Expectation values of position & momentum

(a) Position

The probability density $|\psi_n(x)|^2 = \frac{2}{L}\sin^2\frac{n\pi x}{L}$ is symmetric about $x = L/2$. Hence

$$\langle x \rangle = L/2$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, x^2\, \psi_n(x)\, dx = \frac{2}{L}\int_0^L x^2 \sin^2\frac{n\pi x}{L}\, dx$$

$$= \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

(b) Momentum

$$P_x = -i\hbar \frac{d}{dx}$$

$$\langle P_x \rangle = 0$$

$$\langle P_x^2 \rangle = \frac{n^2\pi^2\hbar^2}{L^2}$$

$$\Delta P_x = \sqrt{\langle P_x^2 \rangle - \langle P_x \rangle^2} = \frac{n\pi\hbar}{L}$$

The uncertainty product

$$\Delta x\, \Delta P_x = n\pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

for $n=1$ i.e., gr. state

$$\boxed{\Delta x\, \Delta P_x = 0.57\hbar} \geq \frac{\hbar}{2}$$

for higher states, the uncertainty product is higher

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2013 ① Determine the probability of finding the particle of mass m between $x=0$ and $x=L/10$ if the particle is described by the normalised wavefunction.

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

for $0 \leq x \leq L$ and is in $n=3$ state.

$$\rightarrow P(x) = \int_0^{L/10} \left[\sqrt{\frac{2}{L}} \sin \frac{3\pi x}{L}\right]^2 dx$$

$$= \frac{2}{L} \int_0^{L/10} \sin^2 \frac{3\pi x}{L}\, dx$$

$$= \frac{1}{L} \int_0^{L/10} \left(1 - \cos \frac{6\pi x}{L}\right) dx$$

$$= \frac{1}{L} \left[x - \frac{L}{6\pi} \sin \frac{6\pi x}{L}\right]_0^{L/10}$$

$$= \frac{1}{L} \left[\frac{L}{10} - \frac{L}{6\pi} \sin \frac{6\pi \cdot \cancel{L}}{10 \cdot \cancel{L}}\right]$$

$$= \left[\frac{1}{10} - \frac{1}{6\pi} \sin \frac{3\pi}{5}\right]$$

$$= \frac{1}{10} - \frac{\sin 108^\circ}{6 \times 3.14} = \frac{1}{10} - \frac{\cos 18^\circ}{18.84}$$

$$\simeq 0.495$$

2013 The wavefunction of a particle confined in a box of linear dimension L along x-axis is

$$\psi(x) = A e^{idx} \quad [0 \leq x \leq L].$$

Find the probability of finding the particle in the distance $0 \leq x \leq L/4$

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$$\rightarrow \cancel{P(x) = \frac{\int_0^{L/4} \psi^*(x)\psi(x)dx}{\int_0^{L} \psi^*(x)\psi(x)dx}}$$

Determination of Normalization constant.

$$\int_0^L \psi^*(x)\,\psi(x)dx = 1$$

$$\Rightarrow \int_0^L A e^{-i\alpha x} \cdot A e^{i\alpha x} dx = 1$$

$$\Rightarrow \int_0^L A^2 dx = 1 \quad \Rightarrow \quad A^2 L = 1$$

$$\Rightarrow A = \frac{1}{\sqrt{L}}$$

$$\therefore \psi(x) = \frac{1}{\sqrt{L}} e^{i\alpha x}$$

Now

$$P(x) = \int_0^{L/4} \psi^*(x)\,\psi(x)dx = \int_0^{L/4} \left(\frac{1}{\sqrt{L}}\right)^2 dx$$

$$= \left(\frac{1}{\sqrt{L}}\right)^2 [x]_0^{L/4}$$

$$= \left(\frac{1}{\sqrt{L}}\right)^2 \cdot \frac{L}{4}$$

$$= \frac{1}{4} = 0.25$$

2011/ If the lowest energy state wave function is $\psi = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$. Determine the probability density at $x = a/3$.

$\rightarrow$ Probability density $= \psi^*(x)\psi(x) = |\psi(x)|^2$

$$= \frac{2}{a} \sin^2 \frac{\pi x}{a}$$

$$= \frac{2}{a} \sin^2 \frac{\pi}{a} \cdot \frac{a}{3} = \frac{2}{a} \sin^2 \frac{\pi}{3}$$

$$= \frac{2}{a} \cdot \frac{3}{4} = \frac{3}{2a}$$

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1) Calculate the energy difference between the gr. state & the first excited state for an e^- in one dimensional rigid box of length 10^{-10} m

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2}. \qquad n = 1, 2, 3, \ldots$$

$$E_n = n^2 \times 0.603 \times 10^{-17} \text{ Joule}$$

$$= 37.7 n^2 \text{ eV}.$$

$$E_2 - E_1 = 150.8 - 37.7 = 113.1 \text{ eV}.$$

(2) Calculate the permitted energy levels of an electron in a box 1 Å wide.

→ $m = 9.1 \times 10^{-31}$ kg

$L = 1 \text{ Å} = 10^{-10}$ m

$h = 6.6 \times 10^{-34}$ J.s

$$E_n = \frac{n^2h^2}{8mL^2} = 37.7 n^2 \text{ eV}.$$

$E_1 = 37.7$ eV

$E_2 = 152$ eV

⋮

(3) A particle is moving in 1-D box of width 10 Å. Calculate the probability of finding the particle within an interval of 1 Å at the centre of the box when it is in the state of least energy

→ At the centre, $x = \frac{L}{2} = \frac{10}{2} \text{ Å} = 5 \text{ Å}$.

for least energy $n = 1$.

$$\therefore \psi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

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Probability $= |\psi_1|^2 \Delta x$

$$= \frac{2}{L} \sin^2 \frac{\pi x}{L} \times \Delta x$$

$$= \frac{2}{L} \sin^2 \frac{\pi}{\cancel{L}} \cdot \frac{\cancel{L}}{2} \cdot \times 10^{-10}$$

$$= \frac{2}{L} \sin^2 \frac{\pi}{2} \times 10^{-10}$$

$$= \frac{2}{L} \times 10^{-10} = \frac{2}{10 \times \cancel{10^{-10}}} \times \cancel{10^{-10}}$$

$$= 0.2.$$

(4) Consider a particle of mass $m = 9.1 \times 10^{-31}$ kg & energy 342 eV confined in a 1-D box of length 1Å.

Calculate

(a) the Q. no. of the State

(b) the energy required to take the system to its next excited state.

(a) $m = 9.1 \times 10^{-31}$ kg

$E = 342 eV = 342 \times 1.6 \times 10^{-19}$ J.

$L = 1 \mathring{A} = 10^{-10}$ m

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$\Rightarrow n^2 = \frac{2mL^2 E}{\pi^2 \hbar^2} \Rightarrow n = 3.$$

(b) $$E_4 - E_3 = \frac{\pi^2 \hbar^2}{2mL^2} (4^2 - 3^2) = 266 eV.$$

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Griffith Ex-2.1. Suppose a particle starts out in a linear combination of just two stationary states.

$$\Psi(x,0) = c_1\psi_1(x) + c_2\psi_2(x).$$

Assume the constants c_n & $\psi_n(x)$ are real.
What is the wavefn $\Psi(x,t)$ at subsequent times?

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

$$|\Psi(x,t)|^2 = \left[c_1\psi_1 e^{+iE_1t/\hbar} + c_2\psi_2 e^{+iE_2t/\hbar}\right]\left[c_1\psi_1 e^{-iE_1t/\hbar} + c_2\psi_2 e^{-iE_2t/\hbar}\right]$$

$$= c_1^2\psi_1^2 + c_2^2\psi_2^2 + 2c_1c_2\psi_1\psi_2\cos\left[(E_2-E_1)t/\hbar\right].$$

$$\boxed{\exp(i\theta) = \cos\theta + i\sin\theta.}$$

Probability density oscillates sinusoidally at an ang. frequency $\frac{E_2-E_1}{\hbar}$. This is certainly not a stationary state.

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Expectation value of Energy :-

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n .$$

Proof:- $H\psi_n = E_n \psi_n$

$$\langle H \rangle = \int \Psi^* H \Psi \, dx = \int \left(\sum c_m \psi_m \right)^* H \left(\sum c_n \psi_n \right) dx$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n E_n \int \psi_m^* \psi_n \, dx$$

$$= \sum_{n=1}^{\infty} |c_n|^2 E_n .$$

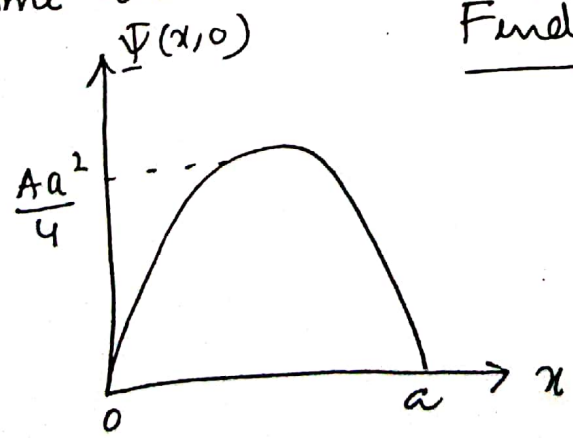
Probability of getting a particular energy is independent of time & hence expectation value of H is also independent of time. This is a manisfestation of Conservation of energy in Quantum mechanics.

Problem Griffiths. A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = Ax(a-x) . \quad [0 \le x \le a] .$$

for some constant A. outside the well $\Psi = 0$.

Find $\Psi(x,t)$??



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Schaum series # 3.26

Consider the wave function $\psi(x) = \frac{N}{x^2 + \alpha^2}$

(a) Calculate Normalization constant N where α is a real constant

(b) find the Uncertainty $\Delta x \, \Delta p$

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Allowed

(4) Find the probability of finding the particle in the rangle $L/4 < x < 3L/4$ at this time when

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \quad \text{for } 0 < x < L$$

$$= 0 \quad \text{otherwise}$$

$$\int_{L/4}^{3L/4} |\psi(x)|^2 \, dx.$$

$$= \int_{L/4}^{3L/4} \frac{2}{L} \sin^2 \frac{\pi x}{L} \, dx$$

$$= \frac{1}{L} \int_{L/4}^{3L/4} \left(1 - \cos \frac{2\pi x}{L}\right) dx$$

$$= \frac{1}{L} \left[x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{L/4}^{3L/4} = \frac{1}{L} \left[\frac{L}{2} + \frac{L}{\pi} \right] = 0.82$$

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(5) A particle limited to the x-axis has the wavefn. $\Psi = ax$ between $x = 0$ and $x = 1$ & $\Psi = 0$ elsewhere.

(a) Find the Probability that the particle can be found between $x = 0.45$ and $x = 0.55$ (b) Find the expectation value $\langle x \rangle$ of the particle's position.

→ (a)

$$\int_{x_1}^{x_2} |\Psi|^2 dx = a^2 \int_{0.45}^{0.55} x^2 dx = a^2 \left[\frac{x^3}{3}\right]_{0.45}^{0.55}$$

$$= 0.0251 a^2$$

(b) $$\langle x \rangle = \int_0^1 x |\Psi|^2 dx = a^2 \int_0^1 x^3 dx = a^2 \left[\frac{x^4}{4}\right]_0^1 = \frac{a^2}{4}.$$

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in the whole space is 1.

Probability Current density

The probability of finding a system described by a wavefn $\psi(\vec{r},t)$ in a finite volume V in space is given by $\int_V \psi^* \psi \, d\tau$ and this changes as the wave function evolves in time

Consider the Schrödinger equation and its complex conjugate form

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi \quad \text{---} \quad (1)$$

and

$$i\hbar \frac{\partial \psi^*}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi^* \quad \text{---} \quad (2)$$

Multiplying eqn (1) by ψ^* and (2) by ψ and subtracting from left-

$$i\hbar\left[\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}\right] = -\frac{\hbar^2}{2m}\left[\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*\right]$$

or, $$\frac{\partial}{\partial t}(\psi^* \psi) = \frac{i\hbar}{2m}\left[\nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)\right]$$

This is in the form of standard continuity equation.

or, $$\frac{\partial \rho}{\partial t} = -\operatorname{div} j$$

where $\rho = (\psi^* \psi)$ & $j = \frac{i\hbar}{2m}\left[\psi \nabla \psi^* - \psi^* \nabla \psi\right]$

Since $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$

& hence $= 0$.

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