Quantum Mechanics (PH101)
Tutorial-1
due on Friday, 12th of February, 2021 (8:00Hrs IST)

1. The lifetime of a given atom in an excited state is 10^{-8} s. It comes to the ground state by emitting a photon of wavelength 5800 $\mathring{A}$. Find the energy uncertainty and wavelength uncertainty of the photon. Use the minimum time-Energy uncertainty principle $\Delta E \Delta t = \hbar/2$.

   Solution:

   Here we will use the time-Energy uncertainty principle $\Delta E \Delta t = \hbar/2$.

   For the given problem the photon can be emitted at any instant during the time interval $\Delta t = 10^{-8}$ s.

   $\therefore$ The energy uncertainty of the photon is

$$\Delta E = \frac{\hbar}{2\Delta t} = \frac{0.527 \times 10^{-34}\ J.s}{10^{-8}\ s} = 0.527 \times 10^{-26}\ J$$

   If λ is the wavelength of the photon then,

$$E = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E} \Rightarrow \Delta\lambda = hc\left(\frac{-\Delta E}{E^2}\right)$$

   So the uncertainty in wavelength is

$$\Delta\lambda = \frac{hc}{E^2}\Delta E = \frac{hc\lambda^2}{h^2c^2}\Delta E = \frac{\lambda^2}{hc}\Delta E$$

$$= \frac{(5.8 \times 10^{-7} m)^2 \times (0.527 \times 10^{-26} J)}{(6.62 \times 10^{-34} Js) \times (3 \times 10^8 m/s)} = 0.89 \times 10^{-14} m \sim 9 \times 10^{-5} \mathring{A}$$

2. Find the uncertainty in the velocity of a particle if the uncertainty in its position is equal to its (a) de Broglie wavelength (b) Compton wavelength. Use the minimum position and momentum uncertainty relation.

   Solution:

   From the uncertainty principle we know that

$$\Delta x \Delta p = \hbar/2$$

$$\Delta v = \frac{\hbar}{2m\Delta x}$$

(a) If the uncertainty in position is equal to the de Broglie wavelength

$$\Delta x = \lambda = h/mv$$

So the uncertainty in velocity is

$$\Delta v = \frac{\hbar}{2m\Delta x} = v/4\pi$$

(b)If the uncertainty in position is equal to the Compton wavelength

$$\Delta x = \lambda_C = \frac{h}{mc}$$

So,

$$\Delta v = \frac{\hbar}{2m\Delta x} = c/4\pi$$

Therefore, the uncertainty in velocity is of the order to the speed of light in vacuum.

3. Check if $\Psi = Ae^{i(kx-\omega t)}$ and $\Psi = Asin(kx - \omega t)$ are acceptable solutions of the time-dependent Schroedinger's equation, where A is constant. Also treat 'U' as a constant. The time-dependent Schroedinger'e equation is given by

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U\Psi$$

Solution:
The time-dependent Schrodinger's equation is given by

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U\Psi$$

For $\Psi = Ae^{i(kx-\omega t)}$**:**

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)} = -i\omega\Psi$$

$$\frac{\partial \Psi}{\partial x} = ik\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = i^2 k^2 \Psi = -k^2 \Psi$$

Inserting these in the Schroedinger's equation yields

$$i\hbar(-i\omega\Psi) = -\frac{\hbar^2}{2m}(-k^2\Psi) + U\Psi$$

$$\Rightarrow \left(\hbar\omega - \frac{\hbar^2 k^2}{2m} - U\right)\Psi = 0$$

Using $E = h\nu = \hbar\omega$ and $p = \hbar k$, we obtain

$$\left(E - \frac{p^2}{2m} - U\right)\Psi = 0$$

Note that the quantity on the left is equal to zero for the non-relativistic case as $E = K.E + U = \frac{p^2}{2m} + U$.

Thus $\Psi = Ae^{i(kx-\omega t)}$ is a solution of the Schroedinger's equation.

For $\Psi = Asin(kx - \omega t)$**:**

Following the similar process as above we will reach at

$$-i\hbar\omega cos(kx - \omega t) = \left(\frac{\hbar^2 k^2}{2m} + U\right) sin(kx - \omega t)$$

This equation is generally not satisfied for all x and t. Hence $\Psi = Asin(kx - \omega t)$ is not an acceptable solution of the time-dependent Schrodinger equation. This function however, is a solution of the classical wave equation.

4. The normalized wave function of the ground state of the Quantum harmonic oscillator is given by $\psi(x) = C_0 e^{-\alpha x^2}$, where $C_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$ and $\alpha = \frac{m\omega}{2\hbar}$. m is the mass and ω is the angular frequency of the oscillator.
Compute the $\Delta x \Delta p$ for this state, where Δx and Δp are the uncertainties in the position x and momentum p, respectively. Please comment over the result whether it is consistent with the uncertainty principle. **Use the Gaussian integral** $\int_{-\infty}^{\infty} e^{-\alpha x^2 + \beta x} dx = \sqrt{\frac{\pi}{\alpha}} e^{\beta^2/4\alpha}$.

Solution: We have $< x >= \int_{-\infty}^{\infty} x|\psi(x)|^2 = 0$ as inegrand is odd function.

$< x^2 >= \int_{-\infty}^{\infty} x^2|\psi(x)|^2 = \frac{1}{4\alpha}C_0^2\left[xe^{-2\alpha x^2}|_{-\infty}^{\infty} + \frac{1}{2\alpha}\int_{-\infty}^{\infty} e^{-2\alpha x^2}\right].$

The first part of the above expression will be zero as e^{-x^2} approaches to zero faster than when x tends to ∞. The second integral is the standard Gaussian integral for which we get $< x^2 >= \frac{\hbar}{2m\omega}$.

Now $\Delta x = \sqrt{< x^2 > - < x >^2} = \sqrt{\frac{\hbar}{2m\omega}}$.

$< p >= -i\hbar\int_{-\infty}^{\infty} \psi^*(x)\frac{d\psi(x)}{dx}dx = 0$. Again inetgrand here is odd function.

$< p^2 >= -\hbar^2\int_{-\infty}^{\infty} \psi^*(x)\frac{d^2\psi(x)}{dx^2}dx = \hbar^2\left[2\alpha\int|\psi|^2dx - 4\alpha^2 < x^2 >\right] = \hbar^2\left[2\left(\frac{m\omega}{2\hbar}\right) - 4\left(\frac{m\omega}{2\hbar}\right)^2\frac{\hbar}{2m\omega}\right].$

So Finally we have,

$< p^2 >= \frac{m\hbar\omega}{2}$.

Therefore, $\Delta p = \sqrt{(< p^2 > - < p >^2)} = \sqrt{\frac{m\hbar\omega}{2}}$.

Now $\Delta x\Delta p = \hbar/2$. This is, for the optimum state (Gaussian state) the product of the uncertainties of position and momentum is the smallest value allowed by Heisenberg's Uncertainty relation:

$\Delta p\Delta x \geq \hbar/2$.

5. An electron is described by the wave function

$$\psi(x) = \begin{cases} 0, & \text{for } x \leq 0 \\ Ce^{-x}(1-e^{-x}), & \text{for } x > 0, \end{cases}$$

where x is in nm and C is a constant.

(a) Determine the value of C that normalizes $\psi(x)$.

(b) Where is the electron most likely to be found?

(c) Calculate the average position or expectation value of the position $< x >$ for the electron. Compare this with the most likely position, and comment on the difference.

Solution:

(a) We have the normalization condition:

$\int_{-\infty}^{\infty} |\psi^2| = 1$. We get $|C| = 2\sqrt{3}\ \ nm^{-1/2}$.

(b)The most likely place x_m for the electron will be where $|\psi(x)|^2$ is maximum, or, in this case where $\psi(x)$ is maximum. We have

$$\frac{d\psi(x)}{dx} = 0 \Rightarrow C[e^{-2x} - e^{-x}(1-e^{-x}) = 0 \Rightarrow x = ln2\ \ nm = 0.693\ \ nm.$$

(c) Since electron state is in the stationary state. Its average position is given by

$$< x >= \int_{-\infty}^{\infty} \psi(x)x\psi^*(x) = C^2 \int_0^{\infty} xe^{-2x}[1-e^{-2x}]^2 = 12 \int_0^{\infty} xe^{-2x}[1-2e^{-x}+e^{-2x}]$$

Using integration by parts we have,

$$< x >= C^2 \left[\frac{1}{4} - \frac{2}{9} + \frac{1}{16}\right] = \frac{13}{12}\ \ nm \simeq 1.083\ \ nm$$

6. A particle is represented by the wavefunction at time $t = 0$ by

$\Psi(x) = A(a^2 - x^2)$ if $-a \le x \le a$ and zero at all other places. Here A and a are constant.

(a) Determine the normalization constant A.
(b) What is the expectation value of x at $t = 0$?
(c) What is the expectation value of p at $t = 0$?
(d) Evaluate $\langle x^2 \rangle$ and $\langle p^2 \rangle$ at $t = 0$.
(e) Obtain the uncertainty relation $(\Delta x \Delta p)$ and comment over your result whether you are getting minimum uncertainty relation or not.

Solution:

(a) The normalization condition is

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\Psi(x)|^2 dx \\ &= \int_{-a}^{a} |\Psi(x)|^2 dx \\ &= \int_{-a}^{a} A^2(a^2-x^2)^2 dx \ = 2A^2\left[a^5 - \frac{2}{3}a^5 + \frac{a^5}{5}\right] = \frac{16}{15}A^2a^5 \end{aligned}$$

$$\Rightarrow A = \sqrt{\frac{15}{16a^5}}$$

(b) The expectation value of x at $t = 0$ is

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi(x)|^2 dx$$

$$\langle x \rangle = \int_{-a}^{a} xA^2(a^2 - x^2)^2 dx$$

This integral is zero since the integrand is an odd function of x.

(c) $\langle p \rangle$ will also be zero due to the above reason given in (b).

(d) Expectation value of x^2 at $t = 0$ is

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(a)x^2\Psi(x)dx = \int_{-\infty}^{\infty} x^2|\Psi(x)|^2 dx$$

$$= \int_{-a}^{a} x^2 A^2(a^2 - x^2)^2 dx = \frac{a^2}{7}$$

(e) Expectation value of p^2 at $t = 0$ is

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(a)p^2\Psi(x)dx = \int_{-a}^{a} \Psi^*(a)\left(-\hbar^2 \frac{d^2}{dx^2}\right)\Psi(x)dx$$

$$= \frac{5\hbar^2}{2a^2}$$

(f) $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle x^2 \rangle = \dfrac{a^2}{7}$

$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \langle p^2 \rangle = \dfrac{5\hbar^2}{2a^2}$

$(\Delta x)^2(\Delta p)^2 = \dfrac{5}{14}\hbar^2$

$\Delta x \Delta p = \sqrt{\dfrac{5}{14}}\hbar$

Note that here we get $\Delta x \Delta p > \hbar/2$ because the given wave function is non-Gaussian.

Quantum Mechanics (PH101)
Tutorial-2
due on Friday, 19th of February, 2021 (8:00Hrs IST)

1. Consider the wave function

$$\Psi(x,t) = \left[Ae^{ipx/\hbar} + Be^{-ipx/\hbar}\right] e^{-ip^2t/2m\hbar}$$

Find the probability current density corresponding to this wave function. Here, p is the momentum of the particle and A and B are complex numbers independent of 'x' and 't'.

Solution:
The probability current density is by definition

$$J(x,t) = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)$$

So,

$$\begin{aligned} J(x,t) = & \frac{\hbar}{2mi}\left[\left(A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}\right)\left(\frac{ip}{\hbar}Ae^{ipx/\hbar} - \frac{ip}{\hbar}Be^{-ipx/\hbar}\right)\right] \\ & - \frac{\hbar}{2mi}\left[\left(Ae^{ipx/\hbar} + Be^{-ipx/\hbar}\right)\left(\frac{-ip}{\hbar}A^*e^{-ipx/\hbar} + \frac{ip}{\hbar}B^*e^{ipx/\hbar}\right)\right] \end{aligned}$$

So we get $J(x,t) = \dfrac{p}{m}(|A|^2 - |B|^2)$.
Note that the wave function $\Psi(x,t)$ is the superpostion of two currents of particles moving in opposite direction. Each of the current is constant and time independents in magnitude. The term $e^{-ip^2t/2m\hbar}$ implies that the particles are of energy $p^2/2m$. The amplitudes of the curents in the left and right directions are respectively A and B.

2. Consider a particle of mass m confined in a potential given by

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a \\ \infty, & \text{if } x < 0 \text{ or } x > a. \end{cases}$$

The energy eigen states of the particle are given by $\psi_n(x) = \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{n\pi}{a}x\right)$ with eigen energy $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$, where $n = 1, 2, 3, ...$

(A) At $t = 0$ an initial wave function is the mixture of two stationary states (first ($\psi_1(x)$) and second ($\psi_2(x)$) energy eigen-states) and given by $\psi(x, t = 0) = \sqrt{\dfrac{1}{3}}\psi_1(x) + \sqrt{\dfrac{2}{3}}\psi_2(x)$.

(i) What is the average energy, $< E >$ of the particle at $t = 0$?

(ii) In a measurement of energy, what is the probability to get the energy $E = E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$?

(iii) What will be the form of state $\psi(x,t)$ at later time t? Note that $\psi(x,t)$ can be written as the superposition of stationary eigen states i.e. $\psi(x,t) = \sum_n C_n \psi_n(x) e^{-iE_nt/\hbar}$, where C_n is the probability amplitude of the finding the state in the n^{th} eigen state.

(iv) What is the value of $< E >$ of the particle at time t?

(B) Consider a particle with energy E_1 in the box.

(i) What is expectation value of the position of the particle?
(ii) What is the probability to find it in the region $0 \leq x \leq \dfrac{a}{2}$?

(C) Repeat the above (part (**B (i) and B(ii)**) for the particle of energy E_2.

Solution:

(A)(i) We have $H\psi_n = E_n\psi_n$ with $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$. The average value of the energy at $t = 0$,

$< E >= \int_o^a \psi(x,t=0)^* H\psi(x,t=0)dx$
$= \int_0^a \Big(\sqrt{\frac{1}{3}}\psi_1(x) + \sqrt{\frac{2}{3}}\psi_2(x)\Big) H \Big(\sqrt{\frac{1}{3}}\psi_1(x) + \sqrt{\frac{2}{3}}\psi_2(x)\Big) dx$
$= \int_0^a \Big(\sqrt{\frac{1}{3}}\psi_1(x) + \sqrt{\frac{2}{3}}\psi_2(x)\Big) \Big(\sqrt{\frac{1}{3}}E_1\psi_1(x) + \sqrt{\frac{2}{3}}E_2\psi_2(x)\Big) dx$
Using the orthonormality condition of the eigen-states $\int \psi_n^*(x)\psi_m(x) = \delta_{mn}$ we have
$< E >= \dfrac{E_1}{3} + \dfrac{2E_2}{3}$.

(ii)The probability to yield E_1 in a measurement is given by

$$P_{E_1} = |\int_0^a \psi(x,t=0)^*\psi_1(x,t=0)dx|^2 = \frac{1}{3}$$

(iii) Time evolution of the energy eigen states are $\psi_n(x,t) = e^{-\frac{E_nt}{\hbar}}\psi_n(x,t=0)$. That gives,

$$\psi(x,t) = \sqrt{\frac{1}{3}}\psi_1(x)e^{\frac{-iE_1t}{\hbar}} + \sqrt{\frac{2}{3}}\psi_2(x)e^{\frac{-iE_2t}{\hbar}}$$

(iv) $< E(t) >= \int_0^a \psi(x,t)^* H\psi(x,t) = \int_0^a \psi(x,0)^* H\psi(x,0) =< E >_{t=0}$.

(B)(i)

$$< x >= \frac{2}{a}\int_0^a x \sin^2\left(\frac{\pi x}{a}\right) dx = \frac{a}{2}$$

(ii)

$$P_{0\le x\le \frac{a}{2}} = \frac{2}{a}\int_0^{a/2} \sin^2\left(\frac{\pi x}{a}\right)dx = \frac{1}{2}$$

(C)(i)

$$< x >= \frac{2}{a}\int_0^{a} x\sin^2\left(\frac{2\pi x}{a}\right)dx = \frac{a}{2}$$

(ii)

$$P_{0\le x\le \frac{a}{2}} = \frac{2}{a}\int_0^{a/2} \sin^2\left(\frac{2\pi x}{a}\right)dx = \frac{1}{2}$$

3. The probability of finding a particle of mass m confined in an infinitely deep potential well of width $2a$ in the ground state, first excited state and second excited state are 60%, 30% and 10% respectively. Find the normalized wave function of the particle and the energy expectation value.

Solution:

Let ψ_1, ψ_2 and ψ_3 be the eigenfunctions and $E_1,\ E_2,$ and E_3 be the energy eigenvalues for the ground state, first excited state and second excited state respectively. The wave function Ψ of the particle is a combination of these three states.

Let $\Psi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3$

where $|c_1|^2 = \frac{60}{100} = \frac{3}{5}$, $|c_2|^2 = \frac{30}{100} = \frac{3}{10}$ and $|c_3|^2 = \frac{10}{100} = \frac{1}{10}$

So, $\Psi = \sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{3}{10}}\psi_2 + \sqrt{\frac{1}{10}}\psi_3$, represents the wave function.

The ground state energy is $E_1 = \frac{\hbar^2\pi^2}{8ma^2}$. So $E_2 = 4E_1$ and $E_3 = 9E_1$.

The energy expectation value is

$$\langle E\rangle = |c_1|^2E_1 + |c_2|^2E_2 + |c_3|^2E_3$$

$$= \tfrac{3}{5}E_1 + \tfrac{3}{10}E_2 + \tfrac{1}{10}E_3$$

$$= \tfrac{3}{5}E_1 + \tfrac{3}{10}4E_1 + \tfrac{1}{10}9E_1 = \tfrac{27}{10}E_1 = \tfrac{27\hbar^2\pi^2}{80ma^2}$$

4. Find the probability that a particle trapped in a box of length L wide can be found between $0.45L$ and $0.55L$ when it is (i)in the ground and (ii) in first excited states.

Solution:

This part of the box is one-tenth of the box's width and is centered on the middle of the box. Classically we would expect the particle to be in this region 10 percent of the time. Quantum mechanics gives quite different predictions that depend on the quantum number of the particle's state.

The probability of finding the particle between x_1 and x_2 when it is in the n^{th} state is give as

$$P_{x_1,x_2} = \int_{x_1}^{x_2} |\psi_n|^2 dx = \frac{2}{L}\int_{x_1}^{x_2} sin^2\ \frac{n\pi x}{L} dx$$

$$= \left[\frac{x}{L} - \frac{1}{2n\pi} sin\ \frac{2n\pi x}{L}\right]_{x_1}^{x_2}$$

Here $x_1 = 0.45L$ and $x_2 = 0.55L$.

(i)For the ground state, which corresponds to $n = 1$, we have

$P_{x_1,x_2} = 0.198 = 19.8\%$. This is about twice the classical probability ($P_{Class} = \int_{x_1}^{x_2} dx = 10\%$).

(ii)For the first excited state which corresponds to $n = 2$, we have

$P_{x_1,x_2} = 0.0065 = 0.65\%$.

Quantum Mechanics (PH101)
Tutorial-3
due on Wednesday, 24th of February, 2021 (8:00Hrs IST)

1. Consider the one-dimensional normalised wave function $\psi_0(x)$ and $\psi_1(x)$ with the properties

$$\psi_0(-x) = \psi_0(x) = \psi_0^*(x), \qquad \psi_1(x) = N\frac{d\psi_0}{dx}.$$

Consider another wave function $\psi(x) = c_1\psi_0(x) + c_2\psi_1(x)$, with $|c_1|^2 + |c_2|^2 = 1$. $N,\ c_1,\ c_2$ are known constants.

(a) Show ψ_0 and ψ_1 are orthogonal and $\psi(x)$ is normalised.
(b) Compute the expectation values of x and p in the states $\psi_0,\ \psi_1$ and ψ.
(c) Compute the expectation value of T, the kinetic energy operator in the state ψ_0

Solution:

(a) For ψ_0 and ψ_1 to be orthogonal we have to show

$$\int_{-\infty}^{\infty} \psi_0^*(x)\psi_1(x)dx = 0$$

Therefore,

$$\int_{-\infty}^{\infty} \psi_0(x)\psi_1(x)dx = N\int dx\psi_0^*\frac{d\psi_0}{dx} = N\int dx\psi_0\frac{d\psi_0}{dx}$$

$$= \frac{N}{2}\int dx\frac{d\psi_0^2}{dx} = \frac{N}{2}\left[\psi_0^2(x)\right]_{-\infty}^{+\infty} = 0 \qquad \text{Owing to the fact that} \quad \psi_0 \to 0 \quad \text{as} \quad x \to \pm\infty.$$

For normalization of $\psi(x)$ we have

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = \int_{-\infty}^{\infty} (c_1\psi_0(x) + c_2\psi_1(x))^*(c_1\psi_0(x) + c_2\psi_1(x))dx$$

$$= \int_{-\infty}^{\infty} (|c_1|^2\psi_0^*\psi_0 + c_1^*\psi_0^*c_2\psi_1 + c_2^*\psi_1^*c_1\psi_0 + |c_2|^2\psi_1^*\psi_1)dx$$

As ψ_0 and ψ_1 are orthogonal (shown before) and with the given condition $|c_1|^2 + |c_2|^2 = 1$ we have

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1.$$

i.e. $\psi(x)$ is normalised.

(b) Expectation value of $\hat{x}$ vanishes in both the states ψ_0 and ψ_1 owing to the oddness of the integrand $x|\psi_0|^2$ and $x|\psi_1|^2$..

$$\langle p\rangle_{\psi_0} = \int_{-\infty}^{\infty} \psi_0^*(x) p \psi_0(x) dx = -i\hbar \int_{-\infty}^{\infty} \psi_0(x) \frac{d\psi_0(x)}{dx} dx$$

$$= \frac{-i\hbar}{N} \int_{-\infty}^{\infty} \psi_0(x)\psi_1(x) dx = 0$$

(As $\psi_1 = N\frac{d\psi_0}{dx}$ and ψ_0 and ψ_1 are orthogonal).

$$\langle p\rangle_{\psi_1} = \int_{-\infty}^{\infty} \psi_1^*(x) p \psi_1(x) dx = -i\hbar \int_{-\infty}^{\infty} \psi_1^*(x) \frac{d\psi_1(x)}{dx} dx$$

$$-i\hbar\frac{N}{N^*} \int_{-\infty}^{\infty} \psi_1(x) \frac{d\psi_1(x)}{dx} dx = -i\hbar\frac{N}{2N^*} \int_{-\infty}^{\infty} \frac{d(\psi_1(x))^2}{dx} dx = -i\hbar\frac{N}{2N^*} \Big[(\psi_1(x))^2\Big]_{-\infty}^{+\infty} = 0$$

(Owing to the fact that $\psi_1 \to 0$ as $x \to \pm\infty$.)

(c) Expectation value of T in ψ_0 is given as

$$\langle T\rangle = \int_{-\infty}^{\infty} \psi_0 T \psi_0 dx = \int_{-\infty}^{\infty} \psi_0 \frac{p^2}{2m} \psi_0 dx = \frac{-\hbar^2}{2m} \int_{-\infty}^{\infty} \psi_0 \frac{d^2\psi_0}{dx^2} dx$$

.

Now consider the term $\frac{d}{dx}\left(\psi_0 \frac{d\psi_0}{dx}\right) = \frac{d\psi_0}{dx}\frac{d\psi_0}{dx} + \psi_0 \frac{d^2\psi_0}{dx^2}$

$$\Rightarrow \psi_0 \frac{d^2\psi_0}{dx^2} = \frac{d}{dx}\left(\psi_0 \frac{d\psi_0}{dx}\right) - \frac{d\psi_0}{dx}\frac{d\psi_0}{dx}$$

$$\Rightarrow \psi_0 \frac{d^2\psi_0}{dx^2} = \frac{1}{N}\frac{d}{dx}\Big(\psi_0\psi_1\Big) - \frac{1}{N^2}\psi_1\psi_1$$

Substituting this in the expression for $\langle T\rangle$ we have ,

$$\langle T\rangle = \frac{-\hbar^2}{2mN} \int_{-\infty}^{\infty} \frac{d}{dx}\Big(\psi_0\psi_1\Big) dx + \frac{\hbar^2}{2mN^2} \int_{-\infty}^{\infty} \psi_1\psi_1 dx$$

$$= \frac{-\hbar^2}{2mN}\Big[\psi_0\psi_1\Big]_{-\infty}^{\infty} + \frac{\hbar^2}{2mN^2}$$

The first term vanishes as $\psi_0,\ \psi_1 \to 0$ as $x \to \pm\infty$ we have

$$\langle T\rangle = \tfrac{\hbar^2}{2mN^2}$$

2. A particle of mass m is confined to a one dimensional infinite well in the region $0 \leq x \leq a$. At $t = 0$ its normalized wave function is

$$\Psi(x,\ t=0) = \sqrt{\frac{8}{5a}}\left[1 + cos\left(\frac{\pi x}{a}\right)\right]\ sin\ \left(\frac{\pi x}{a}\right)$$

(a) What is the wave function at a later time $t = t_0$?

(b) What is the average energy of the system at $t = 0$ and at $t = t_0$?

(c) What is the probability that the particle is found in the left half of the box (i.e., in the region $0 \leq x \leq a/2$) at $t = t_0$?

Solution:

We have the normalized eignefunctions for particle in an infinite well as

$$\psi_n = \sqrt{\frac{2}{a}}\ sin\ \left(\frac{n\pi x}{a}\right)$$

and the energy eigenvalues are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \qquad n = 1,\ 2,\ 3.....$$

As $\Psi(x,\ t=0) = \sqrt{\frac{8}{5a}}\left[1 + cos\left(\frac{\pi x}{a}\right)\right]\ sin\ \left(\frac{\pi x}{a}\right)$

$$= \sqrt{\frac{8}{5a}} sin\ \left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{5a}} sin\ \left(\frac{2\pi x}{a}\right)$$

Comparing this with $\Psi(x,t=0) = \sum_{n=1}^{\infty} c_n\psi_n$ we have

$$c_1 = \frac{2}{\sqrt{5}},\quad c_2 = \frac{1}{\sqrt{5}},\quad c_n = 0 \text{ for } n \neq 1,\ 2,\ ..$$

This suggests that the particle has finite probabilities to be in states with energies E_1 and E_2 only.

(a) Therefore,

$$\Psi(x,t=t_0) = c_1\psi_1(x,0)e^{-iE_1t/\hbar} + c_2\psi_2(x,0)e^{-iE_2t/\hbar}$$

$$= \sqrt{\frac{8}{5a}} sin\ \left(\frac{\pi x}{a}\right) exp\ \left(-i\frac{\pi^2\hbar t_0}{2ma^2}\right) + \sqrt{\frac{2}{5a}} sin\ \left(\frac{2\pi x}{a}\right) exp\ \left(-i\frac{2\pi^2\hbar t_0}{ma^2}\right)$$

(b) Average energy $\langle H\rangle = \int \Psi(x,0)^* H\Psi(x,0)dx$

Since $\Psi(x,0) = c_1\psi_1 + c_2\psi_2$ in this case, we have

$$\langle H\rangle = c_1^2E_1 + c_2^2E_2$$
$$= \frac{4}{5}E_1 + \frac{1}{5}E_2$$
$$= \frac{4\pi^2\hbar^2}{5ma^2}$$

(c) The probability of finding the particle in $0 \le x \le a/2$ at $t = t_0$ is

$$P = \int_0^{a/2} |\Psi(x,t_0)|^2 dx = \frac{1}{2} + \frac{16}{15\pi}\ cos\left(\frac{3\pi^2\hbar t_0}{2ma^2}\right)$$

3. Consider a particle of mass m is held in a one dimensional potential V(x). Suppose that in some region $V(x)$ is constant, $V(x) = V$. For this region, find the stationary state of the particle when (a)$E > V$, (b) $E < V$, and (c)$E = V$. You may leave your answer in the general form.

Solution:
(a) The stationary states are the solutions of

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x) = E\Psi(x)$$

(i) For $E > V$ we introduce the positive constant k defined as $\hbar^2k^2/2m = E - V$ so that we have,

$$\frac{\partial^2\Psi(x)}{\partial x^2} + k^2\Psi(x) = 0$$

The solution can be written as

$$\Psi(x) = Ae^{ikx} + A'e^{-ikx}$$

where A and A' are arbitrary complex constants.
(ii) For $E < V$ we introduce the positive constant q defined by $\hbar^2k^2/2m = V - E$ so we have

$$\frac{\partial^2\Psi(x)}{\partial x^2} - q^2\Psi(x) = 0$$

So the general solution will be

$$\Psi(x) = Be^{qx} + B'e^{-qx}$$

(c)When $E = V$ we have $\dfrac{\partial^2\Psi(x)}{\partial x^2} = 0$. So $\Psi(x) = Cx + C'$, where, C and C' are arbitrary complex constants.

4. Using the uncertainty relation $\Delta p\Delta x \ge \hbar/2$, estimate the ground state energy of the harmonic oscillator.

Solution:

The expectation value of of the energy for quantum harmonic oscillator is

$< \hat{H} >= E = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} < \hat{x}^2 >$

we have $\Delta p^2 =< \hat{p}^2 > - < \hat{p} >^2$ and $\Delta x^2 =< \hat{x}^2 > - < \hat{x} >^2$. For Harmonic oscillator, the eigen state have either even parity or odd parity. So we see that $< \hat{x} >= 0$ and $< \hat{p} >= 0$. Thus we have

$E = \frac{\Delta p^2}{2m} + \frac{m\omega^2}{2}\Delta x^2$. According to the uncertainty relation, the minimal value of the Δp is $\Delta p = \frac{\hbar}{2\Delta x}$; hence,

$E = \frac{\hbar^2}{8m\Delta x^2} + \frac{m\omega^2}{2}\Delta x^2.$

Finally the minimum value of $E(\Delta x)$ is obtained by

$$\frac{dE}{d(\Delta x)} = -\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2\Delta x = 0$$

So, $\Delta x_0 = \sqrt{\frac{\hbar}{2m\omega}}$. Also,

$$\frac{d^2E}{d(\Delta x)^2}|_{\Delta x_0} = \frac{3\hbar^2}{4m(\Delta x)^4} + m\omega^2 > 0.$$

Hence, the minimal value is

$E_{min.} = \frac{\hbar^2}{8m(\Delta x_0)^2} + \frac{m\omega^2}{2}(\Delta x_0)^2 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$

5. Consider that at $t = 0$ the particle is in the state

$$\psi(x) = [c_1\phi_0(x) + c_2\phi_1(x)]$$

where, $\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}$ and $\phi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\sqrt{\frac{2m\omega}{\hbar}}xe^{-m\omega x^2/2\hbar}$ are the stationary state eigenfunction corresponding to the ground and first excited state of the one-dimensional

Harmonic oscillator respectively, and c_1 and c_2 are complex constant. (i) Compute the average potential energy $< \hat{V} >$ and average kinetic energy $< \hat{T} >$ when the system is completely in the ground state, i.e., $c_2 = 0$. (ii) Compute the $< x >$ at time $t > 0$ for the case when $c_1 = c_2$.

Solution:

(i) For $c_2 = 0$ we have $c_1 = 1$.

Here ϕ_0 is even function and hence $|\phi_0|^2$ is also even.

Therefore, $\langle x \rangle = \int x|\phi_0|^2 = 0$.

Hence $\langle p \rangle = md\langle x \rangle/dt = 0$

$$\langle x^2 \rangle = A^2 \int_{-\infty}^{\infty} x^2 |\phi_0|^2 dx = A^2 \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx$$

$$= \frac{\hbar}{2m\omega}$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \phi_0 \left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 \phi_0 dx$$

$$= A^2 \hbar^2 \int_{-\infty}^{\infty} e^{-\alpha x^2/2} \frac{d^2}{dx^2} e^{-\alpha x^2/2} = \frac{m\hbar\omega}{2}$$

$\langle T \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{\hbar\omega}{4}$

$\langle V \rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle = \frac{\hbar\omega}{4}$.

(ii) For $c_1 = c_2$, using the normalization condition of the $\int \psi(x)dx = 1$, we have $c_1 = c_2 = \dfrac{1}{\sqrt{2}}$

Therefore, $\psi(x, 0) = \dfrac{1}{\sqrt{2}}[\phi_0(x) + \phi_1(x)]$.

Thus for $t > 0$ we have

$$\psi(x,t) = \sqrt{\frac{1}{2}} \left[\phi_0(x) e^{-i\omega t/2} + \phi_1(x) e^{-i3\omega t/2} \right]$$

We have $<\hat{x}>= \int_{-\infty}^{\infty} \psi^*(x,t)\hat{x}\psi(x,t) = \frac{1}{2}\Big[\int_{-\infty}^{\infty} \phi_0^*(x)x\phi_0(x)dx + \int_{-\infty}^{\infty} \phi_1^*(x)x\phi_1(x)dx + e^{-i\omega t}\int_{-\infty}^{\infty} \phi_0^*(x)x\phi_1(x)dx + e^{i\omega t}\int_{-\infty}^{\infty} \phi_1^*(x)x\phi_0(x)dx\Big]$

As ϕ_0 is even function and ϕ_1 is odd function the integrand of both the inetgral will be odd function. Thus first and second term will vanish.
The third term will be given by

$\int_{-\infty}^{\infty} \phi_1^*(x)x\phi_0(x)dx = \sqrt{\frac{2}{\pi}}\frac{1}{\lambda^2}\int_{-\infty}^{\infty} x^2 e^{-x^2\lambda^2} = \sqrt{\frac{1}{2\lambda^2}} = \sqrt{\frac{\hbar}{2m\omega}}$ with $\lambda^2 = m\omega/\hbar$

And fourth term,
$\int_{-\infty}^{\infty} \phi_0^*(x)x\phi_1(x)dx = (\int_{-\infty}^{\infty} \phi_1^*(x)x\phi_0(x)dx)^* = \sqrt{\frac{\hbar}{2m\omega}}$

So, finally we obtain

$$<\hat{x}>= \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t)$$