Physics 827: Homework Set No. 8

Due date: Friday, December 2, 2011, 1:00pm in PRB M2043 (Biao Huang's office)

Total point value of set: 110 points

Problem 1 (5 pts.): Exercise 7.4.1 (Shankar, p. 212)

Problem 2 (10 pts.): Exercise 7.4.2 (Shankar, p. 212)

Problem 3 (30 pts.): Exercise 7.4.5 (Shankar, p. 212)

Problem 4 (15 pts.): Exercise 7.4.6 (Shankar, p. 212)

Problem 5 (50 pts.): Exercise 7.5.4 (Shankar, p. 219)

Exercise 7.4.1 (p. 212) (5pts.)

$$\langle n'|\hat{X}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle n'|\hat{a}^+ + \hat{a}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\langle n'|n+1\rangle + \sqrt{n}\,\langle n'|n-1\rangle\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\delta_{n',n+1} + \sqrt{n}\,\delta_{n',n-1}\right) \checkmark$$

$$\langle n'|\hat{P}|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\,\langle n'|\hat{a}^+ - \hat{a}|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n+1}\,\delta_{n',n+1} - \sqrt{n}\,\delta_{n',n-1}\right) \checkmark$$

Exercise 7.4.2 (p. 212) (10pts.)

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}^+ + \hat{a}) \qquad \hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a}^+ - \hat{a})$$

From class

$$\langle n|\hat{X}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\delta_{n,n+1} + \sqrt{n}\,\delta_{n,n-1}\right) = 0$$

$$\langle n|\hat{P}|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{n+1}\,\delta_{n,n+1} - \sqrt{n}\,\delta_{n,n-1}\right) = 0$$

Next

$$\langle n|\hat{X}^2|n\rangle = \frac{\hbar}{2m\omega}\langle n|(\hat{a}^+ + \hat{a})^2|n\rangle = \frac{\hbar}{2m\omega}\langle n|(\hat{a}^+)^2 + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+ + \hat{a}^2|n\rangle$$

($(\hat{a}^+)^2 \sim \delta_{n,n+2} = 0$; $\hat{a}^2 \sim \delta_{n,n-2} = 0$)

$$= \frac{\hbar}{2m\omega}\left(\langle n|\hat{a}^+\hat{a}|n\rangle + \langle n|\hat{a}\hat{a}^+|n\rangle\right)$$

$$= \frac{\hbar}{2m\omega}\left(\langle n|\hat{a}^+\sqrt{n}\,|n-1\rangle + \langle n|\hat{a}\sqrt{n+1}\,|n+1\rangle\right)$$

$$= \frac{\hbar}{2m\omega}\left(\sqrt{n}\cdot\sqrt{n}\,\langle n|n\rangle + \sqrt{n+1}\,\sqrt{n+1}\,\langle n|n\rangle\right) = \frac{(2n+1)\hbar}{2m\omega}$$

$$\langle n|\hat{P}^2|n\rangle = -\frac{m\hbar\omega}{2}\langle n|(\hat{a}^+ - \hat{a})^2|n\rangle = -\frac{m\hbar\omega}{2}\langle n|\hat{a}^{+2} - \hat{a}^+\hat{a} - \hat{a}\hat{a}^+ + \hat{a}^2|n\rangle$$

($\hat{a}^{+2}|n\rangle \to 0$; $\hat{a}^2|n\rangle \to 0$)

$$= +\frac{m\hbar\omega}{2}\langle n|\hat{a}^+\hat{a} + \hat{a}\hat{a}^+|n\rangle = (2n+1)\frac{m\hbar\omega}{2}$$

$$\Rightarrow \Delta P\cdot\Delta X = \sqrt{\left(\langle\hat{X}^2\rangle - \underbrace{\langle\hat{X}\rangle^2}_{0}\right)\left(\langle\hat{P}^2\rangle - \underbrace{\langle\hat{P}\rangle^2}_{0}\right)}$$

$$= (2n+1)\sqrt{\frac{\hbar}{2m\omega}\cdot\frac{m\hbar\omega}{2}} = \left(n+\tfrac{1}{2}\right)\hbar$$

Exercise 7.4.5 (p.212) (30pts)

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

(1) $$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = e^{i(\hat{a}^+\hat{a}+\frac{1}{2})\omega t}|\psi(0)\rangle$$

$$= e^{-i\omega t/2}\sum_{n=0}^{\infty}\frac{(i\omega t)^n}{n!}(\hat{a}^+\hat{a})^n\frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)$$

(5pts) Since $\hat{a}^+\hat{a}|n\rangle = n|n\rangle \Rightarrow (\hat{a}^+\hat{a})^n|0\rangle = 0^n|0\rangle = 0 \quad (n\geq 1)$

$(\hat{a}^+\hat{a})^n|1\rangle = 1^n|1\rangle = |1\rangle \quad (n\geq 0)$

$$= \frac{e^{-i\omega t/2}}{\sqrt{2}}|0\rangle + \frac{e^{-i\omega t/2}}{\sqrt{2}}\underbrace{\sum_{n=0}^{\infty}\frac{(-i\omega t)^n}{n!}}_{e^{-i\omega t}}|1\rangle = \frac{e^{-i\omega t/2}}{\sqrt{2}}|0\rangle + \frac{e^{-3i\omega t/2}}{\sqrt{2}}|1\rangle.$$

(2) $$\langle\psi(0)|\hat{X}|\psi(0)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}\left(\langle 0|+\langle 1|\right)\left(\hat{a}^+ + \hat{a}\right)\left(|0\rangle+|1\rangle\right)$$

$$= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\Big(\underbrace{\langle 0|\hat{a}^+|0\rangle}_{0} + \underbrace{\langle 1|\hat{a}^+|0\rangle}_{1} + \underbrace{\langle 0|\hat{a}^+|1\rangle}_{0} + \underbrace{\langle 1|\hat{a}^+|1\rangle}_{0}$$
$$+ \underbrace{\langle 0|\hat{a}|0\rangle}_{0} + \underbrace{\langle 1|\hat{a}|0\rangle}_{0} + \underbrace{\langle 0|\hat{a}|1\rangle}_{1} + \underbrace{\langle 1|\hat{a}|1\rangle}_{0}\Big)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} = \langle\hat{X}\rangle(0) \quad (\neq 0!)$$

$$\langle\psi(0)|\hat{P}|\psi(0)\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\frac{1}{2}\left(\langle 0|+\langle 1|\right)\left(\hat{a}^+ - \hat{a}\right)\left(|0\rangle+|1\rangle\right)$$

(10pts.) $$= i\sqrt{\frac{m\hbar\omega}{2}}\frac{1}{2}\left(0+1+0+0 - (0+0+1+0)\right) = 0 = \langle\hat{P}\rangle(0)$$

$$\langle\psi(t)|\hat{X}|\psi(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}\left(\langle 0|e^{i\omega t/2} + \langle 1|e^{3i\omega t/2}\right)\left(\hat{a}^+ + \hat{a}\right)\left(e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right)$$

$$= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\Big(e^{i\omega t}\underbrace{\langle 1|\hat{a}^+|0\rangle}_{1} + e^{-i\omega t}\underbrace{\langle 0|\hat{a}|1\rangle}_{1}\Big)$$

(all other matrix elements are zero, see above)

$$= \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t) = \langle\hat{X}\rangle(t)$$

$$\langle\psi(t)|\hat{P}|\psi(0)\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\,\frac{1}{2}\left(\langle 0|e^{i\omega t/2} + \langle 1|e^{3i\omega t/2}\right)(\hat{a}^+ - \hat{a})\left(e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right)$$

$$= \frac{i}{2}\sqrt{\frac{m\hbar\omega}{2}}\left(e^{i\omega t}\langle 1|\hat{a}^+|0\rangle - e^{-i\omega t}\langle 0|\hat{a}|1\rangle\right) \quad \text{(all others are zero)}$$

$$= -\sqrt{\frac{m\hbar\omega}{2}}\sin(\omega t) = \langle\hat{P}\rangle(t)$$

(3) $\frac{d}{dt}\langle\hat{X}\rangle(t) = \frac{i}{\hbar}\langle[\hat{H},\hat{X}]\rangle(t) = \frac{i}{\hbar}\langle\psi(t)|\left[(\hat{a}^+\hat{a}+\frac{1}{2})\hbar\omega, \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^+ + a)\right]|\psi(t)\rangle$

$$= i\omega\sqrt{\frac{\hbar}{2m\omega}}\langle\psi(t)|\underbrace{[\hat{a}^+\hat{a}, \hat{a}^+ + \hat{a}]}_{\hat{a}^+ - \hat{a}\ \text{(see Exercise 7.4.6)}}|\psi(t)\rangle$$

$$= \frac{i}{m}\sqrt{\frac{m\hbar\omega}{2}}\langle\psi(t)|\hat{a}^+ - \hat{a}|\psi(t)\rangle = \frac{\langle\hat{P}\rangle(t)}{m} \qquad (\stackrel{1}{=})$$

(15 pts.)

$\frac{d}{dt}\langle\hat{P}\rangle(t) = \frac{i}{\hbar}\langle[\hat{H},\hat{P}]\rangle(t) = \frac{i}{\hbar}\langle\psi(t)|\left[(\hat{a}^+\hat{a}+\frac{1}{2})\hbar\omega, i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^+ - \hat{a})\right]|\psi(t)\rangle$

$$= -\omega\sqrt{\frac{m\hbar\omega}{2}}\langle\psi(t)|\underbrace{[\hat{a}^+\hat{a}, \hat{a}^+ - \hat{a}]}_{\hat{a}^+ + \hat{a}\ \text{(see Exercise 7.4.6)}}|\psi(t)\rangle$$

$$= -m\omega^2\sqrt{\frac{\hbar}{2m\omega}}\langle\psi(t)|\hat{a}^+ + \hat{a}|\psi(t)\rangle = -m\omega^2\langle\hat{X}\rangle(t) \qquad (\stackrel{2}{=})$$

We solve this by taking another derivative:

$$\frac{d^2\langle\hat{X}\rangle(t)}{dt^2} \stackrel{(1)}{=} \frac{1}{m}\frac{d\langle\hat{P}\rangle(t)}{dt} \stackrel{(2)}{=} -\omega^2\langle\hat{X}\rangle(t) \qquad (\stackrel{3}{=})$$

$$\frac{d^2\langle\hat{P}\rangle(t)}{dt^2} \stackrel{(2)}{=} -m\omega^2\frac{d\langle\hat{X}\rangle(t)}{dt} \stackrel{(1)}{=} -\omega^2\langle\hat{P}\rangle(t) \qquad (\stackrel{4}{=})$$

$(\stackrel{3}{=}) \Rightarrow \langle\hat{X}\rangle(t) = Ae^{i\omega t} + Be^{-i\omega t}$ general solution

$$\left.\begin{aligned}\langle\hat{X}\rangle(0) &= \sqrt{\frac{\hbar}{2m\omega}} = A + B\\ \frac{d}{dt}\langle\hat{X}\rangle\Big|_{t=0} &= \frac{\langle\hat{P}\rangle(0)}{m} = 0 = i\omega(A-B)\end{aligned}\right\}\ \text{initial values}$$

$$\Rightarrow A = B = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}} \Rightarrow \langle\hat{X}\rangle(t) = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1}{2}(e^{i\omega t} + e^{-i\omega t})\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t) \quad \text{as in (2)} \checkmark$$

$(\frac{4}{=}) \Rightarrow \langle \hat{P} \rangle(t) = Ce^{i\omega t} + De^{-i\omega t}$ general solution

$\langle \hat{P} \rangle(0) = 0 = C + D$

$\left.\frac{d\langle P \rangle}{dt}\right|_{t=0} = -m\omega^2 \langle \hat{X} \rangle(0) = -m\omega^2 \sqrt{\frac{\hbar}{2m\omega}} = -\omega\sqrt{\frac{\hbar m\omega}{2}}$ } initial values

$= i\omega(C - D)$

$\Rightarrow C = -D \Rightarrow 2i\omega C = -\omega\sqrt{\frac{\hbar m\omega}{2}}$

$\Rightarrow C = \frac{i}{2}\sqrt{\frac{\hbar m\omega}{2}}$

$\Rightarrow \underbrace{\langle \hat{P} \rangle(t)} = \sqrt{\frac{\hbar m\omega}{2}} \frac{i}{2}\left(e^{i\omega t} - e^{-i\omega t}\right) = \underbrace{-\sqrt{\frac{\hbar m\omega}{2}} \sin\omega t}$

as in part (2) ✓

Exercise 7.4.6 (p. 212) (15 pts.)

$$\langle \hat{a} \rangle(t) = \langle \psi(t) | \hat{a} | \psi(t) \rangle = \langle \psi(0) | \hat{U}^\dagger(t) \hat{a} \hat{U}(t) | \psi(0) \rangle$$

$$= \langle \psi(0) | e^{i\hat{H}t/\hbar} \hat{a} e^{-i\hat{H}t/\hbar} | \psi(0) \rangle$$

$$= \langle \psi(0) | e^{i(\hat{a}^\dagger\hat{a} + \frac{1}{2})\omega t} \hat{a} e^{-i(\hat{a}^\dagger\hat{a} + \frac{1}{2})\omega t} | \psi(0) \rangle$$

Now we know that

$$e^{\hat{L}} \hat{M} e^{-\hat{L}} = \sum_{n=0}^{\infty} \frac{1}{n!} [\hat{L}, \hat{M}]_{(n)}$$

Here $\hat{L} = i\hat{H}t/\hbar$ and $\hat{M} = \hat{a}$, so $[\hat{L}, \hat{M}]_{(n)} = \left(\frac{it}{\hbar}\right)^n [\hat{H}, \hat{a}]_{(n)}$.

$$[\hat{H}, \hat{a}]_{(0)} = \hat{a}$$

$$[\hat{H}, \hat{a}]_{(1)} \overset{\hbar\omega}{=} [\hat{a}^\dagger\hat{a}, \hat{a}] = \left(\hat{a}^\dagger \underbrace{[\hat{a}, \hat{a}]}_{0} + \underbrace{[\hat{a}^\dagger, \hat{a}]}_{-1} \hat{a}\right)\hbar\omega = -\hbar\omega\hat{a}$$

$$[\hat{H}, \hat{a}]_{(2)} = [\hat{H}, [\hat{H}, \hat{a}]_{(1)}] = -[\hat{H}, \hbar\omega\hat{a}] = +(\hbar\omega)^2 \hat{a}$$

$$\Rightarrow [\hat{H}, \hat{a}]_{(n)} = (-\hbar\omega)^n \hat{a}$$

Therefore

$$e^{i(\hat{a}^\dagger\hat{a} + \frac{1}{2})\omega t} \hat{a} e^{-i(\hat{a}^\dagger\hat{a} + \frac{1}{2})\omega t} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{it}{\hbar}(-\hbar\omega)\right)^n \hat{a}$$

$$= \hat{a} \sum_{n=0}^{\infty} (-it\omega)^n = e^{-i\omega t} \hat{a}$$

and

$$\langle \hat{a} \rangle(t) = \langle \psi(0) | e^{-i\omega t} \hat{a} | \psi(0) \rangle = e^{-i\omega t} \langle \psi(0) | \hat{a} | \psi(0) \rangle$$

$$= e^{-i\omega t} \langle \hat{a} \rangle(0)$$

✓

Similarly we show

$$e^{i(\hat{a}^+\hat{a}+\frac{1}{2})\omega t}\hat{a}^+ e^{-i(\hat{a}^+\hat{a}+\frac{1}{2})\omega t} = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{it}{\hbar}\right)^n [\hat{H},\hat{a}^+]_{(n)}$$

where

$$[\hat{H},\hat{a}^+]_{(0)} = \hat{a}^+,$$

$$[\hat{H},\hat{a}^+]_{(1)} = \hbar\omega\left[\hat{a}^+\hat{a},\hat{a}^+\right] = \hbar\omega\left(\hat{a}^+\underbrace{[\hat{a},\hat{a}^+]}_{1} + \underbrace{[\hat{a}^+,\hat{a}^+]}_{0}\hat{a}\right) = \hbar\omega\hat{a}^+,$$

$$[\hat{H},\hat{a}^+]_{(2)} = \hbar\omega[\hat{H},\hat{a}^+] = (\hbar\omega)^2\hat{a}^+,$$

$$\vdots$$

$$[\hat{H},\hat{a}^+]_{(n)} = (\hbar\omega)^n\hat{a}^+$$

thus

$$e^{i(\hat{a}^+\hat{a}+\frac{1}{2})\omega t}\hat{a}^+ e^{-i(\hat{a}^+\hat{a}+\frac{1}{2})\omega t} = \sum_{n=0}^{\infty}\frac{(i\omega t)^n}{n!}\hat{a}^+ = e^{i\omega t}\hat{a}^+$$

and

$$\underbrace{\langle\hat{a}^+\rangle(t)} = \langle\psi(0)|e^{i\hat{H}t/\hbar}\hat{a}^+ e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = \underbrace{e^{i\omega t}\langle\hat{a}^+\rangle(0)} \quad \checkmark$$

Exercise 7.5.4 (p. 219) (50 pts.)

For a system at temperature T ($\beta = \frac{1}{k_B T}$), the Boltzmann distribution

$$P(i) = \frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} \equiv \frac{1}{Z} e^{-\beta E_i}$$

gives the probability to find it in a state i of energy E_i.

(1) Average energy of the system:

$$\bar{E} = \sum_i E_i P(i) = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = \frac{1}{Z} \sum_i E_i e^{-\beta E_i}$$

(5 pts.)
$$\frac{\partial}{\partial \beta} \ln Z = \frac{1}{Z} \frac{\partial Z}{\partial \beta} = \frac{1}{Z} \frac{\partial}{\partial \beta} \left(\sum_i e^{-\beta E_i} \right) = -\frac{1}{Z} \sum_i E_i e^{-\beta E_i}$$

$$\Rightarrow \boxed{\bar{E} = -\frac{\partial}{\partial \beta} \ln Z}$$

(2) If the system is a classical oscillator, the position of the particle in the oscillator potential is described by a continuous variable x, and its momentum by a continuous variable p. A state of the particle is completely specified by specifying x and p:

$$i \longmapsto (x,p) \quad ; \quad \sum_i \longmapsto \int dx\, dp \quad ; \quad E_i \longmapsto E(x,p) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

(10 pts) The "partition function" Z_{cl} is then given by

$$Z_{cl} = \int dx\, dp\, e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2\right)} = \int_{-\infty}^{\infty} dx\, e^{-\frac{\beta m \omega^2}{2} x^2} \cdot \int_{-\infty}^{\infty} dp\, e^{-\frac{\beta}{2m} p^2}$$

$$= \sqrt{\frac{2\pi}{\beta m \omega^2}} \cdot \sqrt{\frac{2m\pi}{\beta}} = \frac{2\pi}{\beta\omega} \checkmark$$

The mean energy of the oscillator is

$$\bar{E}_{cl} = -\frac{\partial}{\partial \beta} \ln Z_{cl} = -\frac{\partial}{\partial \beta} \ln \frac{1}{\beta} = \frac{\partial}{\partial \beta} \ln \beta = \frac{1}{\beta} = k_B T \checkmark$$

A system of N non-interacting classical oscillators has mean thermal energy of $\frac{1}{2}k_BT$ per degree of freedom (x and p (for each dimension (x,y,z)) count as two independent degrees of freedom).

(3) Now look at the corresponding quantum oscillator.
Its states are labeled by the quantum number $n = 0, 1, 2, \ldots$, counting the number of phonon excitations above the ground state:

$$\underset{\sim}{Z}_{qu} = \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} \left(e^{-\beta\hbar\omega}\right)^n \quad \text{(geometric series)}$$

$$= \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} = \underset{\sim}{\frac{e^{\beta\hbar\omega/2}}{e^{\beta\hbar\omega}-1}} \quad \text{(partition function)}$$

and

$$\underset{\sim}{E}_{qu} = -\frac{\partial}{\partial\beta}\ln Z_{qu} = -\frac{1}{Z_{qu}}\frac{\partial}{\partial\beta}Z_{qu} = -\frac{1}{Z_{qu}}\cdot\left[\frac{-e^{\beta\hbar\omega/2}\hbar\omega e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\right.$$

(10pts)

$$= -\frac{1}{Z_{qu}}\left[e^{\beta\hbar\omega/2}\left(\frac{-\hbar\omega e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\right) + \frac{\frac{\hbar\omega}{2}e^{\beta\hbar\omega/2}}{e^{\beta\hbar\omega}-1}\right]$$

$$= -\frac{e^{\beta\hbar\omega/2}}{Z_{qu}}\hbar\omega\,\frac{-e^{\beta\hbar\omega}+\frac{1}{2}(e^{\beta\hbar\omega}-1)}{(e^{\beta\hbar\omega}-1)^2} =$$

$$= -\frac{\hbar\omega}{2}\underbrace{\frac{e^{\beta\hbar\omega/2}}{Z_{qu}}}_{\downarrow}\frac{-e^{\beta\hbar\omega}-1}{(e^{\beta\hbar\omega}-1)^2} =$$

$$= +\frac{\hbar\omega}{2}\left(e^{\beta\hbar\omega}-1\right)\frac{e^{\beta\hbar\omega}-1+2}{(e^{\beta\hbar\omega}-1)^2} = \frac{\hbar\omega}{2} + \hbar\omega\,\frac{1}{e^{\beta\hbar\omega}-1}$$

$$= \hbar\omega\left[\frac{1}{2} + \underbrace{\frac{1}{e^{\beta\hbar\omega}-1}}_{f_{BE}(\hbar\omega)\text{ Bose-Einstein distr.}}\right] \quad \checkmark$$

$\frac{\hbar\omega}{2}$ is the ground state energy, $\hbar\omega\, f_{BE}(\hbar\omega)$ is the thermal excitation energy.

(4) For $T \to \infty$, $\beta \to 0$. In this limit we can Taylor-expand the Bose-Einstein distribution:

$$\bar{E}_{qu} \xrightarrow[\beta \to 0]{T \to \infty} \hbar\omega \left[\frac{1}{2} + \frac{1}{1 + \beta\hbar\omega + \frac{1}{2}(\beta\hbar\omega)^2 + \dots - 1} \right]$$

$$= \hbar\omega \left[\frac{1}{2} + \frac{1}{\beta\hbar\omega} \frac{1}{1 + \frac{1}{2}(\beta\hbar\omega) + \dots} \right]$$

$$\xrightarrow{\beta \to 0} \frac{\hbar\omega}{2} + \frac{1}{\beta}\left(1 - \frac{1}{2}(\beta\hbar\omega) \pm \dots\right)$$

(10 pts)

$$\xrightarrow{\beta \to 0} \frac{1}{\beta}\left(1 + O(\beta\hbar\omega)\right) = k_B T \left(1 + O\left(\frac{\hbar\omega}{k_B T}\right)\right)$$

So we obtain the classical limit as $T \to \infty$, and corrections to the classical limit are of order $\hbar\omega / k_B T$, which is small as long as the thermal energy scale $k_B T$ is much larger than the phonon energy $\hbar\omega$, $k_B T \gg \hbar\omega$ or $\boxed{T \gg \frac{\hbar\omega}{k_B}}$ ✓

(5) For small oscillations we can model a crystal with N_0 atoms as $3N_0$ decoupled oscillators of different frequencies ω_i.

If these oscillators can be treated classically, the mean energy of the crystal is

$$\bar{E}^{cl.}_{crystal} = 3N_0 k_B T$$

since the mean energy stored in each oscillator is $k_B T$ independent of its frequency.

Defining the specific heat as

$$C(T) = \frac{1}{N_0}\frac{\partial \bar{E}}{\partial T}$$

We find

$$\boxed{C_{cl}(T) = \frac{1}{N_0}\frac{\partial}{\partial T}\left(3N_0 k_B T\right) = 3k_B}$$ ✓

independent of T and any crystal parameters, i.e. the same for all crystals made from monatomic molecules (that have no internal degrees of freedom, such as molecular vibrations and rotations).

(15 pts.) If we follow Einstein and treat the oscillators quantum mechanically (even though we can't duplicate his achievement of having done this in 1907, 16 years before the theory of quantum mechanics was discovered!), assuming for simplicity that all crystal normal modes have the same frequency ω, we get instead

$$\bar{E}^{qu}_{crystal}(T) = 3N_0\hbar\omega\left[\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right] \overset{\theta_E \equiv \frac{\hbar\omega}{k_B}}{=} 3N_0 k_B \theta_E\left[\frac{1}{2} + \frac{1}{e^{\theta_E/T}-1}\right]$$

and

$$C_{qu}(T) = \frac{1}{N_0}\frac{\partial}{\partial T}\bar{E}^{qu}_{crystal}(T) = 3k_B\theta_E \frac{-\left(\frac{\theta_E}{T^2}\right)e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2}$$

$$= 3k_B\left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2}$$ ✓

Here $\theta_E = \frac{\hbar\omega}{k_B}$ depends on the crystal frequency and varies from crystal to crystal.

Einstein's theory predict that $C(T)$ approaches zero exponentially as $T \to 0$. Experimentally one finds instead $C(T) \sim T^3$ for small T. Debye realized *) that this discrepancy was due to the (incorrect) assumption of the same ω for all normal modes; he fixed the discrepancy by including a realistic ω-spectrum for the crystal normal modes.

*) after the invention of quantum mechanics.