Physics 829: Homework Set No. 3

Due date: Friday, April 20, 2012, 1:00pm in PRB M2043 (Biao Huang's office)

Total point value of set: 60 points

Problem 1 (10 pts.):
If $\hat{H}(\lambda)$ has eigenvector $|\psi_n(\lambda)\rangle$, prove the *Hellmann-Feynman Theorem*

$$\frac{dE_n(\lambda)}{d\lambda} = \left\langle \psi_n(\lambda) \left| \frac{\partial \hat{H}}{\partial \lambda} \right| \psi_n(\lambda) \right\rangle .$$

Problem 2 (15 pts.): Exercise 17.3.2 (Shankar, p. 466)

Problem 3 (15 pts.): Exercise 17.3.4 (Shankar, p. 470)

Problem 4 (5 pts.): Exercise 18.2.3 (Shankar, p. 478)

Problem 5 (10 pts.): Exercise 18.2.5 (Shankar, p. 478)

Problem 6 (5 pts.): Exercise 18.2.6 (Shankar, p. 478)

Problem 1

$$\frac{dE_n(\lambda)}{d\lambda} = \frac{d}{d\lambda}\langle\psi_n(\lambda)|E_n(\lambda)|\psi_n(\lambda)\rangle \qquad \left(\text{since } \frac{d}{d\lambda}\underbrace{\langle\psi_n(\lambda)|\psi_n(\lambda)\rangle}_{1} = 0\right)$$

$$= \frac{d}{d\lambda}\langle\psi_n(\lambda)|\hat{H}(\lambda)|\psi_n(\lambda)\rangle$$

$$= \left(\frac{d}{d\lambda}\langle\psi_n(\lambda)|\right)\underbrace{\hat{H}(\lambda)|\psi_n(\lambda)\rangle}_{=E_n(\lambda)|\psi_n(\lambda)\rangle} + \langle\psi_n(\lambda)|\frac{\partial\hat{H}}{\partial\lambda}|\psi_n(\lambda)\rangle + \underbrace{\langle\psi_n(\lambda)|\hat{H}(\lambda)}_{E_n(\lambda)\langle\psi_n(\lambda)|}\left(\frac{d}{d\lambda}|\psi_n(\lambda)\rangle\right)$$

$$= \langle\psi_n(\lambda)|\frac{\partial\hat{H}}{\partial\lambda}|\psi_n(\lambda)\rangle + E_n(\lambda)\Big(\underbrace{\left(\frac{d}{d\lambda}\langle\psi_n(\lambda)|\right)|\psi_n(\lambda)\rangle + \langle\psi_n(\lambda)|\left(\frac{d}{d\lambda}|\psi_n(\lambda)\rangle\right)}_{=\frac{d}{d\lambda}\langle\psi_n(\lambda)|\psi_n(\lambda)\rangle = 0}\Big)$$

$$\Rightarrow \frac{dE_n(\lambda)}{d\lambda} = \langle\psi_n(\lambda)|\frac{\partial\hat{H}(\lambda)}{\partial\lambda}|\psi_n(\lambda)\rangle. \quad \checkmark$$

Exercise 17.3.2 (p. 466)

Spin-1 matrices

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S_x^2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$S_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad S_y^2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

$$S_x^2 - S_y^2 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad S_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\hat{H} = \underbrace{A\hat{S}_z^2}_{\hat{H}^0} + \underbrace{B\left(S_x^2 - S_y^2\right)}_{\hat{H}'} \qquad A >> B$$

Use $\hat{S}_z$-eigenbasis to represent $\hat{H}$:

$$\hat{H} \leftrightarrow \underbrace{\begin{pmatrix} A & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & A \end{pmatrix}}_{H^0} + \underbrace{\begin{pmatrix} 0 & 0 & B \\ 0 & 0 & 0 \\ B & 0 & 0 \end{pmatrix}}_{H'} = \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}$$

- Exact eigenvalues and eigenstate of $\hat{H}$:

$$\det\begin{pmatrix} A-\lambda & 0 & B \\ 0 & -\lambda & 0 \\ B & 0 & A-\lambda \end{pmatrix} = -\det\begin{pmatrix} A-\lambda & B & 0 \\ 0 & 0 & -\lambda \\ B & A-\lambda & 0 \end{pmatrix} = +\det\begin{pmatrix} A-\lambda & B & 0 \\ B & A-\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix}$$

$$= \left((A-\lambda)^2 - B^2\right)(-\lambda) = 0$$

$$\Rightarrow \boxed{\lambda_1 = 0} \qquad \text{or} \qquad (\lambda - A)^2 = B^2$$

$$\lambda - A = \pm B$$

$$\boxed{\lambda_{2/3} = A \pm B}$$

- $\lambda_1 = 0$:

$$\begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = 0 \Rightarrow \begin{matrix} A\alpha + B\gamma = 0 \\ \beta = \text{arbitrary} \\ B\alpha + A\gamma = 0 \end{matrix} \Rightarrow \alpha = -\frac{A}{B}\gamma \quad \left\{ \begin{matrix} (A^2 - B^2)\gamma = 0 \\ \Rightarrow \gamma = \alpha = 0 \end{matrix} \right.$$

$$\Rightarrow |1\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$\lambda_2 = A + B$:

$$\begin{pmatrix} -B & 0 & B \\ 0 & -A-B & 0 \\ B & 0 & -B \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} B(-\alpha+\gamma) = 0 \\ (A+B)\beta = 0 \\ B(\alpha-\gamma) = 0 \end{cases} \Rightarrow \beta = 0$$

$$\Rightarrow \gamma = \alpha$$

$$\Rightarrow |2\rangle \longleftrightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$\lambda_3 = A - B$:

$$\begin{pmatrix} B & 0 & B \\ 0 & -A+B & 0 \\ B & 0 & B \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} B(\alpha+\gamma) = 0 \\ (-A+B)\beta = 0 \\ B(\alpha+\gamma) = 0 \end{cases} \Rightarrow \beta = 0$$

$$\Rightarrow \gamma = -\alpha$$

$$\Rightarrow |3\rangle \longleftrightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

- Now the perturbative approach.

  - $\hat{H}^0$ has 2 eigenvalues, 0 and 1, with 1 being two-fold degenerate.

    $\lambda_1^0 = 0$, $\lambda_2^0 = \lambda_3^0 = 1$

  - The corresponding eigenstates are

    $|1^0\rangle \longleftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

    $|2^0\rangle \longleftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

    $|3^0\rangle \longleftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

  The eigenstate $|1^0\rangle$ is stable under the perturbation:

  $$\langle m^0 | \hat{H}' | 1^0 \rangle = (\alpha^* \beta^* \gamma^*)\begin{pmatrix} 0 & 0 & B \\ 0 & 0 & 0 \\ B & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0 \quad \text{for all } \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

  $\Rightarrow \hat{H}'$ has no matrix elements mixing the state $|1^0\rangle$ with the other eigenstates of $\hat{H}^0$.

  - To see the eigenstates in the degenerate subspace $\{|2^0\rangle, |3^0\rangle\}$ that are stable under the perturbation, we must diagonalise the truncated Hamiltonian

$$\hat{\bar{H}} = \hat{P}\hat{H}\hat{P} = \hat{P}(\hat{H}^0 + \hat{H}')\hat{P} \quad \longleftrightarrow \quad \begin{matrix} |2^0\rangle & |3^0\rangle \\ A & B \\ B & A \end{matrix} \begin{matrix} \leftarrow |2^0\rangle \\ \leftarrow |3^0\rangle \end{matrix}$$

$\langle 3^0|\hat{H}|2^0\rangle$

in this degenerate subspace.

To find the eigenvalues $\bar{\lambda}$ of $\hat{\bar{H}}$ we compute

$$\det(\hat{\bar{H}} - \bar{\lambda}\hat{\mathbb{1}}) = 0 \Rightarrow \begin{vmatrix} A-\bar{\lambda} & B \\ B & A-\bar{\lambda} \end{vmatrix} = 0 \Rightarrow (A-\bar{\lambda})^2 - B^2 = 0$$

$$\Rightarrow (\bar{\lambda}-A)^2 = B^2 \Rightarrow \boxed{\bar{\lambda}_{2,3} = A \pm B}$$

These are the exact eigenvalues $\lambda_{2,3}$ of $\hat{H}$!

The corresponding eigenstates are (in the $\{|2^0\rangle, |3^0\rangle\}$ subspace)

$$\begin{pmatrix} \langle 2^0|\bar{2}\rangle \\ \langle 3^0|\bar{2}\rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad ; \quad \begin{pmatrix} \langle 2^0|\bar{3}\rangle \\ \langle 3^0|\bar{3}\rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

(using work from the exact solution)

$$\Rightarrow |\bar{2}\rangle = |2\rangle \;, \quad |\bar{3}\rangle = |3\rangle$$

The eigenstates that diagonalize $\hat{H}$ in the degenerate subspace corresponding to $\lambda^0_{2,3} = 1$ are the exact eigenstates of $\hat{H}$, with the exact eigenvalues $\bar{\lambda}_{2,3} = \lambda_{2,3}$. This is so since $\hat{H}$ has zero matrix elements between the degenerate subspace $\{|2^0\rangle, |3^0\rangle\} = \{|2\rangle, |3\rangle\}$ and the rest of its Hilbert space (i.e. the 1-d subspace spanned by $|1^0\rangle = |1\rangle$).

Exercise 17.3.4 (p. 470)

(1) Consider $\hat{H}(\lambda) = \hat{H}_0 + \lambda\hat{H}' \equiv \hat{H}_{coulomb}(e^2) + \frac{\lambda}{\hat{r}} = \hat{H}_{coulomb}(e^2 - \lambda)$

where $\hat{H}_{coulomb}(e^2) = \frac{\hat{p}^2}{2m} - \frac{e^2}{\hat{r}}$

We want $\left\langle \frac{1}{\hat{r}} \right\rangle_{nlm} = \langle \psi_{nlm} | \hat{H}' | \psi_{nlm} \rangle$

We can compute the eigenenergies of $\hat{H}(\lambda)$ exactly; they are

$$E_n(\lambda) = -\frac{m(e^2-\lambda)^2}{2\hbar^2 n^2} = -\frac{me^4}{2\hbar^2 n^2} + \frac{me^2\lambda}{\hbar^2 n^2} - \frac{m\lambda^2}{2\hbar^2 n^2}$$

This contains corrections of order λ and λ^2 to $E_n(0) = -\frac{me^4}{2\hbar^2 n^2}$

The term $\sim \lambda$ can be identified with the first order correction

$$\lambda E_n^{(1)} = \langle \psi_{nlm}(\lambda=0) | \frac{\lambda}{\hat{r}} | \psi_{nlm}(\lambda=0) \rangle$$

$$\Rightarrow \boxed{\left\langle \frac{1}{r} \right\rangle_{nlm} = +\frac{me^2}{\hbar^2 n^2} = \frac{1}{n^2 a_0}}$$

(2) Now consider $\tilde{\hat{H}}(\lambda) = \hat{H}_0 + \lambda\tilde{\hat{H}}' = \hat{H}_{coulomb} + \frac{\lambda}{\hat{r}^2}$

In the coordinate representation, the term $\lambda\hat{H}' = \frac{\lambda}{r^2}$ has the same r-dependence as the centrifugal term $\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$. So the exact eigenfunctions of $\tilde{\hat{H}}(\lambda)$ are hydrogen eigenfunctions whose radial wavefunctions are obtained from a modified radial differential equation where

$$\frac{\ell(\ell+1)}{r^2} \longrightarrow \frac{\tilde{\ell}(\tilde{\ell}+1)}{r^2} = \frac{\ell(\ell+1)}{r^2} + \frac{2m\lambda}{\hbar^2 r^2}$$

or $\tilde{\ell}(\tilde{\ell}+1) = \ell(\ell+1) + \frac{2m\lambda}{\hbar^2} \Rightarrow (2\tilde{\ell}+1)\,d\tilde{\ell} = \frac{2m}{\hbar^2}\,d\lambda$

l enters the energy eigenvalue through the main quantum $n = k + l + 1$ where k is the number of nodes of the radial wavefunction:

$$\tilde{E}_{n\tilde{l}m}(\lambda) = -\frac{me^4}{2\hbar^2(k+\tilde{l}(\lambda)+1)^2} = \langle n\tilde{l}m;\lambda | \hat{\tilde{H}}(\lambda) | n\tilde{l}m;\lambda \rangle$$

The Hellmann-Feynman theorem gives

$$\frac{d\tilde{E}_{n\tilde{l}m}}{d\lambda}(\lambda) = \langle n\tilde{l}m;\lambda | \frac{\partial \hat{\tilde{H}}(\lambda)}{\partial\lambda} | n\tilde{l}m;\lambda \rangle =$$

$$= \langle n\tilde{l}m;\lambda | \frac{1}{\hat{r}^2} | n\tilde{l}m;\lambda \rangle$$

So we get $\left\langle \frac{1}{r^2} \right\rangle_{nlm}$ by evaluating this at $\lambda = 0$:

$$\left\langle \frac{1}{r^2} \right\rangle_{nlm} = \frac{dE_{n\tilde{l}m}}{d\lambda}\Big|_{\lambda=0} = + \frac{me^4}{\hbar^2(k+\tilde{l}+1)^3} \frac{d\tilde{l}}{d\lambda}\Big|_{\lambda=0}$$

$$= \frac{me^4}{\hbar^2(k+l+1)^3} \frac{2m}{\hbar^2} \frac{1}{2l+1} = \frac{2m^2e^4}{\hbar^4 n^3} \frac{1}{2l+1}$$

$$= \frac{2}{a_0^2 n^3} \frac{1}{2l+1} = \frac{1}{l+\frac{1}{2}} \frac{1}{a_0^2 n^3}$$

To compare with (17.3.11) we multiply with e^4:

$$\left\langle \frac{e^4}{r^2} \right\rangle_{nlm} = \frac{4m^2e^8}{4\hbar^4 n^4} \cdot \frac{n}{l+\frac{1}{4}} = \frac{4n}{l+\frac{1}{2}} \left(-\frac{me^4}{2\hbar^2 n^2} \right)^2 = \frac{4n E_0^2}{l+\frac{1}{2}} \checkmark$$

(3) Consider $\left\langle \frac{1}{r^3} \right\rangle_{nlm}$. The radial part of the kinetic energy operator in coordinate representation reads

$$\frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}$$

Define $\hat{p}_r \leftrightarrow -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) = -i\hbar\left(\frac{1}{r}\frac{\partial}{\partial r} r\right)$

which is shorthand for

$$\langle r|\hat{p}_r|\psi\rangle = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}\left(r\langle r|\psi\rangle\right) = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}\left(r\psi(r)\right)$$

Then

$$\langle r|\frac{\hat{p}_r^2}{2m}|\psi\rangle = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r} r\left(\frac{1}{r}\frac{\partial}{\partial r}(r\psi(r)\right) = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi(r))$$

$$= -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r}\left(r\psi' + \psi\right) = -\frac{\hbar^2}{2m}\left(\psi'' + \frac{2}{r}\psi'\right).$$

while

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r} r^2\frac{\partial\psi}{\partial r} = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\psi'\right) = -\frac{\hbar^2}{2m}\left(\psi'' + \frac{2}{r}\psi'\right)$$

So the two are the same expressions.

Hence $\frac{\hat{p}_r^2}{2m}$ is the radial kinetic energy operator.

In an energy eigenstate

$$\langle n\ell m|[\hat{H}, \hat{p}_r]|n\ell m\rangle = \underbrace{\langle n\ell m|\hat{H}\hat{p}_r|n\ell m\rangle}_{=E_n\langle n\ell m|} - \underbrace{\langle n\ell m|\hat{p}_r\hat{H}|n\ell m\rangle}_{=E_n|n\ell m\rangle}$$

$$= \langle n\ell m|\hat{p}_r|n\ell m\rangle(E_n - E_n) = 0$$

On the other hand,

$$[\hat{H}, \hat{p}_r] = \left[\frac{\hat{p}_r^2}{2m} + \frac{1}{2mr^2}\hat{\vec{L}}^2 - \frac{e^2}{\hat{r}}, \hat{p}_r\right] =$$

$$= \left[\hat{p}_r, \frac{e^2}{\hat{r}} - \frac{\hat{L}^2}{2m\hat{r}^2}\right] \qquad (\hat{L}^2 \text{ and } \tfrac{1}{r^2} \text{ commute})$$

$$\Rightarrow 0 = \langle n\ell m | [\hat{H}, \hat{p}_r] | n\ell m \rangle = \int d^3r\, \psi^*_{n\ell m}(\vec{r}) (-i\hbar)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\left(\frac{e^2}{r} - \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right)\psi_{n\ell m}(\vec{r})$$

$$- \int d^3r\, \psi^*_{n\ell m}(\vec{r})\left(\frac{e^2}{r} - \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)(-i\hbar)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\psi_{n\ell m}(\vec{r})$$

(we used that $\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r)\, Y_{\ell m}(\vartheta,\varphi)$

and $\hat{L}^2 Y_{\ell m}(\vartheta,\varphi) = \hbar^2 \ell(\ell+1) Y_{\ell m}(\vartheta,\varphi)$)

$$= -i\hbar \int d^3r\, \psi^*_{n\ell m}(\vec{r})\left(-\frac{e^2}{r^2} + \frac{\hbar^2\ell(\ell+1)}{mr^3}\right)\psi_{n\ell m}(\vec{r})$$

(all other terms cancel)

$$= -i\hbar\left[\left\langle -\frac{e^2}{r^2}\right\rangle_{n\ell m} + \frac{\hbar^2\ell(\ell+1)}{m}\left\langle\frac{1}{r^3}\right\rangle_{n\ell m}\right]$$

$$\Rightarrow \left\langle\frac{1}{r^3}\right\rangle_{n\ell m} = \frac{me^2}{\hbar^2}\frac{1}{\ell(\ell+1)}\left\langle\frac{1}{r^2}\right\rangle_{n\ell m} = \frac{1}{\ell(\ell+1)\,a_0}\left\langle\frac{1}{r^2}\right\rangle_{n\ell m}$$

Plugging in the result from (2) this becomes

$$\left\langle\frac{1}{r^3}\right\rangle_{n\ell m} = \frac{1}{a_0^3 n^3}\frac{1}{\ell(\ell+\frac{1}{2})(\ell+1)} \qquad (17.3.20)$$

(4) Consider $\hat{H}(\lambda) = \hat{H}_{\text{coulomb}} + \lambda\frac{\hat{\vec{p}}^2}{2m} \equiv \hat{H}_0 + \lambda\hat{H}'$

We want $\langle H'\rangle_{n\ell m} = \left\langle\frac{\hat{\vec{p}}^2}{2m}\right\rangle_{n\ell m}$

We compute the eigenvalues of $\hat{H}(\lambda)$ exactly:

$$\hat{H}(\lambda) = \hat{H}_{\text{coulomb}}\left(\mu = \frac{m}{1+\lambda}\right)$$

$$\Rightarrow E_n(\lambda) = -\frac{me^4}{2\hbar^2(1+\lambda)n^2} = E_n^0 + \lambda \left.\frac{dE_n(\lambda)}{d\lambda}\right|_{\lambda=0} + \dots$$

$$= E_n^0 + \lambda E_n' + \dots$$

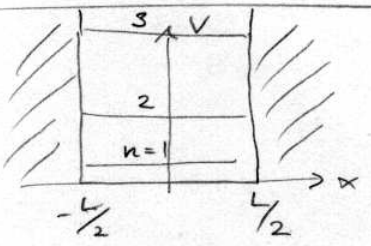
$$\Rightarrow E_n^{(1)} = \langle H' \rangle_{nlm} = \left.\frac{dE_n(\lambda)}{d\lambda}\right|_{\lambda=0} = \left. + \frac{me^4}{2\hbar^2(1+\lambda)^2 n^2}\right|_{\lambda=0}$$

$$= \frac{me^4}{2\hbar^2 n^2} = -E_n^0 = -\langle H^0 \rangle_{nlm}$$

$$\Rightarrow \langle \hat{T} \rangle_{nlm} = -\langle \hat{T} + \hat{V} \rangle_{nlm} \Rightarrow \boxed{\langle T \rangle_{nlm} = -\frac{1}{2}\langle \hat{V} \rangle_{nlm}}$$

Virial theorem for hydrogen (Coulomb potential) (13.1.33)

Exercise 18.2.3 (p. 478)



The semiclassical argument for the natural time period for a particle in the ground state of this box is given in the text on p. 479, Eq. (18.2.19)

Let's assume the box doubles its size in time $\tau \ll T \simeq \frac{mL^2}{\pi\hbar}$. This is a rapid change, and we can use the sudden approximation that $|\psi_{after}\rangle = |\psi_{before}\rangle = |\psi_{n=1,L}\rangle$ right after the change. The probability of catching the particle in the ground state of the new box is

$$P_{n=1}(2L) = \left|\langle n=1, 2L \,|\, n=1, L\rangle\right|^2$$

$$= \left| \int_{-\infty}^{\infty} dx \sqrt{\frac{2}{2L}} \cos\left(\frac{\pi x}{2L}\right) \Theta(L-|x|) \cdot \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right) \Theta\left(L-\left|\frac{x}{2}\right|\right) \right|^2$$

$$= \frac{2}{L^2} \left| \int_{-L/2}^{L/2} dx \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{2L}\right) \right|^2 \qquad \xi = \frac{\pi x}{L}$$

$$= 2 \left| \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} d\xi \cos(\xi) \cos(\xi/2) \right|^2$$

$$= 2 \left| \frac{1}{2\pi} \int_{0}^{\pi/2} d\xi \underbrace{\left(e^{i\xi} + e^{-i\xi}\right)\left(e^{i\xi/2} + e^{-i\xi/2}\right)}_{e^{3i\xi/2} + e^{i\xi/2} + e^{-i\xi/2} + e^{-3i\xi/2}} \right|^2$$

$$= 2 \left| \frac{1}{\pi} \int_{0}^{\pi/2} d\xi \left(\cos(3\xi/2) + \cos(\xi/2)\right) \right|^2$$

$$= \frac{2}{\pi^2} \left| \underbrace{\frac{2}{3}\sin\left(\frac{3\pi}{4}\right) + 2\sin\left(\frac{\pi}{4}\right)}_{4\sqrt{2}/3} \right|^2 = \left(\frac{8}{3\pi}\right)^2 \approx 0.721 = 72.1\%$$

Exercise 18.2.5 (p.478)

$$\hat{H} = \hat{H}^0 + \hat{H}' = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\hat{x}^2 - fx\,\theta(-t)$$

The external force f is abruptly turned off at $t=0$, and we can therefore use the sudden approximation that at $t=0^+$ the particle is still in the ground state of

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\left(\hat{x} - \frac{f}{m\omega^2}\right)^2 - \frac{1}{2}\frac{f^2}{m\omega^2}$$

Its energy is $E_0 = \hbar\omega/2 - \frac{f^2}{2m\omega^2}$, and its wavefunction is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}\left(x - \frac{f}{m\omega^2}\right)^2}$$

The corresponding state vector is

$$|0\rangle = \hat{T}\left(\frac{f}{m\omega^2}\right)|0^0\rangle = e^{-\frac{i}{\hbar}\frac{f}{m\omega^2}\hat{P}}|0^0\rangle \qquad (17.2.9)$$

where $|0^0\rangle$ is the ground state of $\hat{H}^0 = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\hat{x}^2$.

We want

$$P(n) = |\langle n^0|0\rangle|^2 = \left|\langle n^0| e^{-\frac{i}{\hbar}\frac{f}{m\omega^2}\hat{P}}|0^0\rangle\right|^2$$

$$= \left|\langle n^0| e^{-\frac{i}{\hbar}\frac{f}{m\omega^2}\sqrt{\frac{\hbar m\omega}{2}}\frac{\hat{a}-\hat{a}^\dagger}{i}}|0^0\rangle\right|^2$$

$$= \left|\langle n^0| e^{\frac{f}{\sqrt{2\hbar m\omega^3}}(\hat{a}^\dagger - \hat{a})}|0^0\rangle\right|^2 = \left|\langle n^0| e^{\sqrt{\lambda}(\hat{a}^\dagger - \hat{a})}|0^0\rangle\right|^2$$

where $\lambda = \frac{f^2}{2m\hbar\omega^3}$.

Now $e^{\sqrt{\lambda}(\hat{a}^\dagger - \hat{a})} = e^{\sqrt{\lambda}\hat{a}^\dagger} e^{-\sqrt{\lambda}\hat{a}} e^{-\frac{1}{2}\left[\sqrt{\lambda}\hat{a}^\dagger, -\sqrt{\lambda}\hat{a}\right]}$ $\qquad [\hat{a}^\dagger, \hat{a}] = -1$

$$= e^{-\lambda/2} e^{\sqrt{\lambda}\hat{a}^\dagger} e^{-\sqrt{\lambda}\hat{a}}$$

and $e^{-\sqrt{\lambda}\hat{a}}|0^o\rangle = |0^o\rangle$

$$\Rightarrow P(n) = e^{-\lambda}\left|\langle n^o| e^{\sqrt{\lambda}\hat{a}^+}|0^o\rangle\right|^2 = e^{-\lambda}\left|\langle n^o|\sum_{m=0}^{\infty}\frac{\lambda^{m/2}}{m!}(\hat{a}^+)^m|0^o\rangle\right|$$

Now $|m^o\rangle = \frac{(\hat{a}^+)^m}{\sqrt{m!}}|0^o\rangle$ and $\langle n^o|m^o\rangle = \delta_{mn}$

$$P(n) = e^{-\lambda}\left|\langle n^o|\sum_{m=0}^{\infty}\frac{\lambda^{m/2}}{\sqrt{m!}}|m^o\rangle\right|^2$$

$$= e^{-\lambda}\left|\sum_{m=0}^{\infty}\frac{\lambda^{m/2}}{\sqrt{m!}}\underbrace{\langle n^o|m^o\rangle}_{\delta_{mn}}\right|^2 = e^{-\lambda}\left|\frac{\lambda^{n/2}}{\sqrt{n!}}\right|^2$$

$$\Rightarrow P(n) = \frac{e^{-\lambda}\lambda^n}{n!}$$ as desired

Exercise 18.2.6 (p.478)

$$\int_{t=0^-}^{t=0^+}: \quad i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle = \left(H^0 + \hat{H}'\delta(t)\right)|\psi(t)\rangle$$

$$|\psi(0^+)\rangle - |\psi(0^-)\rangle = -\frac{i}{\hbar} \lim_{\varepsilon \to 0} \int_{-\varepsilon/2}^{\varepsilon/2} \left(\hat{H}^0 + \hat{H}'\delta(t)\right)|\psi(t)\rangle \, dt$$

$$= -\frac{i}{\hbar}\hat{H}'|\psi(0)\rangle \qquad (*)$$

If at $t = 0^-$ $|\psi(0^-)\rangle = |i^0\rangle$, and we expand $|\psi(0^+)\rangle$ in eigenstates of $\hat{H}^0$,

$$|\psi(0^+)\rangle = \sum_n c_n |n^0\rangle,$$

then (using the fact that $|\psi(0)\rangle = |\psi(0^-)\rangle + O(\hat{H}') = |i^0\rangle + O(\hat{H}')$

$$c_f = \langle f^0|\psi(0^+)\rangle = \underbrace{\langle f^0|i^0\rangle}_{=0 \text{ since } f \neq i} - \frac{i}{\hbar}\langle f^0|\hat{H}'|i^0\rangle + \text{higher orders}$$

$$\Rightarrow \boxed{c_f^{(1)} = -\frac{i}{\hbar}\langle f^0|\hat{H}'|i^0\rangle}$$

This only good to first order in $\hat{H}'$, since we made the replacement $|\psi(0)\rangle \to |i^0\rangle$ on the r.h.s. of $(*)$.