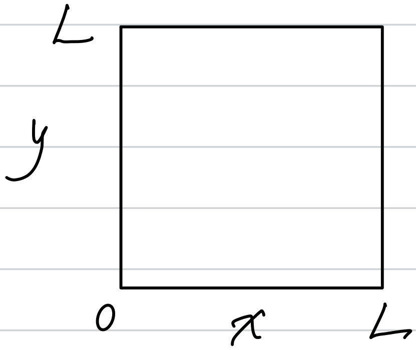
PHYS 418 Solutions Problem Set 7

1) <u>particle in a box</u> - <u>fixed b.c.</u>



$\psi = 0$ on boundary surfaces at $\begin{cases} x = 0, L \\ y = 0, L \\ z = 0, L \end{cases}$

$$-\frac{\hbar^2}{2m}\nabla^2 \psi = \varepsilon \psi \quad \text{energy eigenstates}$$

we know solutions to Schrodinger's equation are

$$\phi_k = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \quad \text{with energy } \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

But these <u>do not</u> satisfy the desired boundary conditions.

To see how to construct solutions that will obey the desired boundary conditions, consider first a particle in a <u>one dimensional</u> box.

For each k there are two degenerate plane wave solutions

$$\phi_k = \frac{e^{ikx}}{\sqrt{L}} \quad \text{and} \quad \phi_{-k} = \frac{e^{-ikx}}{\sqrt{L}} \quad \text{both with } \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

Any linear combination of these

two is then also a solution with $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$

Let's consider $\psi_k = \frac{\phi_k - \phi_{-k}}{\sqrt{2}} = \sqrt{\frac{2}{L}} \sin(kx)$

$$\tilde{\psi}_k = \frac{\phi_k + \phi_{-k}}{\sqrt{2}} = \sqrt{\frac{2}{L}} \cos(kx)$$

Now $\tilde{\psi}_k(0) \neq 0$ so that one is no good.

But $\psi_k(0) = 0$, so this is a contender!

We also need $\psi_k(L) = 0$. This will happen if $k = \frac{\pi}{L} m$ for m integer $1, 2, 3, \ldots$

Note, we do not allow $m = 0$ because that would give $\psi_k = 0$. And we do not allow integer $m < 0$ since

$$\sin\left(-m\frac{\pi}{L}x\right) = -\sin\left(\frac{m\pi}{L}x\right)$$

is not a new solution.

We can now construct a solution for the three dimensional problem that satisfies the desired boundary conditions

$$\psi_{\vec{k}}(\vec{r}) = \sqrt{\frac{8}{V}} \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

where $k_x = \frac{\pi}{L} m_x$, $k_y = \frac{\pi}{L} m_y$, $k_z = \frac{\pi}{L} m_z$

$m_x, m_y, m_z = 1, 2, 3, \ldots$ integer

The spacing between allowed values of any component of $\vec{k}$ is

$$\Delta k = \frac{\pi}{L}$$

and we must have $k_x, k_y, k_z > 0$

The energy of such a state is

$$\varepsilon_{\vec{k}} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

Number of states

The number of states with $\varepsilon_{\vec{k}} < E$ will be the number of allowed $\vec{k}$ that lie within the volume of a sphere in k-space of radius $k = \sqrt{\frac{2mE}{\hbar^2}}$

Since we require all $k_\mu > 0$, we are only interested in the octant of the sphere with $k_x, k_y, k_z > 0$. This has volume $\frac{1}{8}\frac{4}{3}\pi k^3 = \frac{\pi}{6}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$

since the spacing between allowed k_μ is $\frac{\pi}{L}$, the volume of k-space per allowed value of $\vec{k}$ is $\left(\frac{\pi}{L}\right)^3$. So we then have

$$\# \text{ states} = \frac{\frac{\pi}{6}\left(\frac{2mE}{\hbar^2}\right)^{3/2}}{\left(\frac{\pi}{L}\right)^3}$$

$$= \frac{V}{6\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

and finally the number of states per unit volume is

$$\boxed{G(E) = \frac{1}{6\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}}$$

Periodic boundary conditions

For this case the energy eigenstates are

$\phi_k = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$ where $k_x = \frac{2\pi}{L} n_x$,

$k_y = \frac{2\pi}{L} m_y$, $k_z = \frac{2\pi}{L} m_z$

with $m_x, m_y, m_z = 0, \pm 1, \pm 2, \ldots$

all integers, positive and negative.

The energy of this state is $\varepsilon_k = \frac{\hbar^2}{2m} k^2$

The number of allowed states with $\varepsilon_k < \varepsilon$ is then the number of allowed $\vec{k}$ within a sphere in k-space of radius

$$k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$$

Since k_x, k_y, k_z can include negative values, we take the volume of the entire sphere $\frac{4}{3}\pi k^3 = \frac{4}{3}\pi \left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2}$

Now the spacing between allowed values of k_μ is $\frac{2\pi}{L}$, so the volume of k-space per allowed value of $\vec{k}$ is $\left(\frac{2\pi}{L}\right)^3$

The number of allowed states with $\varepsilon_k < \varepsilon$ is therefore

$$\# \text{ states} = \frac{\frac{4}{3}\pi\left(\frac{2mE}{\hbar^2}\right)^{3/2}}{\left(\frac{2\pi}{L}\right)^3}$$

$$= \frac{V}{6\pi^6}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

So the number of states per unit volume is

$$\boxed{G(E) = \frac{1}{6\pi^6}\left(\frac{2mE}{\hbar^2}\right)^{3/2}}$$

This is exactly the same as we found for the <u>fixed boundary</u> conditions!

2)

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

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

$$\frac{\sqrt{\langle n^2 \rangle - \langle n \rangle^2}}{\langle n \rangle} = e^{\beta\hbar\omega/2} \geq 1$$

so fluctuations are always large

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

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

a) Classically, use the equipartition theorem

$$\langle \tfrac{1}{2} m \omega_0^2 x^2 \rangle = \tfrac{1}{2} k_B T$$

as x is a quadratic degree of freedom, it contributes $\frac{1}{2} k_B T$ 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

$$\langle \tfrac{p^2}{2m} \rangle = \langle \tfrac{1}{2} m \omega_0^2 x^2 \rangle = \tfrac{1}{2} \langle H \rangle$$

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

again $\langle x \rangle = 0$

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

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

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

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

$$= \frac{\hbar}{m\omega_0}\left[\frac{k_B T}{\hbar\omega_0} + \frac{1}{2}\right]$$

ignore since $\frac{1}{\beta\hbar\omega_0} \gg 1$

$$\simeq \frac{k_B T}{m\omega_0^2}$$ 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.