

$$\psi(x) = N \times \exp\left(-\frac{1}{2}\alpha x^2\right)$$

(a) Normalize \rightarrow

$$\int_{-\infty}^{+\infty} \psi^* \psi dx = 1$$

$$\Rightarrow \int_{-\infty}^{+\infty} N^2 x^2 \exp(-\alpha x^2) dx = 1.$$

Even function

$$2 \int_0^{\infty} N^2 x^2 \exp(-\alpha x^2) dx = 1. \quad \text{--- (1)}$$

We know

$$\int_0^{\infty} e^{-\alpha x^2} x^n dx = \frac{(n-1)!}{2^{\frac{n}{2}+1} \alpha^{\frac{n}{2}}} \sqrt{\frac{\pi}{\alpha}} \quad \text{For } n \text{ even}$$

$$= \frac{\left[\frac{1}{2}(n-1)\right]!}{2 \alpha^{\frac{(n+1)/2}{2}}} \quad \text{For } n \text{ odd.}$$

$$\text{From (1)} \Rightarrow 2N^2 \frac{1}{2^2 \alpha} \sqrt{\frac{\pi}{\alpha}} = 1.$$

$$N^2 \frac{1}{2\alpha} \sqrt{\frac{\pi}{\alpha}} = 1.$$

$$N = \left[\sqrt{\frac{\alpha}{\pi}} \cdot 2\alpha \right]^{\frac{1}{2}}$$

$$= \left(\frac{2\alpha^{\frac{3}{2}}}{\pi^{\frac{1}{2}}} \right)^{\frac{1}{2}} = \frac{\sqrt{2\alpha}^{\frac{3}{4}}}{\pi^{\frac{1}{4}}}$$

$$N = \frac{\sqrt{2\alpha}^{\frac{3}{4}}}{\pi^{\frac{1}{4}}}$$

What is $\langle \hat{x} \rangle$ and $\langle \hat{x}^2 \rangle$

$$\begin{aligned}\langle \hat{x} \rangle &= \int_{-\infty}^{+\infty} \psi^* \hat{x} \psi dx = N^2 \int_{-\infty}^{+\infty} x \exp\left(-\frac{1}{2}kx^2\right) dx \\ &= N^2 \int_{-\infty}^{+\infty} x^3 \exp\left(-kx^2\right) dx \quad \boxed{\text{odd}}\end{aligned}$$

$$\boxed{\langle \hat{x} \rangle = 0}$$

$$\begin{aligned}\langle \hat{x}^2 \rangle &= \int_{-\infty}^{+\infty} \psi^* \hat{x}^2 \psi dx = N^2 \int_{-\infty}^{+\infty} x^4 \exp\left(-kx^2\right) dx \quad \boxed{\text{Even}} \\ &= 2N^2 \int_0^{+\infty} x^4 \exp\left(-kx^2\right) dx.\end{aligned}$$

Apply the formulation mentioned in box for $\boxed{n=4}$

⑥ $\langle \hat{p} \rangle$ and $\langle \hat{p}^2 \rangle$

$$\begin{aligned}\langle \hat{p} \rangle &= \int_{-\alpha}^{+\alpha} \hat{\psi}^* \hat{p} \hat{\psi} dx = N^2 \int_{-\alpha}^{+\alpha} x \exp\left(-\frac{1}{2} \kappa x^2\right) \left(-i\hbar \frac{d}{dx}\right) \exp\left(-\frac{1}{2} \kappa x^2\right) dx \\ &= N^2 \int_{-\alpha}^{+\alpha} (-i\hbar) \times \exp\left(-\frac{\kappa x^2}{2}\right) \left[1 + x \left(-\frac{1}{2} \kappa \cdot 2x\right)\right] \exp\left(-\frac{\kappa x^2}{2}\right) dx \\ &= N^2 \int -i\hbar \left[x \exp\left(-\kappa x^2\right) - \kappa x^3 \exp\left(-\kappa x^2\right) \right] dx\end{aligned}$$

\uparrow odd \uparrow odd

$$\boxed{\langle \hat{p} \rangle = 0}$$

$$\begin{aligned}\langle \hat{p}^2 \rangle &= \int_{-\alpha}^{+\alpha} \hat{\psi}^* \hat{p}^2 \hat{\psi} dx = \int_{-\alpha}^{+\alpha} \hat{\psi}^* (-i\hbar) \frac{d^2}{dx^2} \hat{\psi} dx \\ &= -\hbar^2 \int_{-\alpha}^{+\alpha} \hat{\psi}^* \frac{d^2 \hat{\psi}}{dx^2} dx.\end{aligned}$$

⊕

On evaluation of $\hat{\psi}^* \frac{d^2 \hat{\psi}}{dx^2}$
 you will get even integrand.
 It can be ^{integrated} easily via the
 formula for Gaussian integration.

(d) For $v(x)=0 \rightarrow \langle H \rangle = ?$

$$\begin{aligned} \langle H \rangle &= \left\langle \frac{p^2}{2m} + V(x) \right\rangle = \left\langle \frac{p^2}{2m} \right\rangle + \underbrace{\int \psi^* \frac{\partial^2}{\partial x^2} \psi dx}_{=0} \\ &= -\frac{\hbar^2}{2m} \int \psi^* \frac{\partial^2}{\partial x^2} \psi dx \end{aligned}$$

Putting $\psi(x) = N e^{-\alpha x^2}$

You can work out the value of $\langle H \rangle$

(e) Find $v(x) = ?$

$$H \psi(x) = E \psi(x)$$

$$\left[+ \frac{\hbar^2}{2m} + V(x) \right] \psi(x) = E \psi(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x)$$

$$\text{Now, } \psi(x) = N x \exp -\frac{\alpha x^2}{2}$$

$$\frac{d\psi}{dx} = N \exp -\frac{\alpha x^2}{2} + N x (-\alpha x) \exp -\frac{\alpha x^2}{2}$$

$$= N \exp -\frac{\alpha x^2}{2} - N \alpha x^2 \exp -\frac{\alpha x^2}{2}$$

$$\frac{d^2\psi}{dx^2} = N (-\alpha x) \exp -\frac{\alpha x^2}{2} - 2N \alpha x \exp -\frac{\alpha x^2}{2}$$

$$+ N \alpha^2 x^2 \exp -\frac{\alpha x^2}{2}$$

$$= \left(3N \alpha x + N \alpha^2 x^3 \right) \exp -\frac{\alpha x^2}{2}$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x) \psi(x) = E \psi(x)$$

$$-\frac{\hbar^2}{2m} \left(-3N \alpha x + N \alpha^2 x^3 \right) \exp -\frac{\alpha x^2}{2} + V(x) N x \exp -\frac{\alpha x^2}{2}$$

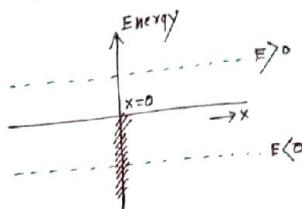
$$= N E x \exp -\frac{\alpha x^2}{2}$$

Equation. Taking $V(x) = \frac{\hbar^2 \alpha^2 x^2}{2m} \rightarrow \text{satisfies } v(0) = 0$

we get $\Rightarrow \boxed{E = \frac{3\hbar^2 \alpha}{2m}}$

\Rightarrow A delta-function is an infinitely high, infinitesimal narrow spike.

$$\Rightarrow \text{Form} = N(x) = -\alpha \delta(x)$$



\Rightarrow Schrödinger eqⁿ

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha \delta(x)\psi = E\psi(x) \quad \text{--- (1)}$$

looking only for $E < 0$ cases. Forget about $E > 0$.

\Rightarrow For $x > 0$ and $x < 0$, $N(x) = 0$

$$\Rightarrow \text{Eq}^1 \text{ becomes } \rightarrow \boxed{\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi} \rightarrow \frac{d^2\psi}{dx^2} = k^2\psi \quad \text{where } k^2 = -\frac{2mE}{\hbar^2}$$

\Rightarrow Since $E < 0$; k^2 is always positive.

$$\Rightarrow \text{By Solving, we get } \boxed{\begin{aligned} \psi &= B e^{kx} && \text{at } x < 0 \\ &\text{and } \psi &= F e^{-kx} & \text{at } x > 0 \end{aligned}}$$

$$\Rightarrow \text{Continuity at } x=0 \text{ claims } \Rightarrow \left. \psi \right|_{x < 0} = \left. \psi \right|_{x > 0} \quad \text{at } x=0 \Rightarrow B = F$$

\Rightarrow Taking (1) and integrating

$$\begin{aligned} -\frac{\hbar^2}{2m} \int_{-t}^t \frac{d^2\psi}{dx^2} dx - \kappa \int_{-t}^t S(x)\psi(x) dx &= E \int_{-t}^t \psi(x) dx \\ -\frac{\hbar^2}{2m} \left[\frac{d\psi}{dx} \Big|_{-t}^t - \frac{d\psi}{dx} \Big|_{-t}^t \right] - \kappa \psi(0) &= 0 \end{aligned}$$

Make it narrow

$$\boxed{4 \left(\frac{d\psi}{dx} \Big|_{-t}^t \right) = -\frac{2m\alpha}{\hbar^2} \psi(0)}$$

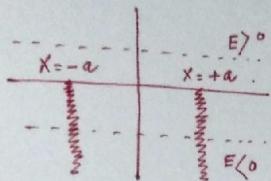
$$\Rightarrow x < 0 : \left. \frac{d\psi}{dx} \right|_{-t}^t = BK \quad ; \quad x > 0 : \left. \frac{d\psi}{dx} \right|_t = -BK, \quad \psi(0) = B$$

$$\Rightarrow 4 \left(\frac{d\psi}{dx} \Big|_{-t}^t \right) = 2BK = -\frac{2m\alpha}{\hbar^2} B \Rightarrow \boxed{k = \frac{m\alpha}{\hbar^2}}$$

$$\boxed{E = -\frac{m\alpha^2}{2\hbar^2}}$$

Double Delta

Problem NO. 2



$$V(x) = -K \left[\delta(x+a) + \delta(x-a) \right] \quad \text{where } \alpha = \frac{\hbar^2}{ma}$$

$$\textcircled{(2)} \quad x < -a : \psi(x) = A e^{kx}$$

$$-a \leq x \leq a : \psi(x) = C e^{kx} + D \bar{e}^{-kx}$$

$$k^2 = -\frac{2mE}{\hbar^2}$$

$$x > a : \psi(x) = F \bar{e}^{-kx}$$

$$\text{Continuity at } x = -a \Rightarrow \boxed{A e^{-ka} = C \bar{e}^{-ka} + D e^{ka}} \quad \text{--- (A)}$$

$$x = +a \Rightarrow \boxed{F \bar{e}^{-ka} = C e^{ka} + D \bar{e}^{-ka}} \quad \text{--- (B)}$$

Discontinuity of $\frac{d\psi}{dx}$ at $x = -a$

$$k \left(C \bar{e}^{-ka} - D e^{ka} \right) - k A \bar{e}^{-ka} = -\frac{2m\alpha}{\hbar^2} A \bar{e}^{-ka} = -\frac{2}{a} A \bar{e}^{-ka}$$

$$\text{at } x = +a \Rightarrow \boxed{-k F \bar{e}^{-ka} - k \left(C e^{ka} + D \bar{e}^{-ka} \right)} = -\frac{2m\alpha}{\hbar^2} F \bar{e}^{-ka} = -\frac{2}{a} F \bar{e}^{-ka}$$

Discontinuous equations can be simplified as

$$\text{For } x = -a : A \bar{e}^{-ka} \left(k - \frac{2}{a} \right) = k \left(C \bar{e}^{-ka} - D e^{ka} \right) \quad \text{--- (C)}$$

$$x = +a : F \bar{e}^{-ka} \left(\frac{2}{a} - k \right) = k \left(C e^{ka} + D \bar{e}^{-ka} \right) \quad \text{--- (D)}$$

Eliminating C and D for A and F

$$C \bar{e}^{-ka} = D e^{ka} \left(ka - 1 \right) \rightarrow C^2 = D^2 \Rightarrow \boxed{C = \pm D}$$

$$D \bar{e}^{-ka} = C e^{ka} \left(ka - 1 \right)$$

$$\text{For } C = D : \psi = C \left(e^{kx} + \bar{e}^{-kx} \right) = C' \cosh kx$$

$$C = -D : \psi = C \left(e^{kx} - \bar{e}^{-kx} \right) = C' \sinh kx$$

Solving for Bound States

$$\text{Even } C = D : \boxed{\bar{e}^{-2ka} = ka - 1}$$

$$\text{odd } C = -D : \boxed{\bar{e}^{-2ka} = 1 - ka}$$

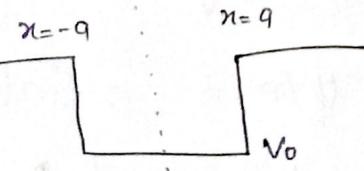
From intersection work out the value of ka and get E_{Bound} .

3 (9). for finite square well potential.

$$V(n) = \begin{cases} -V_0 & \text{for } -a \leq x \leq a \\ 0 & \text{otherwise} \quad (|x| > a) \end{cases}$$

Sol:-

(i) In Region $|x| < a$, Schrödinger eqⁿ



$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = E \psi \quad V=0 \quad \text{in this Region}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi$$

$$\text{Let } K = \sqrt{-\frac{2mE}{\hbar^2}}$$

$$\frac{\partial^2 \psi}{\partial x^2} = K^2 \psi$$

solution of this eqⁿ.

$$\psi(n) = A e^{Kn} + B e^{-Kn}$$

But $x \rightarrow \infty$, ~~first~~ first term blows up and similarly $x \rightarrow -\infty$, second term diverge.

so,

$$\psi(n) = \begin{cases} A e^{-Kn} & \text{for } x < a \\ B e^{Kn} & \text{for } x > a \end{cases}$$

(ii) Now in Region $-a \leq x \leq a$ $V(n) = -V_0$
Schrödinger eqⁿ

$$\left(-\frac{\hbar^2}{2m} \nabla^2 - V_0 \right) \psi(n) = E \psi(n).$$

$$\frac{\partial^2 \psi'}{\partial n^2} = -\frac{2m(E + V_0)}{\hbar^2} \psi \quad \text{Let } l = \sqrt{\frac{2m(E + V_0)}{\hbar^2}}$$

$$\frac{\partial^2 \psi'}{\partial n^2} = -l^2 \psi$$

Solution of this equation, i.e.

$$\psi(n) = C \sin(lnx) + D \cos(ln)$$

So, A, B, C and D. ~~C and D~~ can be determined by using boundary conditions.

(i) Continuous at $x=a$ and $n=-a$

(ii) $\frac{\partial \psi}{\partial x}$ continuous at $x=a$ and $n=-a$

As we know that potential is symmetric about $x=0$

so,

$$(i) B e^{-ka} = C \cos(la)$$

$$(ii) -ka B e^{-ka} = C \sin(la) \cdot (-l)$$

$$\frac{k}{l} = \tan(la)$$

Now for sufficiently deep well, we given that

$$Z_0 = \frac{a}{\hbar} \sqrt{2mV_0} \text{ is fairly large}$$

$$z = la \text{ and } Z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$$

and we know that value of k and l

$$k^2 + l^2 = 2mV_0/\hbar^2$$

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \quad \text{if } z_0 \rightarrow \infty$$

So, $\tan(z) = \tan\left(\frac{(2n+1)\pi}{2}\right)$

So,

$$l a \approx \frac{(2n+1)\pi}{2}$$

$$\sqrt{\frac{2m(E + V_0)}{\hbar^2}} a = \frac{(2n+1)\pi}{2}$$

$$\frac{2m(E + V_0)}{\hbar^2} a^2 = \frac{(2n+1)^2 \pi^2}{4}$$

$$E = \frac{(2n+1)^2 \pi^2 \hbar^2}{8ma^2} - V_0$$

$$E = \frac{(2n+1)^2 \pi^2 \hbar^2}{2m(2a)^2} - V_0$$

for finite V_0 , only finite no. of bound states will be possible as long as $E < 0$

or

$$\boxed{\frac{(2n+1)^2 \pi^2 \hbar^2}{2m(2a)^2} < V_0}$$

$$\underline{4a.} \quad \psi(n) = e^{i\alpha} \phi(n)$$

where $\phi(n)$ is real and $\alpha = \text{constant}$.

Sol^h

$$\langle p \rangle = \int_{-\infty}^{\infty} \bar{e}^{i\alpha} \phi(n) - i\hbar \frac{\partial}{\partial n} e^{i\alpha} \phi(n) dn$$

$$= -i\hbar \int_{-\infty}^{\infty} \phi(n) \frac{\partial}{\partial n} \phi(n) dn$$

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \phi(n) \cdot \phi'(n) dn.$$

So, as p is hermitian operator so, ~~eigen~~ expectation value of $(\langle p \rangle)$ p must be real.

and $\phi(n)$ is Real ~~one~~ function. So,

$$\int_{-\infty}^{\infty} \phi(n) \phi'(n) dn = \text{Real value.}$$

$$\langle p \rangle = -i\hbar \underbrace{(\text{Real value})}_{\text{Imaginary value}} \quad \{ \langle p \rangle = a + ib \} \text{ for Ex.}$$

so,

$$\langle p \rangle = 0$$

4b.

$$\psi(n) = \phi_1(n) + e^{i\alpha} \phi_2(n)$$

similarly

$$\langle p \rangle = \int_{-\infty}^{\infty} (\phi_1(n) + \bar{e}^{i\alpha} \phi_2(n)) - i\hbar \frac{\partial}{\partial n} (\phi_1(n) + e^{i\alpha} \phi_2(n)) dn.$$

$$\langle b \rangle = -i\hbar \left[\int_{-\infty}^{\infty} \phi_1(n) \phi_1^*(n) e^{i\alpha} + \int_{-\infty}^{\infty} \phi_1(n) \phi_2^*(n) e^{i\alpha} \right. \\ \left. + \int_{-\infty}^{\infty} \phi_2(n) \phi_1^*(n) e^{-i\alpha} + \int_{-\infty}^{\infty} \phi_2(n) \phi_2^*(n) dn \right]$$

Because of these both term will give us real value.

$$\langle b \rangle = -i\hbar e^{i\alpha} \int_{-\infty}^{\infty} \phi_1(n) \phi_2^*(n) dn \\ + -i\hbar \int_{-\infty}^{\infty} e^{-i\alpha} \phi_2(n) \phi_1^*(n) dn$$

$\langle b \rangle =$ ~~real~~ real value.

$$\int_{-\infty}^{\infty} \phi_i(n) \phi_j^*(n) = \text{real value}$$

$$\text{So, if } \alpha = \pi/2(2n+1) \quad e^{\pm i\alpha} = \pm i$$

So,

$$\langle b \rangle = \text{Non zero when } \alpha = \left(\frac{2n+1}{2}\right)\pi$$

Problem 5: The 1-D Schrödinger eqn.

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + v(x) \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t),$$

It can also be written as

$$\hat{H} \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t), = i\hbar \dot{\psi}(x,t)$$

where the Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial}{\partial x^2} + v(x)$$

(a) The probability density is

$$\rho(x,t) = \psi^* \psi.$$

Then

$$\frac{\partial \rho}{\partial t} = \dot{\psi}^* \psi + \psi^* \dot{\psi}.$$

$$\begin{aligned} &= \left[(\hat{H}\psi)^* \psi - \psi^* (\hat{H}\psi) \right] \frac{i}{\hbar} \\ &= \left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) \right] \frac{i}{\hbar} \\ &\quad + \underbrace{\left[v(x,t) \psi^* \psi - \psi^* v(x,t) \psi \right]}_{\approx 0} \frac{i}{\hbar} \end{aligned}$$

Now



$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{\hbar}{2im} \left(\frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) \\ &= -\frac{\partial}{\partial x} \left[\frac{\hbar}{2im} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) \right] \\ &= -\frac{\partial}{\partial x} \left[\frac{\hbar}{2im} 2i \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial x} \right) \right] = -\frac{\partial}{\partial x} J \end{aligned}$$

where the probability current is defined as

$$J(x,t) = \frac{\hbar}{m} \operatorname{Im} \left(\Psi^* \frac{\partial \Psi}{\partial x} \right),$$

Therefore we have shown.

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0.$$

Note $\int dx \Psi^* \Psi = 1$ is unit free.

Then, the $\rho = \Psi^* \Psi$ has the unit L^{-1} .

Similarly

$$\left[\Psi^* \frac{\partial \Psi}{\partial x} \right] = \frac{1}{L^2}, \quad [\hbar] = \frac{ML^2}{T}, \quad \left[\frac{\hbar}{m} \right] = \frac{L^2}{T}.$$

Then $[J] = \frac{1}{T} \Rightarrow$ probability per unit time.

(b) Now we demonstrate the conservation of probability — in time.

Say, $N(t)$ is the integral of the $\rho(x,t)$ throughout the space —

$$N(t) \equiv \int_{-\infty}^{\infty} \rho(x,t) dx.$$

The change in probability now is then

$$\begin{aligned} \frac{dN(t)}{dt} &= \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t} dx = - \int_{-\infty}^{\infty} \frac{\partial J}{\partial x} dx \\ &= - (J(\infty, t) - J(-\infty, t)) \end{aligned}$$

The $\frac{dN(t)}{dt}$ vanishes if the probability current vanishes at infinity, $|x| \rightarrow \infty$. (3)

Recall

$$J = \frac{\hbar}{2im} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right).$$

The current indeed vanishes as we restrict the wave fn. to satisfy

$$\lim_{x \rightarrow \pm\infty} \psi = 0 \quad \text{or} \quad \lim_{x \rightarrow \pm\infty} \frac{\partial \psi}{\partial x} \text{ is bounded.}$$

Therefore, we prove $\frac{dN}{dt} = 0$.

Now we go for probability in a region $[a, b]$, and is given by

$$P_{ab}(t) = + \int_a^b \rho(x, t) dx.$$

The change in the probability -

$$\frac{dP_{ab}(t)}{dt} = - \int_a^b \frac{\partial J(x, t)}{\partial x} dt = - J(b, t) + J(a, t)$$

- $J(b, t)$ → probability flowing out at $x = b$,

$J(a, t)$ → probability flowing in at $x = a$.