PHYS 418 Solutions Problem Set 7

1) photon occupation number

$$\langle n \rangle = \frac{\sum_n e^{-\beta\hbar\omega n}\, n}{\sum_n e^{-\beta\hbar\omega n}} = \frac{\sum_n e^{-\beta\hbar\omega n}\, n}{w}$$

where $w = \sum_n e^{-\beta\hbar\omega n}$

a) $$\frac{\partial\langle n\rangle}{\partial\beta} = \frac{1}{w}\sum_n e^{-\beta\hbar\omega n}\, n\,(-\hbar\omega n)$$

$$- \frac{1}{w^2}\left(\sum_n e^{-\beta\hbar\omega n}\, n\right)\frac{\partial w}{\partial\beta}$$

$$= \frac{-\hbar\omega\sum_n e^{-\beta\hbar\omega n}\, n^2}{w}$$

$$- \frac{1}{w^2}\left(\sum_n e^{-\beta\hbar\omega n}\, n\right)\left(\sum_n e^{-\beta\hbar\omega n}(-\hbar\omega n)\right)$$

$$= -\hbar\omega\langle n^2\rangle + \hbar\omega\langle n\rangle^2$$

So $$\boxed{-\frac{1}{\hbar\omega}\frac{\partial\langle n\rangle}{\partial\beta} = \langle n^2\rangle - \langle n\rangle^2}$$

b) For photons, $\langle n \rangle = \dfrac{1}{e^{\beta\hbar\omega}-1}$

so $$\frac{\partial\langle n\rangle}{\partial\beta} = \frac{-\hbar\omega\, e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

So
$$\langle n^2\rangle - \langle n\rangle^2 = \frac{-1}{\hbar\omega}\,\frac{\partial\langle n\rangle}{\partial\beta} = \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

and
$$\frac{\langle n^2\rangle - \langle n\rangle^2}{\langle n\rangle^2} = \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\cdot(e^{\beta\hbar\omega}-1)^2$$

$$= e^{\beta\hbar\omega}$$

Relative fluctuation is
$$\frac{\sqrt{\langle n^2\rangle - \langle n\rangle^2}}{\langle n\rangle} = e^{\beta\hbar\omega/2} \geqslant 1$$

so fluctuations are always large

The bigger is $\beta\hbar\omega$, ie the smaller is $\frac{k_B T}{\hbar\omega}$, the larger the fluctuations are.

2) $H = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2$ x is displacement from equilibrium position

a) Classically, use the equipartition theorem

$$\left\langle \frac{1}{2} m\omega_0^2 x^2 \right\rangle = \frac{1}{2} k_B T$$

as x is a quadratic degree of freedom, it contributes $\frac{1}{2}k_BT$ to the average energy

$$\Rightarrow \boxed{\langle x^2 \rangle = \frac{k_B T}{m\omega_0^2}}$$

by symmetry $\langle x \rangle = 0$
so $\langle (\Delta x)^2 \rangle = \langle x^2 \rangle$

b) Quantum mechanically: use the quantum virial theorem

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{1}{2} m\omega_0^2 x^2 \right\rangle = \frac{1}{2}\langle H \rangle$$

$$\langle x^2 \rangle = \frac{\langle H \rangle}{m\omega_0^2}$$

again $\langle x \rangle = 0$

To comute $\langle H \rangle$, we know that $\langle H \rangle = \hbar\omega_0 \left[\langle n \rangle + \frac{1}{2} \right]$

where

$$\langle n \rangle = \frac{1}{e^{\beta\hbar\omega_0} - 1}$$

is the average excitation number of the oscillator

so

$$\boxed{\langle x^2 \rangle = \frac{\hbar\omega_0}{m\omega_0^2} \left[\frac{1}{e^{\beta\hbar\omega_0} - 1} + \frac{1}{2} \right]}$$

$$= \frac{\hbar}{2m\omega_0} \left[\frac{e^{\beta\hbar\omega_0} + 1}{e^{\beta\hbar\omega_0} - 1} \right]$$

c) We expect the quantum result to reduce to the classical result when $k_B T \gg \hbar\omega_0$
ie when thermal energy is much greater than the quantum energy level spacing

So when $k_B T \gg \hbar\omega_0 \Rightarrow \beta\hbar\omega_0 \ll 1$

$$\langle x^2 \rangle \simeq \frac{\hbar}{m\omega_0}\left[\frac{1}{1+\beta\hbar\omega_0 - 1} + \frac{1}{2}\right] \quad \text{as } e^x \sim 1 + x + \cdots \text{ as } x \to 0$$

$$= \frac{\hbar}{m\omega_0}\left[\frac{k_B T}{\hbar\omega_0} + \underbrace{1/2}_{\text{ignore since } \frac{1}{\beta\hbar\omega_0} \gg 1}\right]$$

$$\simeq \frac{k_B T}{m\omega_0^2} \quad \text{same as classical result}$$

We could also have done the quantum calculation a more straightforward way. The position operator for the quantum oscillator is

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}}\,(a^{+} + a)$$

So

$$\hat{x}^2 = \frac{\hbar}{2m\omega_0}(a^{+}+a)(a^{+}+a)$$

$$= \frac{\hbar}{2m\omega_0}(a^{+}a^{+} + aa^{+} + a^{+}a + aa)$$

The thermal average is then

$$\langle \hat{x}^2 \rangle = Tr[\hat{\rho}\,\hat{x}^2]$$

which is most easily evaluated in the energy eigenstate basis

$$\langle \hat{x}^2 \rangle = \sum_n \rho_n \langle n | \hat{x}^2 | n \rangle$$

where $$\rho_n = \frac{e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

and $E_n = \hbar\omega(n+1/2)$ are the energy eigenvalues

We have

$$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega_0}\langle n|a^\dagger a^\dagger + aa^\dagger + a^\dagger a + aa|n\rangle$$

now $\langle n|a^\dagger a^\dagger|n\rangle = \langle n|aa|n\rangle = 0$

and $[a, a^\dagger] = 1 \Rightarrow aa^\dagger = a^\dagger a + 1$

So

$$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega_0}\langle n|\,2a^\dagger a + 1\,|n\rangle$$

Now $a^\dagger a = \hat{n}$ is just the number operator, so

$$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega_0}(2n+1)$$

$$= \frac{\hbar}{m\omega_0}(n + 1/2) = \frac{E_n}{m\omega_0^2}$$

So

$$\langle \hat{x}^2\rangle = \sum_n \rho_n \frac{E_n}{m\omega_0^2} = \frac{1}{m\omega_0^2}\langle E\rangle$$

where $\langle E\rangle = \hbar\omega_0(\langle n\rangle + 1/2)$

using $\langle n\rangle = \dfrac{1}{e^{\beta\hbar\omega_0} - 1}$

we recover our previous result.