}^a} = M_a{}^b\,X_b \qquad , \qquad M_a{}^b = \left.\frac{\partial x^b}{\partial \tilde{x}^a}\right|_{\boldsymbol{x}_e} \quad . \tag{8.10}$$

8.1.2 Structure constants

From the relation $\frac{\partial D}{\partial x^b} = S_b{}^c\,X_c\,D$ we derive

$$\begin{aligned}\frac{\partial}{\partial x^a}\left[\frac{\partial D}{\partial x^b}\,D^{-1}\right] - \frac{\partial}{\partial x^b}\left[\frac{\partial D}{\partial x^a}\,D^{-1}\right] &= \frac{\partial D}{\partial x^b}\,\frac{\partial D^{-1}}{\partial x^a} - \frac{\partial D}{\partial x^a}\,\frac{\partial D^{-1}}{\partial x^b} \\ &= \left(\frac{\partial S_b{}^c}{\partial x^a} - \frac{\partial S_a{}^c}{\partial x^b}\right) X_c\end{aligned} \tag{8.11}$$

[6]In mathematics texts, the generators are taken to be $\{X_a\}$, whereas in physics texts they are taken to be $\{T_a\}$.

On the other hand, since $D(\boldsymbol{x})D^{-1}(\boldsymbol{x}) = \mathbb{1}$ for all $\boldsymbol{x}$, taking the differential we have $dD^{-1} = -D^{-1}\,(dD)\,D^{-1}$, and the above equation becomes

$$\frac{\partial D}{\partial x^a}\,D^{-1}\,\frac{\partial D}{\partial x^b}\,D^{-1} - \frac{\partial D}{\partial x^b}\,D^{-1}\,\frac{\partial D}{\partial x^a}\,D^{-1} = \left(\frac{\partial S_b{}^c}{\partial x^a} - \frac{\partial S_a{}^c}{\partial x^b}\right) X_c \quad . \tag{8.12}$$

Now evaluate the above equation at $\boldsymbol{x} = \boldsymbol{x}_e$ to obtain the result

$$\big[X_a\,,\,X_b\big] = f_{ab}{}^c\,X_c \tag{8.13}$$

where

$$f_{ab}{}^c = \left(\left.\frac{\partial S_b{}^c}{\partial x^a}\right|_{\boldsymbol{x}_e} - \left.\frac{\partial S_a{}^c}{\partial x^b}\right|_{\boldsymbol{x}_e}\right) \quad . \tag{8.14}$$

We see that the structure constants are independent of the representation D, but are dependent on the coordinatization of G. Note that all the business in the above equation is evaluated in the vicinity of $\boldsymbol{x}_e$, so we don't need to worry about chart labels – the only chart on G which matters is the one containing the identity e.

8.1.3 Exponential map

Next, consider a curve $\boldsymbol{x}(t)$ on some open interval $t \in (-\tau, \tau)$ satisfying $\dot{x}^a\,S_a{}^b(\boldsymbol{x}) = \theta^b$, with $\boldsymbol{x}(0) = \boldsymbol{x}_e$ and where $\boldsymbol{\theta}$ is t-independent. This satisfies the dynamical system $\dot{x}^a = \theta^b\big[S^{-1}(\boldsymbol{x})\big]_b{}^a$; we assume $S(\boldsymbol{x})$ is invertible. Then $D_{\boldsymbol{\theta}}(t) \equiv D(\boldsymbol{x}(t))$ satisfies

$$\frac{dD_{\boldsymbol{\theta}}(t)}{dt} = \sum_a \theta^a\,X_a\,D_{\boldsymbol{\theta}}(t) \quad , \tag{8.15}$$

the solution to which is $D_{\boldsymbol{\theta}}(t) = \exp(\theta^a X_a\,t)$. Without loss of generality, we may set $t = 1$, for which

$$D(\boldsymbol{\theta}) \equiv D_{\boldsymbol{\theta}}(1) = \exp(\theta^a X_a) = \exp(-i\theta^a T_a) \quad , \tag{8.16}$$

with implied sum on a. This is called the *exponential map*. Cartan proved that the exponential map is surjective if G is a compact, connected Lie group, *i.e.* for any $g \in G$, the representative $D(g)$ may be written as an exponential[7].

The generators $\{X_a\}$ may be viewed as basis vectors in a vector space. Recall that an algebra is a vector space over a field (in our case, $\mathbb{R}$ or $\mathbb{C}$) which acts on itself via addition and multiplication. An abstract Lie algebra $\mathfrak{g}$ is defined by three conditions: (i) $\mathfrak{g}$ is a vector space over some field $\mathbb{F}$, with multiplication

[7] For a counterexample in the case of a noncompact Lie group, consider the case of $\mathsf{SL}(2,\mathbb{R})$, whose Lie algebra $\mathsf{sl}(2,\mathbb{R})$ is the set of all traceless 2×2 real matrices. Suppose $M \in \mathsf{sl}(2,\mathbb{R})$. If M has two distinct eigenvalues, they must be paired $(\lambda, -\lambda)$ because $\mathsf{Tr}\,M = 0$. Then $\exp(M)$ has eigenvalues $\exp(\pm\lambda)$. If $\mathsf{det}M = -\lambda^2 < 0$, then λ is real, whereas if $\mathsf{det}M > 0$, then $\lambda = i\beta$ with β real. In both cases, the exponential does not correspond to any matrix of the form $\mathsf{diag}(-K, -K^{-1}) \in \mathsf{sl}(2,\mathbb{R})$, which has two negative real eigenvalues. If $\mathsf{det}M = 0$, then $M^2 = 0$, which follows from the Cayley-Hamilton theorem, which says that any 2×2 matrix M satisfies its own characteristic equation, *i.e.* $P(M) = 0$ where $P(\lambda) = \lambda^2 - \lambda\mathsf{Tr}\,M + \mathsf{det}M$. But then M is conjugate to $\begin{pmatrix} 0 & a \\ 0 & 0 \end{pmatrix}$ and $\exp(M)$ is conjugate to $\begin{pmatrix} 1 & e^a \\ 1 & 0 \end{pmatrix}$, which is degenerate with 1 the only eigenvalue.

defined by the *Lie bracket* $[\bullet,\bullet]:\mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$, which is (ii) antisymmetric, *i.e.* $[X,Y]=-[Y,X]\;\forall\;X,Y\in\mathfrak{g}$, and (iii) satisfies the Jacobi identity,

$$\big[X,[Y,Z]\big]+\big[Y,[Z,X]\big]+\big[Z,[X,Y]\big]=0\quad . \tag{8.17}$$

Note that none of these three axioms makes any reference to an underlying Lie group! This may prompt the question of whether every real Lie algebra is the Lie algebra of some matrix Lie group. It turns out that if $\mathfrak{g}$ is finite-dimensional, then the answer to this question is yes[8]. For example, the vector space $\mathbb{R}^3$ endowed with the vector cross product as the Lie bracket is a Lie algebra. The corresponding Lie group is $\mathsf{SO}(3)$. With generators $(\Sigma_a)_{ij}=-\epsilon_{aij}$, one has $\big[\Sigma_a,\Sigma_b\big]=\epsilon_{abc}\,\Sigma_c$, and a general element of the Lie algebra may be written $X=x^a\Sigma_a$, so that $\big[X,Y\big]=(\boldsymbol{x}\times\boldsymbol{y})^c\,\Sigma_c$, and the general Lie group element is given by the exponential map $g=\exp(x^a\Sigma_a)\in\mathsf{SO}(3)$.

For matrix Lie algebras, the Lie bracket is the familiar commutator: $[X,Y]=XY-YX$. Why not define multiplication by the usual product XY? For starters, unless we are talking about matrix Lie algebras, such a composition is in general not well-defined. Even if one embeds the Lie group within $\mathsf{GL}(\mathcal{V})$ and its Lie algebra within $\mathsf{End}(\mathcal{V})$, while the composition XY will be well-defined, it will still depend on the embedding[9]. Furthermore, there is no guarantee that XY will be an element of $\mathfrak{g}$. Consider, for example, the Lie group $\mathsf{SL}(n,\mathbb{R})$ consisting of $n\times n$ matrices with unit determinant. Its Lie algebra, $\mathsf{sl}(n,\mathbb{R})$, consists of all real traceless $n\times n$ matrices. But if $\mathsf{Tr}\,X=\mathsf{Tr}\,Y=0$, there is no guarantee that $\mathsf{Tr}\,(XY)=0$. On the other hand, $\mathsf{Tr}\,(XY)=\mathsf{Tr}\,(YX)$, and thus $\mathsf{Tr}\,[X,Y]=0$ and $[X,Y]\in\mathsf{sl}(n,\mathbb{R})$.

8.1.4 Baker-Campbell-Hausdorff formula

Suppose $X=\sum_a x^aX_a$ and $Y=\sum_a y^aX_a$ are sums over generators of $\mathfrak{g}$, then e^X and e^Y are elements of $D(G)$, and so, then, must be $\exp(X)\exp(Y)\equiv\exp(Z)$. In §1.4.5, we presented Dynkin's expression of the Baker-Campbell-Hausdorff (BCH) formula[10],

$$\ln\left(e^X\,e^Y\right)=\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\sum_{\substack{r_1,s_1\\ r_1+s_1>0}}\cdots\sum_{\substack{r_n,s_n\\ r_n+s_n>0}}\frac{\big[X^{r_1}Y^{s_1}X^{r_2}Y^{s_2}\cdots X^{r_n}Y^{s_n}\big]}{\sum_{i=1}^n(r_i+s_i)\cdot\prod_{j=1}^n r_j!\,s_j!}\quad , \tag{8.18}$$

where

$$\big[X^{r_1}Y^{s_1}X^{r_2}Y^{s_2}\cdots X^{r_n}Y^{s_n}\big]=\underbrace{[X,[X,\cdots[X}_{r_1},\underbrace{[Y,[Y,\cdots[Y}_{s_1},\cdots\underbrace{[X,[X,\cdots[X}_{r_n},\underbrace{[Y,[Y,\cdots[Y}_{s_n}]]\cdots]]\quad . \tag{8.19}$$

Thus,

$$\exp(X)\exp(Y)=\exp\Big(X+Y+\tfrac{1}{2}\,[X,Y]+\tfrac{1}{12}\,[X,[X,Y]]+\tfrac{1}{12}\,[Y,[Y,X]]+\ldots\Big)\quad . \tag{8.20}$$

Every term inside the round bracket on the RHS, other than $X+Y$, formed from nested commutators. Thus if $[X,Y]\in\mathfrak{g}$ for all $X,Y\in\mathfrak{g}$, then the product $e^X\,e^Y=e^Z$ with $Z\in\mathfrak{g}$.

[8] See B. C. Hall, *Lie Groups, Lie Algebras, and Representations*, chapter 5.
[9] See W. Fulton and J. Harris, *Representation Theory*, p. 108.
[10] See https://en.wikipedia.org/wiki/Baker-Campbell-Hausdorff_formula.

Let's denote for the moment the Lie bracket operation as $\star$, *i.e.* $X \star Y = [X, Y]$. Then, restating the conditions of antisymmetry and the Jacobi identity,

$$\begin{aligned} X \star Y &= -Y \star X \\ (X \star Y) \star Z &= X \star (Y \star Z) + Y \star (Z \star X) \quad . \end{aligned} \tag{8.21}$$

Thus, we see that multiplication within a Lie algebra, via the Lie bracket, is neither commutative nor associative!

8.2 Vector fields and the Lie algebra

8.2.1 Smooth vector fields

Antisymmetry and the Jacobi identity are properties of all smooth *vector fields* over a manifold M. A vector field X may be expressed as a first order differential operator,

$$X = \sum_{i=1}^{n} X^i \, \frac{\partial}{\partial x^i} \quad , \tag{8.22}$$

where, in our typical physicists' callow approach to mathematics, we shall assume $X^i(\boldsymbol{x})$ is a smooth map from M to $\mathbb{R}^n$ (*i.e.*, $i \in \{1, \ldots, n\}$). Acting on a function $f(\boldsymbol{x}) : M \to \mathbb{R}$, we obtain another function[11],

$$X(f)(\boldsymbol{x}) = \sum_{i=1}^{n} X^i(\boldsymbol{x}) \, \frac{\partial f(\boldsymbol{x})}{\partial x^i} \quad . \tag{8.24}$$

If f and g are functions on M and c is a constant, then

$$\begin{aligned} X(cf + g) &= c\, X(f) + X(g) \\ X(fg) &= f\, X(g) + g\, X(f) \quad . \end{aligned} \tag{8.25}$$

If $Y = \sum_{i=1}^{n} Y^i \, \frac{\partial}{\partial x^i}$, then XY is in general not a vector field, but the *Lie bracket* $[X, Y]$ is:

$$[X, Y] = \sum_{i=1}^{n} A^i \, \frac{\partial}{\partial x^i} \qquad , \qquad A^i = \sum_{j=1}^{n} \left(X^j \, \frac{\partial Y^i}{\partial x^j} - Y^j \, \frac{\partial X^i}{\partial x^j} \right) \quad . \tag{8.26}$$

This is also called the *Lie derivative* of Y with respect to X: $\pounds_X(Y) = [X, Y]$.

[11] We are engaging here in a very standard abuse of notation. The coordinates $\{x^1, \ldots, x^n\}$ should be thought of as the components of $\varphi_\alpha : U_\alpha \to \mathbb{R}^n$, coming from the chart $(\varphi_\alpha, U_\alpha)$. When we write $\partial f(\boldsymbol{x})/\partial x^i$, what we really mean is

$$\left. \frac{\partial f(\boldsymbol{x})}{\partial x^i} \right|_p \equiv \left. \frac{\partial}{\partial x^i} \left(f \circ \varphi^{-1} \right) \right|_{\varphi(p)} \quad , \tag{8.23}$$

where $p \in M$ and $\varphi(p) \in U \subseteq \mathbb{R}^n$. Furthermore, the quantities X^i are really functions on M, which at the point $p \in M$ take the values $X^i(p)$.

The space of linear differential operators $v_p = \sum_i v^i \left.\frac{\partial}{\partial x^i}\right|_p$ at a particular point $p \in M$ is called the *tangent space* to M at p, and denoted T_pM. Each such v_p is a *tangent vector* to M at p. Note that $\dim(T_pM) = \dim M = n$, because n components v_i must be specified to fix v_p. The collection $TM = \coprod_p T_pM$ of all the tangent spaces of M is called the *tangent bundle* of M. Its dimension is $\dim(TM) = 2n$, because one now must specify a location p as well as the tangent vector at p. A vector field X is then a choice of tangent vector at each point $p \in M$, hence $X : M \to TM$ is a map from a manifold M to its tangent bundle. The space of all smooth vector fields[12] on M is denoted $\mathfrak{X}(M)$ and is an infinite-dimensional space (provided $\dim M \geq 1$), because specification of a vector field X requires specification of n independent *functions* $X^i : M \to \mathbb{R}$.

Suppose M and N are smooth manifolds and $F : M \to N$ be a smooth map. Let $f : N \to \mathbb{R}$ be a smooth function on N. We can pull back f to M by defining

$$F^*f = f \circ F \quad . \tag{8.27}$$

Thus if $p \in M$ then $(F^*f)(p) = f(F(p))$, with $F(p) \in N$. The function $F^*f : M \to \mathbb{R}$ is called the *pullback* of f.

Let $X \in \mathfrak{X}(M)$ be a vector field on M. Then we can push forward X to $\mathfrak{X}(N)$ using the map F in the following natural way. Again let $f : N \to \mathbb{R}$ be a smooth function on N. Then define

$$(F_*X)(f) = X(f \circ F) \quad . \tag{8.28}$$

Thus $F_* : \mathfrak{X}(M) \to \mathfrak{X}(N)$. Note that $f \circ F$ is a smooth function on M. The expression F_*X thus denotes a smooth vector field on M, *i.e.* an element of $\mathfrak{X}(M)$, and is the *pushforward* of X. Thus pushforward of a tangent vector v_p is called the *differential map* and is denoted $dF_p : T_pM \to T_{F(p)}N$, *viz.*

$$dF_p(v_p)(f) = v_p(f \circ F) \quad . \tag{8.29}$$

The tangent vector $dF_p(v_p) \in T_{F(p)}N$ is the pushforward of the tangent vector $v_p \in T_pM$. Note that v_p eats smooth functions on M in the vicinity of p and excretes real numbers. Correspondingly, $dF_p(v_p)$ eats smooth functions on N in the vicinity of $F(p)$ and excretes real numbers. The relation between the differential map of a tangent vector and the pushforward of a vector field is thus

$$dF_p(X_p)(f) = X_p(f \circ F) = X(f \circ F)(p) \quad . \tag{8.30}$$

To unpack this expression, note that $X = \sum_i X^i \frac{\partial}{\partial x^i}$ is a vector field and $X_p = \sum_i X^i(p) \left.\frac{\partial}{\partial x^i}\right|_p$ is a tangent vector at $p \in M$. Acting on a function $f(F(q))$ with q in the vicinity of p, it yields $X_p(f \circ F)$, which is the function $X(f \circ F)$ evaluated at p.

Let $\gamma : I \to M$ take some interval $I \subset \mathbb{R}$ to M. The *velocity vector* $\dot\gamma(t_0) \in T_{\gamma(t_0)}M$ is defined by

$$\dot\gamma(t_0)(f) = d\gamma_{t_0}\left(\left.\frac{d}{dt}\right|_{t_0}\right)(f) = \left.\frac{d}{dt}\,(f \circ \gamma)\right|_{t_0} \quad . \tag{8.31}$$

which says that the differential $d\gamma_{t_0}$ is a map $d\gamma_{t_0} : T_{t_0}I \to T_{\gamma(t_0)}M$.

[12] A vector field which is not smooth, and hence not in $\mathfrak{X}(M)$, is called a *rough vector field*.

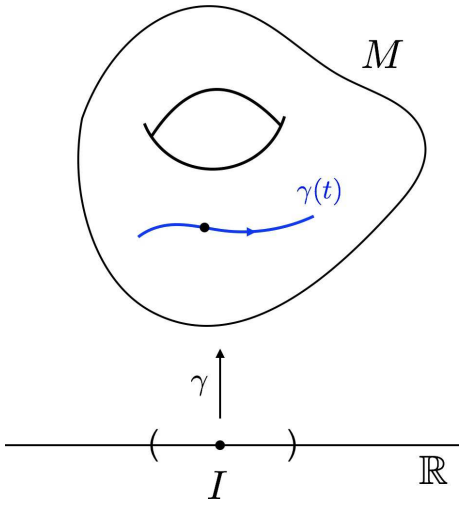


Figure 8.2: A smooth curve $\gamma(t)$ on a manifold M.

As we have stressed, an essential feature of Lie groups is that the action of group multiplication furnishes us with a natural map from the group to itself. That is, we may define $L_g : G \to G$ as left multiplication by g, *i.e.* $L_g h = gh$. Thus, the pushforward $L_{g*}X$ of a vector field $X \in \mathfrak{X}(G)$ is another vector field $(L_{g*}X) \in \mathfrak{X}(G)$. This naturally gives rise to the notion of a *left-invariant vector field* X which satisfies $L_{g*}X = X$ for all $g \in G$. Thus, $X_{gh} = (dL_g)_h(X_h)$ for all $g, h \in G$. Now let $h = e$, so we have

$$X_g = (dL_g)_e(X_e) \quad . \tag{8.32}$$

This means that we can construct a left-invariant vector field simply by left-translating the tangent vector X_e by g, for all values of $g \in G$. The space of left-invariant vector fields on G, $\mathfrak{X}^L(G)$, is a subspace of $\mathfrak{X}(G)$. It is a linear subspace, in that if $X, Y \in \mathfrak{X}^L(G)$, then so is $cX + Y$ where $c \in \mathbb{R}$ is a constant. To construct $\mathfrak{X}^L(G)$, we may employ the following method[13]. Let $\gamma : I \to G$ be a smooth curve with $I \subset \mathbb{R}$ an interval containing $t = 0$, $\gamma(0) = e$, and $\dot\gamma(0) = X_e$ with $X_e \in T_eG$. Let $f \in C^\infty(G)$ be a smooth function on G. Then if $X_g = (dL_g)_e(X_e)$, this means

$$\begin{aligned}\big(X(f)\big)(g) = X_g(f) = (dL_g)_e(X_e)(f) = X_e(f \circ L_g) = \frac{d}{dt}\Big|_{t=0} (f \circ L_g \circ \gamma)(f) \\ = \frac{d}{dt}\Big|_{t=0} f\big(g\,\gamma(t)\big) \quad .\end{aligned} \tag{8.33}$$

Thus, we have constructed a map from T_eG to $\mathfrak{X}(G)$. The finite-dimensional subspace $\mathfrak{X}^L(G) \subset \mathfrak{X}(G)$ is the image of this map. Indeed, $\mathfrak{X}^L(G)$ is a vector space and as such is isomorphic to T_eG. Furthermore, if $X, Y \in \mathfrak{X}^L(G)$, then[14]

$$L_{g*}[X, Y] = [L_{g*}X, L_{g*}Y] = [X, Y] \in \mathfrak{X}^L(G) \quad . \tag{8.34}$$

[13] See T. Kemp, *Introduction to Smooth Manifolds & Lie Groups*, ch. 12.

[14] In general, let $F\colon M \to N$ and $f\colon N \to \mathbb{R}$. Let $X \in \mathfrak{X}(M)$ be a vector field on M. In general, $Y_{F(p)} = dF_p(X_p)$ does not define a vector field on N because F may not be surjective. In the case where it is, Y is said to be F-*related* to X. If $Y_1, Y_2 \in \mathfrak{X}(N)$ are F-related, respectively, to $X_1, X_2 \in \mathfrak{X}(M)$, then $X_1X_2(f \circ F) = X_1(Y_2(f) \circ F) = (Y_1Y_2(f)) \circ F$. Thus $F_*[X_1, X_2] = [Y_1, Y_2] = [F_*X_1, F_*X_2]$.

This leads us to the following interpretation of the Lie algebra of G: $\mathfrak{g}$ *is the space of left-invariant vector fields on* G.

8.2.2 Integral curves and the exponential map

Let $\gamma : I \to M$ be a smooth curve on M and $X \in \mathfrak{X}(M)$ a vector field on M. If

$$\dot\gamma(t) = X_{\gamma(t)} \tag{8.35}$$

for all $t \in I$, then $\gamma(t)$ is said to be an *integral curve* of X. This means that at every point p which $\gamma(t)$ passes through, its tangent vector is X_p *i.e.*

$$\dot\gamma(t_0) = d\gamma_{t_0}\left(\frac{d}{dt}\Big|_{t_0}\right) = X_{\gamma(t_0)} \quad . \tag{8.36}$$

Identifying the components of the basis vectors $\frac{\partial}{\partial x^i}$ at each point $p \in M$, we have that any integral curve is the solution of a dynamical system, *i.e.* a set of n coupled ordinary differential equations, *viz.*

$$\frac{d\gamma^i(t)}{dt} = X^i\big(\gamma^1(t), \ldots, \gamma^n(t)\big) \quad . \tag{8.37}$$

For example, on $M = \mathbb{R}^2$, let $X = x\,\frac{\partial}{\partial y} - y\,\frac{\partial}{\partial x}$, in which case we obtain

$$\frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -y \\ +x \end{pmatrix} \qquad \Longrightarrow \qquad \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} x_0\cos t - y_0 \sin t \\ x_0 \sin t + y_0 \cos t \end{pmatrix} \quad . \tag{8.38}$$

This is the unique integral curve of X which passes through (x_0, y_0), where its tangent vector is given by $\dot{\boldsymbol{x}}(0) = \begin{pmatrix} -y_0 \\ +x_0 \end{pmatrix}$. If the flow is global, meaning t may be extended to the entire real line, the vector field is called *complete*. As an example of a vector field whose flow is *incomplete*, consider the case $M = \mathbb{R}^1$ and $X = x^2\,\frac{\partial}{\partial x}$. Then we have $\dot x = x^2$ with solution $x(t) = x_0/(1 - x_0 t)$. This blows up at finite time $t = 1/x_0$ and can therefore not be extended to the entire real line $t \in \mathbb{R}$. For complete flows, we define the curve $\gamma_p(t)$ to be the solution to $\dot\gamma(t) = X_{\gamma(t)}$ with $\gamma(0) = p$. Then $\gamma_p(t+s) = \gamma_q(s)$ where $q = \gamma_p(t)$. This simply says that we can extend the solution of our coupled ODEs by choosing new initial conditions as our most recent final conditions.

If $M = G$ is a Lie group, all left-invariant vector fields $X \in \mathfrak{X}^L(G)$ are complete. This is because one can always find an integral curve $\gamma^e(t)$ for X on $t \in (-\delta, +\delta)$ with $\gamma^e(0) = e$, or some finite positive δ. But if X is left-invariant, this solution may be translated about G by left multiplication: $\gamma^g(t) \equiv L_g\gamma^e(t) = g\gamma^e(t)$ is an integral curve on $(-\delta, +\delta)$ with initial conditions $\gamma^g(0) = g$. We can then stitch these finite curves starting at different values of g together to yield a global flow[15] Now consider the integral curve $\gamma(t)$ of X, with $\gamma(0) = e$, defined for all $t \in \mathbb{R}$. This entails $\gamma(s+t) = \gamma(s)\,\gamma(t)$, which yields a group homomorphism $\gamma : \mathbb{R} \to G$, called a *one-parameter subgroup*. As an example, suppose $G \subseteq \mathsf{GL}(n, \mathbb{F})$ is

[15] For a less callow description, see Kemp, lemma 13.1.

a Lie subgroup of $\mathsf{GL}(n,\mathbb{F})$[16], with $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$. This basically accounts for all the matrix Lie groups discussed in §1.4.2. Then differentiating $\gamma(s+t)$ with respect to s and setting $s = 0$ yields

$$\dot\gamma(t) = \dot\gamma(0)\,\gamma(t) \quad . \tag{8.39}$$

Here we are using as (global) coordinates the matrix elements themselves. We have $A \equiv \dot\gamma(0) \in T_eG = \mathfrak{g}$. Then [insert mathy discussion about ODEs, convergence] we have that the unique solution to the above equation is $\gamma(t) = \exp(At)$.

So much in differential geometry can be either clarified or obscured by notation. Warner[17] denotes the map $\gamma : \mathbb{R} \to G$ as exp_X, which I like because it makes the connection to $X \in \mathfrak{X}(G)$ explicit. The exponential map $\exp$ is then defined by $\exp(X) = \mathsf{exp}_X(1)$.

8.3 Representations of Lie Algebras

Let us now shrink back from all this mathy talk and return to the more practical aspects of characterizing Lie algebras.

8.3.1 Properties of the structure constants

We noted above that if $A \in \mathfrak{g}$ and $B \in \mathfrak{g}$, then so is their Lie bracket $[A,B]$. Thus, if $\{X^a\}$ is a basis for $\mathfrak{g}$, we must have

$$\big[X_a, X_b\big] = f_{ab}{}^c\, X_c \quad , \tag{8.40}$$

where the $f_{ab}{}^c$ are the *structure constants* for the Lie algebra. Owing to the antisymmetry of the Lie bracket and the Jacobi identity, the structure constants satisfy the relations

$$\begin{aligned} 0 &= f_{ab}{}^c + f_{ba}{}^c \\ 0 &= f_{bc}{}^d\, f_{da}{}^e + f_{ab}{}^d\, f_{dc}{}^e + f_{ca}{}^d\, f_{db}{}^e \quad . \end{aligned} \tag{8.41}$$

What happens if we choose a different parameterization for G, resulting in a different set of generators? From eqn. 8.10, the new generators are $\widetilde{X}_a = M_a{}^b\, X_b$ with $M_a{}^b = (\partial x^b/\partial\tilde x^a)\big|_{\boldsymbol{x}_e}$. Thus

$$\big[\widetilde{X}_a, \widetilde{X}_b\big] = M_a{}^r\, M_b{}^s\, \big[X_r, X_s\big] = M_a{}^r\, M_b{}^s\, f_{rs}{}^c\, X_c = M_a{}^r\, M_b{}^s\, f_{rs}{}^t\, (M^{-1})_t{}^c\, \widetilde{X}_c = \tilde f_{ab}{}^c\, \widetilde{X}_c \quad , \tag{8.42}$$

and we conclude

$$\tilde f_{ab}{}^c = M_a{}^r\, M_b{}^s\, f_{rs}{}^t\, (M^{-1})_t{}^c \quad . \tag{8.43}$$

Lie algebras in which all elements commute are *abelian*. In an abelian Lie algebra, all the structure constants vanish: $f_{ab}{}^c = 0$ for all a, b, c.

[16] A Lie subgroup G of a Lie group G' is, as its name connotes, itself a Lie group, and which is also topologically an embedded submanifold of G'. If you are seriously interested in the precise definition of an embedded submanifold, you probably should not be reading these notes.

[17] F. W. Warner, *Foundations of Differential Manifolds and Lie Groups*, p. 102.

Recall the "physics generators" T_a are given by $T_a = iX_a$, where the X_a are the "math generators". Thus the physics generators satisfy $\big[T_a, T_b\big] = i{f_{ab}}^c\, T_c$. The reason we physicists choose this convention is that unitary representations $D(G)$ of a Lie group result Hermitian generators of the Lie algebra. We may deduce this from the exponential map $D(\boldsymbol{\theta}) = \exp(\theta_a X_a) = \exp(-i\theta_a T_a)$. In the math convention, the X_a are then antihermitian. In either case, the structure constants are then real, since

$$\begin{aligned}\big[T_a, T_b\big]^\dagger &= -i\big({f_{ab}}^c\big)^*\, T_c \\ &= \big[T_b, T_a\big] = -i{f_{ab}}^c\, T_c \quad .\end{aligned} \tag{8.44}$$

Thus $\big({f_{ab}}^c\big)^* = {f_{ab}}^c$. Using the T_a as basis vectors, if $Y = y^a\, T_a$ and $Z = z^b\, T_b$, then the Lie bracket of Y and Z is given by

$$\big[Y, Z\big] = y^a\, z^b\, \big[T_a, T_b\big] = i{f_{ab}}^c\, y^a\, z^b\, T_c \quad . \tag{8.45}$$

Another way to write this in component notation is $\big[Y, Z\big]^c = i{f_{ab}}^c\, y^a\, z^b$.

8.3.2 Representations

A finite-dimensional real (or complex) *representation* of a Lie group a homomorphism $\Pi : G \to \mathsf{GL}(\mathcal{V})$, where $\mathcal{V}$ is a finite-dimensional real/complex vector space. Similarly, a finite-dimensional real/complex representation of a real/complex Lie algebra $\mathfrak{g}$ is a homomorphism $\pi : \mathfrak{g} \to \mathsf{gl}(\mathcal{V})$. When $\mathcal{V}$ is an n-dimensional vector space over a field $\mathbb{F}$ (= $\mathbb{R}$ or $\mathbb{C}$ for our purposes), $\mathsf{GL}(\mathcal{V}) = \mathsf{GL}(n, \mathbb{F})$, where $\mathsf{GL}(n, \mathbb{F})$ is the set of all $n \times n$ invertible matrices. Then $\mathsf{gl}(\mathcal{V}) = \mathsf{gl}(n, \mathbb{F})$, where $\mathsf{gl}(n, \mathbb{F})$ is the set of all $n \times n$ matrices, with the matrix commutator as the Lie bracket. If the homomorphism Π is injective (one-to-one), the representation is said to be *faithful*. This means that the collection of matrices $\{\Pi(g)\}$ with $g \in G$ under matrix multiplication is itself a group isomorphic to G.

A proper subspace $\mathcal{W} \subset \mathcal{V}$ is said to be *invariant* if $\Pi(g)\,\omega \in \mathcal{W}$ for all $g \in G$ and $\omega \in \mathcal{W}$. A similar definition holds for Lie algebras. If there is no proper invariant subspace, a representation is said to be *irreducible*. Two representations $\Pi(G) : G \to \mathsf{GL}(\mathcal{V})$ and $\Sigma(G) : G \to \mathsf{GL}(\mathcal{V}')$ are said to be *equivalent* if $\mathcal{V} \cong \mathcal{V}'$ and there exists $\phi : \mathcal{V} \to \mathcal{V}'$ such that $\phi\big(\Pi(g)\, v\big) = \Sigma(g)\, \phi(v)$ for all $g \in G$ and $v \in \mathcal{V}$.

8.3.3 Matrix Lie groups and their Lie algebras

A *matrix Lie group* $G \subseteq \mathsf{GL}(n, \mathbb{C})$ has the property that if A_n is a sequence of matrices in G which converges to A, then either $A \in G$ or A is noninvertible[18]. Recall that the Lie algebra $\mathfrak{g}$ of a matrix Lie group G is the set of all matrices X such that $\exp(tX) \in G$ for all $t \in \mathbb{R}$. What is the relation between $\Pi(G)$ and $\pi(\mathfrak{g})$? From $\Pi(e^X) = e^{\pi(X)}$, we have that

$$\pi(X) = \frac{d}{dt}\bigg|_{t=0} \Pi(e^{tX}) \quad . \tag{8.46}$$

Note that $\pi(gXg^{-1}) = \Pi(g)\,\pi(X)\,\Pi(g^{-1})$. So long as G is connected, $\Pi(G)$ is irreducible if and only if $\pi(\mathfrak{g})$ is irreducible. Thus, $\mathfrak{g}$ is a vector space; indeed it is the *tangent space* to G at its identity E, which

[18] A sequence of matrices A_n converges to A if each element of A_n converges to the corresponding element of A.

is to say the set of derivatives of all smooth curves in G passing through E. Recall $\mathsf{SL}(n,\mathbb{F})$ is the set of matrices with unit determinant, *i.e.* $\det \exp(tX) = 1$. This entails $\mathsf{Tr}\, X = 0$, hence $\mathsf{sl}(n,\mathbb{F})$ is the set of all real traceless $n \times n$ matrices. Similarly, for the orthogonal and unitary groups $\mathsf{O}(n)$ and $\mathsf{U}(n)$, we have their algebras $\mathsf{o}(n)$ and $\mathsf{u}(n)$ are the sets of all real antisymmetric and complex antihermitian matrices, respectively[19].

What are we doing?

WHY are we studying matrix representations of matrix Lie groups? *For God's sake they're already matrices!* The point is that representations act on vector spaces whose dimensions are not necessarily the same as the n in $\mathsf{GL}(n,\mathbb{C})$. For example, SU(3) obviously acts on $\mathbb{R}^3$, but it can act on other vector spaces as well. Our interest shall be finite-dimensional complex IRREPs of MLGs. The task of identifying such representations is almost completely reduced to finding finite-dimensional complex IRREPs of their associated Lie algebras.

8.3.4 Some examples

Some common examples of representations of matrix Lie groups and their associated Lie algebras:

TRIVIAL REPRESENTATION : In the *trivial representation*, $\Pi(g) = \mathbb{1}$ for all $g \in G$. Then $\Pi(e^X) = e^{\pi(X)} = \mathbb{1}$ and we have $\pi(X) = 0$ for all $X \in \mathfrak{g}$.

STANDARD REPRESENTATION: In the *standard representation*, $\Pi(g) = g$ for all $g \in G \subseteq \mathsf{GL}(n,\mathbb{F})$. We then have $\pi(X) = X$ for all $X \in \mathfrak{g} \subseteq \mathsf{gl}(n,\mathbb{F})$.

ADJOINT REPRESENTATION : In the *adjoint representation*, define the Lie group homomorphism $\mathtt{Ad} : G \to \mathsf{GL}(\mathfrak{g})$ by $\mathtt{Ad}_g(X) = gXg^{-1}$. Here $\mathsf{GL}(\mathfrak{g})$ is the space of linear operations acting on the Lie algebra $\mathfrak{g}$. Note that $\mathtt{Ad}$ is a Lie group homomorphism because

$$\mathtt{Ad}_g\, \mathtt{Ad}_h(X) = ghXh^{-1}g^{-1} = \mathtt{Ad}_{gh}(X) \quad . \tag{8.47}$$

The corresponding Lie algebra representation $\mathtt{ad} : \mathfrak{g} \to \mathsf{gl}(\mathfrak{g})$ is then given by $\mathtt{ad}_X(Y) = [X,Y]$. If this seems abstract, recall the explicit construction of the adjoint representation of any Lie algebra is given in terms of its structure constants[20]. If the basis vectors of $\mathfrak{g}$, *i.e.* the generators of the algebra, are taken to be the set $\{X_a\}$, and $\big[X_a, X_b\big] = f_{ab}{}^c\, X_c$, where the $f_{ab}{}^c$ are the structure constants, then from the Jacobi identity one readily derives that the matrices $(X_a)_{bc} = -f_{ab}{}^c$ satisfy the above relation, and therefore provide a representation of $\mathfrak{g}$, which is the adjoint representation. We can give the adjoint representation more of a "physics flavor" by identifying each generator X_a with a ket vector $|\, X_a \,\rangle$, such that

$$\big|\, \alpha X_a + \beta X_b \,\big\rangle = \alpha \,\big|\, X_a \,\big\rangle + \beta \,\big|\, X_b \,\big\rangle \quad . \tag{8.48}$$

The action of $\mathtt{ad}_X$ is then that of an operator, for which $\mathtt{ad}_X \,|\, Y \,\rangle = |\, [X,Y] \,\rangle$. Thus,

$$\mathtt{ad}_{X_a} \,\big|\, X_b \,\big\rangle = \big|\, [X_a, X_b] \,\big\rangle = f_{ab}{}^c \,\big|\, X_c \,\big\rangle \quad , \tag{8.49}$$

[19] Math convention here.
[20] See §1.4.6.

abc	$f_{ab}{}^{c}$	abc	$f_{ab}{}^{c}$	abc	$f_{ab}{}^{c}$
123	1	246	$\frac{1}{2}$	367	$-\frac{1}{2}$
147	$\frac{1}{2}$	257	$\frac{1}{2}$	458	$\frac{\sqrt{3}}{2}$
156	$-\frac{1}{2}$	345	$\frac{1}{2}$	678	$\frac{\sqrt{3}}{2}$

Table 8.1: Nonzero structure constants for $\mathsf{su}(3)$. Index permutation is totally antisymmetric.

which says $f_{ab}{}^{c} = \langle\, X_c \,|\, \mathsf{ad}_{X_a} \,|\, X_b \,\rangle$.

For the group $G = \mathsf{SU}(2)$, the Lie algebra $\mathsf{su}(2)$ has three generators, which may be taken to be the Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$. These satisfy $\big[\sigma_a, \sigma_b\big] = 2i\epsilon_{abc}\,\sigma_c$, hence $f_{ab}{}^{c} = 2\,\epsilon_{abc}$. The generators of the adjoint representation of $\mathsf{su}(2)$ are then $(T_a)_{bc} = i(X_a)_{bc} = -if_{ab}{}^{c}$, hence

$$T_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad , \quad T_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad , \quad T_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{8.50}$$

This is the same Lie algebra as $\mathsf{so}(3)$, because, as we have seen, $\mathsf{SU}(2)$ is a double cover of $\mathsf{SO}(3)$, so locally in the vicinity of the identity both Lie groups look the same. The three generators T_a are of course the generators of rotations in three-dimensional space.

8.3.5 SU(3)

Recall that the Lie algebra $\mathsf{su}(N)$ consists of $N \times N$ Hermitian matrices (physics convention). For $N = 2$, the canonical basis is that of the Pauli matrices σ_a. It is convenient to define the generators $S_a = \frac{1}{2}\sigma_a$. This basis for the Lie algebra is normalized according to $\mathsf{Tr}(S_a\,S_b) = \frac{1}{2}$
$delta_{ab}$, and the structure constants are defined by $\big[S_a\,,\,S_b\big] = i\epsilon_{abc}\,S_c$. We can then read off $f_{ab}{}^{c} = \epsilon_{abc}$.

For $N = 3$, the canonical basis is given by the *Gell-mann matrices*,

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad , \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad , \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad , \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{8.51}$$
$$\lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad , \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad , \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \quad .$$

Define $T_a = \frac{1}{2}\lambda_a$, in which case $\mathsf{Tr}(T_aT_b) = \frac{1}{2}\delta_{ab}$. One can check that the nonzero structure constants are given by the following table: The structure constants in Tab. 8.1 are totally antisymmetric under index permutation, so that $f_{ab}{}^{c} = -f_{ac}{}^{b} = f_{ca}{}^{b}$: *etc.*

Note that the generators $\{T_1, T_2, T_3\}$ generate an $\mathsf{su}(2)$ subgroup, called the isospin group. There are two

other such su(2) subgroups contained within su(3):

$$\big[T_4\,,\,T_5\big] = \frac{i}{2}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix} = i\,(T_3 + \sqrt{3}\,T_8) \tag{8.52}$$

and

$$\big[T_6\,,\,T_7\big] = \frac{i}{2}\begin{pmatrix}0&0&0\\0&1&0\\0&0&-1\end{pmatrix} = i\,(-T_3 + \sqrt{3}\,T_8) \quad . \tag{8.53}$$

Note also that the three su(3) subalgebras are overlapping, *i.e.* the generators T_3 and T_8 are partially shared among all three. Finally, observe that $\big[T_3\,,\,T_8\big] = 0$. The pair $\{T_3, T_8\}$ comprises the *maximal set of commuting generators*, also known as the *Cartan subalgebra* (CSA), about which we shall have much more to say in §8.5 below. For su(2), the Cartan subalgebra consists of a single generator (which always commutes with itself), which is conventionally taken to be S_3.

Taking a cue from su(2), we define the ladder matrices

$$T_\pm \equiv T_1 \pm i\,T_2 \quad , \quad U_\pm \equiv T_6 \pm i\,T_7 \quad , \quad V_\pm \equiv T_4 \pm i\,T_5 \quad , \tag{8.54}$$

which satisfy $Z_+^\dagger = Z_-$, where $Z = T, U, V$. We also give special names $H_1 \equiv T_3$ and $H_2 \equiv T_8$ to the elements of the CSA. One then readily obtains the commutation relations

$$\begin{aligned}\big[T_+\,,\,T_-\big] &= 2\,H_1 \\ \big[U_+\,,\,U_-\big] &= \sqrt{3}\,H_2 - H_1 \\ \big[V_+\,,\,V_-\big] &= \sqrt{3}\,H_2 + H_1 \quad .\end{aligned} \tag{8.55}$$

as well as

$$\begin{aligned}\big[H_1\,,\,T_\pm\big] &= \pm T_\pm & \big[H_2\,,\,T_\pm\big] &= 0 \\ \big[H_1\,,\,U_\pm\big] &= \mp\tfrac{1}{2}U_\pm & \big[H_2\,,\,U_\pm\big] &= \pm\tfrac{\sqrt{3}}{2}\,U_\pm \\ \big[H_1\,,\,V_\pm\big] &= \pm\tfrac{1}{2}V_\pm & \big[H_2\,,\,V_\pm\big] &= \pm\tfrac{\sqrt{3}}{2}\,V_\pm \quad .\end{aligned} \tag{8.56}$$

and, finally,

$$\begin{aligned}\big[T_+\,,\,U_+\big] &= V_+ & \big[T_+\,,\,U_-\big] &= 0 \\ \big[U_+\,,\,V_+\big] &= 0 & \big[U_+\,,\,V_-\big] &= T_- \\ \big[V_+\,,\,T_+\big] &= 0 & \big[V_+\,,\,T_-\big] &= -U_+ \quad ,\end{aligned} \tag{8.57}$$

plus the corresponding six relations obtained by Hermitian conjugation.

Now let's consider a representation π of su(3) in which the representatives $\pi(T_a)$ act on some Hilbert space $\mathcal{H}$. They could just as well be matrices acting on a vector space $\mathcal{V}$ - a Hilbert space is nothing more than a vector space along with an inner product - but the point is that the dimension of $\mathcal{H}$ or $\mathcal{V}$ is arbitrary and is not constrained to be the 3 of su(3). Accordingly, we define

$$\hat{t}_\pm = \pi(T_\pm) \quad , \quad \hat{u}_\pm = \pi(U_\pm) \quad , \quad \hat{v}_\pm = \pi(V_\pm) \quad , \quad \hat{h}_{1,2} = \pi(H_{1,2}) \quad . \tag{8.58}$$

Since $\big[\hat{h}_1\,,\,\hat{h}_2\big] = 0$, these operators may be simultaneously diagonalized. We write their normalized common eigenvectors as $|\,h_1,h_2\,\rangle$, where

$$\hat{h}_j\,|\,h_1,h_2\,\rangle = h_j\,|\,h_1,h_2\,\rangle \tag{8.59}$$

for $j = 1,2$. The eigenvalues h_1 and h_2 are called *weights*, and $\boldsymbol{h} = \{h_1,h_2\}$ the *weight vector*. The number of components of the weight vector is the dimension of the Cartan subalgebra. The commutation relations listed above for the generators also hold for their representatives. Thus,

$$\begin{aligned}
\hat{h}_1\,\hat{t}_\pm\,|\,h_1,h_2\,\rangle &= \big[\hat{h}_1\,,\,\hat{t}_\pm\big]\,|\,h_1,h_2\,\rangle + \hat{t}_\pm\,\hat{h}_1\,|\,h_1,h_2\,\rangle = (h_1 \pm 1)\,\hat{t}_\pm\,|\,h_1,h_2\,\rangle \\
\hat{h}_1\,\hat{u}_\pm\,|\,h_1,h_2\,\rangle &= \big[\hat{h}_1\,,\hat{u}_\pm\big]\,|\,h_1,h_2\,\rangle + \hat{u}_\pm\,\hat{h}_1\,|\,h_1,h_2\,\rangle = (h_1 \mp \tfrac{1}{2})\,\hat{u}_\pm\,|\,h_1,h_2\,\rangle \\
\hat{h}_1\,\hat{v}_\pm\,|\,h_1,h_2\,\rangle &= \big[\hat{h}_1\,,\,\hat{v}_\pm\big]\,|\,h_1,h_2\,\rangle + \hat{v}_\pm\,\hat{h}_1\,|\,h_1,h_2\,\rangle = (h_1 \pm \tfrac{1}{2})\,\hat{v}_\pm\,|\,h_1,h_2\,\rangle
\end{aligned} \tag{8.60}$$

and

$$\begin{aligned}
\hat{h}_2\,\hat{t}_\pm\,|\,h_1,h_2\,\rangle &= \big[\hat{h}_2\,,\,\hat{t}_\pm\big]\,|\,h_1,h_2\,\rangle + \hat{t}_\pm\,\hat{h}_2\,|\,h_1,h_2\,\rangle = h_2\,\hat{t}_\pm\,|\,h_1,h_2\,\rangle \\
\hat{h}_2\,\hat{u}_\pm\,|\,h_1,h_2\,\rangle &= \big[\hat{h}_2\,,\hat{u}_\pm\big]\,|\,h_1,h_2\,\rangle + \hat{u}_\pm\,\hat{h}_2\,|\,h_1,h_2\,\rangle = (h_2 \mp \tfrac{\sqrt{3}}{2})\,\hat{u}_\pm\,|\,h_1,h_2\,\rangle \\
\hat{h}_2\,\hat{v}_\pm\,|\,h_1,h_2\,\rangle &= \big[\hat{h}_2\,,\,\hat{v}_\pm\big]\,|\,h_1,h_2\,\rangle + \hat{v}_\pm\,\hat{h}_2\,|\,h_1,h_2\,\rangle = (h_2 \pm \tfrac{\sqrt{3}}{2})\,\hat{v}_\pm\,|\,h_1,h_2\,\rangle \quad .
\end{aligned} \tag{8.61}$$

We see that the operator $\hat{t}_+$ shifts the weights (h_1,h_2) by $(1,0)$. Accordingly, we define the *rootvector* of the generator T_+ to be $\boldsymbol{\alpha}_{T_+} = (1,0)$. The full set of root vectors may now be read off from the above equations:

$$\boldsymbol{\alpha}_{T_\pm} = \pm\Big(1\,,\,0\Big) \quad , \quad \boldsymbol{\alpha}_{U_\pm} = \pm\Big(-\tfrac{1}{2}\,,\,\tfrac{\sqrt{3}}{2}\Big) \quad , \quad \boldsymbol{\alpha}_{V_\pm} = \pm\Big(\tfrac{1}{2}\,,\,\tfrac{\sqrt{3}}{2}\Big) \quad . \tag{8.62}$$

These are sketched below in Fig. 8.3.

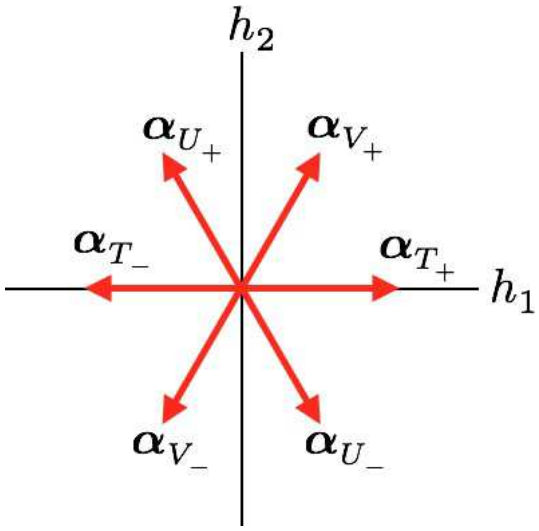


Figure 8.3: SU(3) root vectors.

In the adjoint representation, these results take the form

$$\begin{aligned} \mathsf{ad}_{H_1} \big| T_\pm \big\rangle &= \pm \big| T_\pm \big\rangle & \mathsf{ad}_{H_2} \big| T_\pm \big\rangle &= 0 \\ \mathsf{ad}_{H_1} \big| U_\pm \big\rangle &= \mp \tfrac{1}{2} \big| U_\pm \big\rangle & \mathsf{ad}_{H_2} \big| U_\pm \big\rangle &= \pm \tfrac{\sqrt{3}}{2} \big| U_\pm \big\rangle \\ \mathsf{ad}_{H_1} \big| V_\pm \big\rangle &= \pm \tfrac{1}{2} \big| V_\pm \big\rangle & \mathsf{ad}_{H_2} \big| V_\pm \big\rangle &= \pm \tfrac{\sqrt{3}}{2} \big| V_\pm \big\rangle \quad . \end{aligned} \tag{8.63}$$

If the representation π is of finite dimension, then there must be a *highest weight state* $|\,\psi_0\,\rangle$, analogous to $|\,j,j\,\rangle$ in $\mathsf{su}(2)$, which is annihilated by $\hat{t}_+$, $\hat{u}_+$, and $\hat{v}_+$.

8.4 Classification of Semisimple Lie Algebras

We now consider the general problem of classifying Lie algebras. As it turns out, Lie algebras come in different flavors, and we shall be most interested in real (or complex) Lie algebras which are *semisimple*.

8.4.1 Real, complex, simple, and semisimple

REAL AND COMPLEX LIE ALGEBRAS : The Lie algebra $\mathfrak{g}$ formed by the vector space of generators X_a over $\mathbb{R}$ is called a *real Lie algebra*. Now $\mathfrak{g}$ is a vector space, and any vector space $\mathcal{V}$ over $\mathbb{R}$ may be *complexified* to a vector space $\mathcal{V}^{\mathbb{C}}$, by writing a complex vector as $\phi = (v_1, v_2) \in \mathcal{V}^{\mathbb{C}}$, where $v_{1,2} \in \mathcal{V}$. Alternatively, we can write $\phi = v_1 + iv_2$. Thus, $\mathsf{dim}(\mathcal{V}^{\mathbb{C}}) = 2\,\mathsf{dim}(\mathcal{V})$, and $\mathcal{V} \subset \mathcal{V}^{\mathbb{C}}$ is a real subspace of $\mathcal{V}^{\mathbb{C}}$. The Lie bracket on $\mathfrak{g}$ has a unique extension to $\mathfrak{g}^{\mathbb{C}}$:

$$[X_1 + iX_2\,,\,Y_1 + iY_2] = \big([X_1\,,\,Y_1 - [X_2\,,\,Y_2]\big) + i\big([X_1\,,\,Y_2] + [X_2\,,\,Y_1]\big) \quad . \tag{8.64}$$

This complexified bracket satisfies antisymmetry and the Jacobi identity and renders $\mathfrak{g}^{\mathbb{C}}$ a Lie algebra in its own right, called the *complexification* of $\mathfrak{g}$. If $\mathfrak{g}$ is a real matrix Lie algebra contained within $M_n(\mathbb{C})$, the space of all $n \times n$ complex-valued matrices[21], and if for every $X \in \mathfrak{g}$ it is the case that $iX \notin \mathfrak{g}$, then $\mathfrak{g}^{\mathbb{C}} \subseteq M_n(\mathbb{C})$ is isomorphic to the set $\big\{X + iY \,|\, X, Y \in \mathfrak{g}\big\}$. In such cases, complexification of the algebra $\mathfrak{g}$ is tantamount from extending the field $\mathbb{F}$ from $\mathbb{R}$ to $\mathbb{C}$.

The orthogonal group $\mathsf{O}(n+1)$ and the Lorentz group $\mathsf{O}(n,1)$ have different (real) Lie algebras, but the same complex Lie algebra. Explicitly, consider the case of $\mathsf{SO}(3)$, whose Lie algebra $\mathsf{so}(3)$ is the set of matrices R which satisfy (math convention) $R^{\mathsf{T}} = -R$. This algebra has three generators,

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad , \quad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{8.65}$$

The nonzero Lie brackets are given by

$$[X_1\,,X_2] = X_3 \quad , \quad [X_2\,,X_3] = X_1 \quad , \quad [X_3\,,X_1] = X_2 \quad . \tag{8.66}$$

[21] $M_n(\mathbb{C})$ is identical to $\mathsf{gl}(n,\mathbb{C})$.

Now consider $\mathsf{SO}(1,2)$, where $R \in \mathsf{so}(1,2)$ requires $R^{\mathsf{T}} = -\Lambda R \Lambda$, where $\Lambda = \mathsf{diag}(1,-1,-1)$. Again, there are three generators,

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad X_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad , \quad X_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{8.67}$$

The nonzero Lie brackets are given by

$$[X_1\,,X_2] = X_3 \quad , \quad [X_2\,,X_3] = -X_1 \quad , \quad [X_3\,,X_1] = X_2 \quad . \tag{8.68}$$

Evidently the structure constants of $\mathsf{so}(1,2)$ are different than those of $\mathsf{so}(3)$, but they can be made the same by redefining the generators as $\{\widetilde{X}_1, \widetilde{X}_2, \widetilde{X}_3\} \equiv \{X_1, iX_2, iX_3\}$. Thus $\mathsf{so}(1,2)^{\mathbb{C}} \cong \mathsf{so}(3)^{\mathbb{C}}$. Indeed, $\mathsf{so}(p,q,\mathbb{R})^{\mathbb{C}} \cong \mathsf{so}(p+q,\mathbb{C})$ for all p,q.

Another example: $\mathsf{u}(n)^{\mathbb{C}} \cong \mathsf{gl}(n,\mathbb{C})$. To see this[22], note that $\mathsf{u}(n)$ contains $n \times n$ complex matrices which are antihermitian (again, math convention): $R^\dagger = -R$. Since $(iR)^\dagger = -iR^\dagger = +iR$, if $R \in \mathsf{u}(n)$ then necessarily $iR \notin \mathsf{u}(n)$. Now note that a general complex matrix $R \in \mathsf{gl}(n,\mathbb{C})$ may always be written as a complex sum of two antihermitian matrices, $R = R_1 + iR_2$, with $R_1 = (R - R^\dagger)/2$ and $R_2 = (R + R^\dagger)/2i$. Therefore $\mathsf{u}(n)^{\mathbb{C}} = \mathsf{gl}(n,\mathbb{C})$. Some other common complexifications:

$$\begin{aligned} \mathsf{gl}(n,\mathbb{R})^{\mathbb{C}} \cong \mathsf{gl}(n,\mathbb{C}) \quad , \quad \mathsf{sl}(n,\mathbb{R})^{\mathbb{C}} \cong \mathsf{sl}(n,\mathbb{C}) \quad , \quad \mathsf{su}(n)^{\mathbb{C}} \cong \mathsf{sl}(n,\mathbb{C}) \\ \mathsf{o}(n)^{\mathbb{C}} \cong \mathsf{so}(n,\mathbb{C}) \quad , \quad \mathsf{sp}(n,\mathbb{R})^{\mathbb{C}} \cong \mathsf{sp}(n,\mathbb{C}) \quad , \quad \mathsf{sp}(n)^{\mathbb{C}} \cong \mathsf{sp}(n,\mathbb{C}) \quad . \end{aligned} \tag{8.69}$$

LIE SUBALGEBRA : $\mathfrak{h} \subseteq \mathfrak{g}$ is a *Lie subalgebra* of $\mathfrak{g}$ if it is closed with respect to both addition $+$ and the Lie bracket $[\bullet,\bullet]$. *Ado's theorem* says that any finite-dimensional Lie algebra over $\mathbb{F}$ is isomorphic to some subalgebra of $\mathsf{gl}(n,\mathbb{F})$ for some n.

IDEALS : $\mathfrak{h} \subseteq \mathfrak{g}$ is an *ideal* of $\mathfrak{g}$ if $[A\,,X] \in \mathfrak{h}$ for all $A \in \mathfrak{h}$ and $X \in \mathfrak{g}$. For Lie subalgebras, there is no distinction between left and right ideals. An ideal $\mathfrak{h}$ is also called an *invariant subalgebra*. Ideals are useful for constructing *quotient algebras* $\mathfrak{g}/\mathfrak{h}$.

SIMPLE AND SEMISIMPLE LIE GROUPS : A Lie group G said to be *simple* if it contains no nontrivial invariant Lie subgroups (*i.e.* other than G itself). Examples include $(\mathbb{R},+,0)$, which is abelian and noncompact, and the special orthogonal group in odd dimensions, $\mathsf{SO}(2n+1,\mathbb{R})$, which is compact. G is said to be *semisimple* if it c ontainsno invariant *abelian* subgroups, including G itself. Thus $(\mathbb{R},+,0)$ is simple but not semisimple (it is abelian). Other examples of semisimple Lie groups include $\mathsf{SO}(n,\mathbb{R})$ for $n > 1$[23] and $\mathsf{Sp}(2n,\mathbb{R})$. In a sense, semisimple Lie groups are maximally nonabelian.

SIMPLE AND SEMISIMPLE LIE ALGEBRAS : A Lie algebra $\mathfrak{g}$ is *simple* if it contains no nontrivial ideals. A Lie algebra $\mathfrak{g}$ is *semisimple* if it contains no abelian ideals, including $\mathfrak{g}$ itself. Any one-dimensional Lie algebra is then simple but not semisimple. Semisimple Lie algebras, like semisimple Lie groups, are, in a sense, "maximally nonabelian".

SOLVABLE LIE ALGEBRA : Given a Lie algebra $\mathfrak{g}$, define $\mathfrak{g}^{(0)} = \mathfrak{g}$ and then iteratively define

$$\mathfrak{g}^{(n+1)} = \left[\mathfrak{g}^{(n)}, \mathfrak{g}^{(n)}\right] \quad , \tag{8.70}$$

[22] See B. C. Hall, *Lie Groups, Lie Algebras, and Representations*, p. 66.

[23] $\mathsf{SO}(2)$ is abelian, hence not semisimple.

i.e. $\mathfrak{g}^{(n+1)}$ consists of all $[A,B]$ where $A,B \in \mathfrak{g}^{(n)}$. This is called the *derived series* of $\mathfrak{g}$. We say that $\mathfrak{g}$ is *solvable* if $\mathfrak{g}^{(n)} = 0$ for some n. If $\mathfrak{g}^{(1)} = 0$, then $\mathfrak{g}$ is abelian. Every abelian Lie algebra is solvable. The Lie algebra $\mathfrak{t}(n,\mathbb{F})$ of upper triangular matrices with elements in $\mathbb{F}$ is solvable. Semisimple Lie algebras are never solvable. To see this, note that by the definition of semisimplicity that any semisimple Lie algebra $\mathfrak{g}$ may be written as a direct sum of simple Lie algebras, *viz.*

$$\mathfrak{g} = \bigoplus_{i=1}^{n} \mathfrak{g}_i \quad , \tag{8.71}$$

where each $\mathfrak{g}_i$ is simple, and at least one of the $\mathfrak{g}_i$ is nonabelian. Without loss of generality we may assume that $\mathfrak{g}_1$ is nonabelian. For simplicity[24], assume $n = 2$, and compute

$$\begin{aligned} \mathfrak{g}^{(1)} = \big[\mathfrak{g}\,,\,\mathfrak{g}\big] &= \big[\mathfrak{g}_1 \oplus \mathfrak{g}_2\,,\,\mathfrak{g}_1 \oplus \mathfrak{g}_2\big] \\ &= \big[\mathfrak{g}_1\,,\,\mathfrak{g}_1\big] \oplus \big[\mathfrak{g}_2\,,\,\mathfrak{g}_2\big] = \mathfrak{g}_1 \oplus \mathfrak{g}_2^{(1)} \quad , \end{aligned} \tag{8.72}$$

which follows from the fact that $\mathfrak{g}_1$ is simple and nonabelian, hence $\big[\mathfrak{g}_1\,,\,\mathfrak{g}_1\big] = \mathfrak{g}_1$. Therefore $\mathfrak{g}$ is not solvable.

TRUE FACT : Simple Lie groups have simple Lie algebras, and semisimple Lie groups have semisimple Lie algebras.

8.4.2 The Killing form and Cartan's criterion

How can we classify Lie algebras? We might hope to do so based on their structure constants ${f_{ab}}^c$, but these depend on our parameterization of G. We seek a more useful and robust classification. To this end, define the *Killing form*,

$$g_{ab} = \mathsf{Tr}(\hat{X}_a\,\hat{X}_b) = {f_{ar}}^s\,{f_{bs}}^r \quad , \tag{8.73}$$

where $(\hat{X}_a)_{bc} = -{f_{ab}}^c$ is the generator $\hat{X}^a$ in the adjoint representation. Note that $g_{ab} = g_{ba}$ is symmetric. Define the contravariant tensor g^{ab} to be the matrix inverse of g_{ab}, ***if the inverse*** g^{ab} ***exists***. In this case $g_{ab}\,g^{bc} = {\delta_a}^c$, and we may use g_{ab} and g^{ab} to lower and raise indices, respectively. Thus,

$$f_{abc} \equiv {f_{ab}}^r\,g_{rc} = {f_{ab}}^r\,{f_{rd}}^e\,{f_{ce}}^d \quad . \tag{8.74}$$

It is left as an exercise to the student[25] to confirm that f_{abc} is a totally antisymmetric tensor, which means it reverses sign under exchange of any two of its three indices. Thus

$$f_{abc} = f_{bca} = f_{cab} = -f_{bac} = -f_{acb} = -f_{cba} \quad . \tag{8.75}$$

Under a coordinate transformation, the Killing form transforms as

$$\widetilde{g}_{ab} = {M_a}^r\,{M_b}^s\,g_{rs} = {M_a}^r\,g_{rs}\,(M^{\mathsf{T}})^s{}_b \quad . \tag{8.76}$$

Now because g_{ab} is symmetric, it can be diagonalized by an orthogonal transformation, *viz.*

$${O_a}^r\,{O_b}^s\,g_{rs} = {O_a}^r\,g_{rs}\,(O^{\mathsf{T}})^s{}_b = \mathsf{diag}(\beta_1,\ldots,\beta_{n_1},-\tilde{\beta}_1,\ldots,-\tilde{\beta}_{n_2},0_1,\ldots,0_{n_3}) \quad , \tag{8.77}$$

[24] No pun intended!

[25] Hint: you will need to invoke the Jacobi identity.

where $n_1 + n_2 + n_3 = n$ and each β_i and $\tilde{\beta}_j$ is real and positive. This is the most general case for g_{ab}, with n_1 positive eigenvalues, n_2 negative eigenvalues, and n_3 zero eigenvalues. Now consider *dilations*, which are coordinate transformations which do not preserve lengths. There is nothing illegal about choosing a dilated set of coordinates to describe our group manifold! Dilations are equivalent to an M matrix of the form $M = \mathsf{diag}(\alpha_1, \alpha_2, \ldots, \alpha_n)$ where α_i is for each i a nonzero real number[26]. Combining dilations and orthogonal transformations, consider the matrix $M_a{}^b = D_a\, O_a{}^b$, with no sum on a, and where

$$D_a = \big((\lambda_1/\beta_1)^{1/2}\,,\,\ldots\,,\,(\lambda_{n_1}/\beta_{n_1})^{1/2}\,,\,(\tilde{\lambda}_1/\tilde{\beta}_1)^{1/2}\,,\,\ldots\,,\,(\tilde{\lambda}_{n_2}/\tilde{\beta}_{n_2})^{1/2}\,,\,1_1\,,\,\ldots\,,\,1_{n_3}\big) \quad , \tag{8.78}$$

where the λ_i and $\tilde{\lambda}_j$ are arbitrary positive real numbers. Then we have

$$\widetilde{g}_{ab} = M_a{}^r\, M_b{}^s\, g_{rs} = D_a\, D_b\, O_a{}^r\, O_b{}^s\, g_{rs} = \mathsf{diag}(\boldsymbol{\lambda}_{n_1}, -\tilde{\boldsymbol{\lambda}}_{n_2}, \mathbf{0}_{n_3}) \quad . \tag{8.79}$$

Now comes an important result due to E. Cartan:

CARTAN CRITERION : The Killing form of a Lie algebra $\mathfrak{g}$ is nonsingular, *i.e.* $\det g \neq 0$, if and only if $\mathfrak{g}$ is semisimple.

Thus, $n_3 = 0$ for semisimple Lie algebras, and only for semisimple Lie algebras. In addition, if G is compact, then $n_1 = 0$ and the Killing form is negative definite. Thus, for compact semisimple Lie groups, by rotating and rescaling coordinates, the Killing form of the associated Lie algebra may be chosen to be $g_{ab} = \lambda_a\, \delta_{ab}$ (no sum on a), where $\lambda_a < 0$.

8.4.3 Casimirs

While some of the structure constants $f_{ab}{}^c$ may vanish, is there a way of constructing certain combinations of the generators which happen to commute with *all* elements of the Lie algebra? Such entities would be particularly valuable in classifying Lie algebras and their representations. For semisimple Lie algebras, it is indeed possible. Such elements are called *Casimir elements*, or *Casimirs* for short, after the Dutch physicist Hendrik Casimir, who in 1931 first recognized of the existence, for general semisimple Lie algebras, of quantities analogous to $\boldsymbol{L}^2$ for the angular momentum algebra $\mathsf{so}(3)$. For this, he was made a Catholic saint[27]. The general expression for a $p^{\rm th}$ *order Casimir* is

$$C_p = \kappa^{a_1 a_2 \cdots a_p}\, X_{a_1} X_{a_2} \cdots X_{a_p} \quad . \tag{8.80}$$

where

$$\kappa^{a_1 a_2 \cdots a_p} = f^{a_1 b_1}{}_{b_2}\, f^{a_2 b_2}{}_{b_3} \cdots f^{a_p b_p}{}_{b_1} \quad . \tag{8.81}$$

Note that $f^{ab}{}_c = g^{ar}\, g^{bs}\, g_{ct}\, f_{rs}{}^t$. The claim is that $[C_p\,, X_c] = 0$ for all generators X_c. Let's check this for the case $p = 2$ where

$$\kappa^{ab} = f^{ar}{}_s\, f^{bs}{}_r = g^{ab} \quad , \tag{8.82}$$

[26] Without loss of generality, we may assume $\alpha_i > 0$ as well, since mirror operations are included in the set of orthogonal transformations.

[27] I jest. St. Casimir (1458 – 1484), was a Polish prince and second oldest son of King Casimir IV. For some strange reason, in his iconography, he is often depicted with three hands, suggesting he may have been a sly poker player, or an expert juggler. See https://en.wikipedia.org/wiki/Saint_Casimir.

which is the Killing form. Thus, $C_2 = g^{ab}\,X_a\,X_b = X^a\,X_a$, which should look familiar. Now

$$\begin{aligned}[X^a X_a\,,X_c] &= X^a\,[X_a,X_c] + [X^a,X_c]\,X_a \\ &= f_{ac}{}^d\,X^a\,X_d + f^a{}_c{}^d\,X_d X_a = f^a{}_c{}^d\,(X_a X_d + X_d X_a) = 0 \quad ,\end{aligned} \tag{8.83}$$

because $f^a{}_c{}^d = -f^d{}_c{}^a$, because $f^a{}_c{}^d = g_{cb}\,f^{abd}$ and f^{abd} is totally antisymmetric.

What about C_3? We have

$$C_3 = f^{ar}{}_s\,f^{bs}{}_t\,f^{ct}{}_r\,X_a\,X_b\,X_c \quad . \tag{8.84}$$

Consider the case of $\mathfrak{g} = \mathsf{so}(3)$, where we may take $f_{abc} = 2^{-1/2}\,\epsilon_{abc}$ so that $g_{ab} = \delta_{ab}$. Since the Killing form is the unit matrix, raising and lowering indices doesn't do anything, hence $X^a = X_a$ and $f_{abc} = f_{ab}{}^c = f^a{}_b{}^c = \cdots = 2^{-1/2}\,\epsilon_{abc}$. Now

$$\epsilon_{ars}\,\epsilon_{bst}\,\epsilon_{ctr} = \epsilon_{ars}\big(\delta_{br}\,\delta_{sc} - \delta_{bc}\,\delta_{rs}\big) = \epsilon_{abc} \tag{8.85}$$

hence the cubic Casimir is

$$C_3 = 2^{-3/2}\,\epsilon_{abc}\,X_a\,X_b\,X_c = 2^{-3/2}\,X_a\,X_a = 2^{-3/2}\,C_2 \quad . \tag{8.86}$$

So the cubic Casimir for $\mathsf{so}(3)$ is the same as the quadratic Casimir, up to a multiplicative factor. Indeed, it turns out that C_2 is the *only* independent Casimir invariant for $\mathsf{so}(3)$.

Derivation

Let $\pi : \mathfrak{g} \to \mathsf{gl}(\mathcal{V})$ be an IRREP of $\mathfrak{g}$ and let $\widetilde{\pi} : \mathfrak{g} \to \mathsf{gl}(\widetilde{\mathcal{V}})$ be a fiducial[28] representation, with generators X_a and $\widetilde{X}_a$, respectively. Now consider the construction

$$\Xi_a = X_a \otimes \widetilde{\mathbb{1}} + \mathbb{1} \otimes \widetilde{X}_a \quad . \tag{8.87}$$

It is easy to show that the $\{\Xi_a\}$ form a representation acting on the product vector space $\mathcal{V} \times \widetilde{\mathcal{V}}$, *i.e.*

$$\big[\Xi_a\,,\,\Xi_b\big] = f_{ab}{}^c\,\Xi_c \quad . \tag{8.88}$$

Now define

$$Q = X_a \otimes \widetilde{X}^a = g^{ab} X_a \otimes \widetilde{X}_b \tag{8.89}$$

where g^{ab} is the inverse Killing form. One then discovers

$$\begin{aligned}\big[\Xi_a\,,\,Q\big] &= \big[X_a\,,\,X_b\big] \otimes \widetilde{X}^b + X_b \otimes \big[\widetilde{X}_a\,,\,\widetilde{X}^b\big] \\ &= f_{ab}{}^c\,X_c \otimes \widetilde{X}^b + f_a{}^b{}_c\,X_b \otimes \widetilde{X}^c = f_{abc}\big(X^c \otimes \widetilde{X}^b + X^b \otimes \widetilde{X}^c\big) = 0 \quad .\end{aligned} \tag{8.90}$$

It then follows that $\big[\Xi_a\,,\,Q^p\big] = 0$ for all $p \in \mathbb{N}$[29], *i.e.*

$$\big[X_{a_1} X_{a_2} \cdots X_{a_p}\,,\,X_b\big] \otimes \widetilde{X}^{a_1}\widetilde{X}^{a_2}\cdots\widetilde{X}^{a_p} \;+\; X_{a_1} X_{a_2} \cdots X_{a_p} \otimes \big[\widetilde{X}^{a_1}\widetilde{X}^{a_2}\cdots\widetilde{X}^{a_p}\,,\,\widetilde{X}_c\big] = 0 \tag{8.91}$$

[28] Fiducial means "accepted as a fixed basis of reference or comparison".

[29] $\mathbb{N} = \mathbb{Z}_+ = \{1, 2, 3, \ldots\}$ denotes the natural numbers, *i.e.* the positive integers.

Now define the partial trace

$$\kappa^{a_a \cdots a_p} = \widetilde{\mathsf{Tr}} \left(\widetilde{X}^{a_1} \cdots \widetilde{X}^{a_p} \right) \quad . \tag{8.92}$$

In taking the partial trace of eqn. 8.91 over the $\widetilde{\mathcal{V}}$ subspace, the second term vanishes because the trace of a commutator is zero. We therefore conclude that

$$C_p = \kappa^{a_a \cdots a_p} X_{a_1} \cdots X_{a_p} \tag{8.93}$$

satisfies $\big[C_p\,,\,X_c\big] = 0$ for all generators X_c. In eqn. 8.80, we take the fidicial representation $\widetilde{\pi}$ to be the adjoint representation.

Note that the Casimirs are not themselves elements of the Lie algebra. Indeed, they must each be proportional to the unit matrix by Schur's lemma. The Lie algebra $\mathsf{so}(n,\mathbb{R})$, for example, consists of *antisymmetric* matrices of dimension n. What the Casimirs do for us is help classify IRREPs of a Lie algebra.

For semisimple Lie algebras, there can be no linear Casimirs. To see this, note that $\big[C_1\,,\,X_a\big] = 0$ for all a means ad_{C_1}=0. Then the Jacobi identity then guarantees that for all a and b,

$$\big[C_1\,,\,[X_a\,,\,X_b]\big] = \big[X_a\,,\,[C_1\,,\,X_b]\big] - \big[X_b\,,\,[C_1\,,\,X_a]\big] = 0 \quad , \tag{8.94}$$

and so $\mathsf{ad}_{C_1}\mathsf{ad}_{X_a} = 0$. Suppose $C_a = \zeta^a X_a$ is a linear Casimir, where the $\{\zeta^a\}$ are constants. Then $\mathsf{ad}_{C_1} = \zeta^b\,\mathsf{ad}_{X_b}$ and $\mathsf{ad}_{C_1}\mathsf{ad}_{X_a} = \zeta^b\,\mathsf{ad}_{X_b}\mathsf{ad}_{X_a} = 0$. Now take the trace, to obtain

$$\zeta^b\,\mathsf{Tr}\,\mathsf{ad}_{X_b}\mathsf{ad}_{X_a} = \zeta^b\,g_{ba} = 0 \quad . \tag{8.95}$$

But if $\mathfrak{g}$ is semisimple, the Killing form has no nullspaces. Hence $C_1 = 0$.

8.5 The Cartan Subalgebra