Physics 491
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Lecture # 3

If we measure the position of n identically prepared Q.M. objects (e.g. e^-) we can calculate the position expectation value. Identically prepared = same $\Psi(x,t)$.

$$\langle x \rangle = \int_{-\infty}^{\infty} x\, \psi^* \psi \, dx$$

← default limits if left out

$$\frac{d}{dt}\langle x \rangle = \int_{-\infty}^{\infty} x \frac{\partial}{\partial t}\left(\psi^* \psi\right) dx$$

x is integration variable, not a classical trajectory $x(t)$!

For a free particle ($V=0$),

note first derivative in time

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

& Complex conjugate (CC) equation

$$\frac{d}{dt}\langle x \rangle = \frac{i\hbar}{2m}\int x \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right] dx$$

integrate by parts and use normalization

$$\psi\big|_{\pm\infty} = 0$$

$$\frac{d}{dt}\langle x\rangle = \frac{-i\hbar}{2m}\int\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx$$

integrate by parts again

$$m\,\frac{d\langle x\rangle}{dt} = \int\psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi\,dx$$

suggests momentum is a (differential) operator

$$\vec{p} \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$$ "is represented by"

In case of V, Ehrenfest's theorem

$$\frac{d}{dt}\langle p\rangle = \left\langle -\frac{\partial V}{\partial x}\right\rangle$$

thus $F_x = \dfrac{dP_x}{dt}$ holds on average.

Time independent equation

For potential without explicit time dependence $V = V(x)$,

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

let $\Psi(x,t) = \phi(t)\psi(x)$

define $\dot{\phi} \equiv \frac{d\phi}{dt}$, $\psi' \equiv \frac{d\psi}{dx}$

$$i\hbar \psi \dot{\phi} = \left(-\frac{\hbar^2}{2m}\psi'' + V\psi\right)\phi$$

$$\frac{i\hbar\dot{\phi}}{\phi} = \frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\psi'' + V\psi\right) \equiv E \quad \text{constant}$$

$$\Psi(x,t) = e^{-iEt/\hbar}\psi_E(x)$$

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)\psi_E = E\psi_E}$$

"stationary state"

ψ_E energy eigenstate, E eigenvalue

with $\hat{p} \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$, write

Hamiltonian operator $\hat{H}$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V$$

Free particle solutions:

for $V(x) = \text{constant} \equiv 0$

$$\Psi = A e^{i(kx - \omega t)} \quad \text{plane wave}$$

$$k = \frac{p}{\hbar} = \frac{\sqrt{2mE}}{\hbar} \; ; \; \omega = \frac{E}{\hbar}$$

technically, plane wave is not a solution since

$$\int_{-L/2}^{L/2} \Psi^* \Psi \, dx = L|A|^2$$

$$A = \frac{1}{\sqrt{L}} \rightarrow_{L \to \infty} 0$$

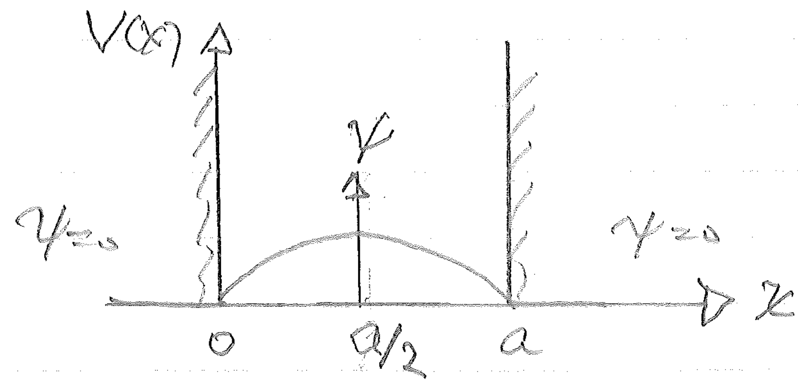
Since wave equation is linear, any wave packet is a superposition of plane waves.

$$j = \frac{\hbar}{2mi}\left(\underbrace{\psi^* \psi'}_{\hookrightarrow ik\psi} - \psi \psi^{*\prime}\right) = |A|^2 \frac{\hbar k}{m}$$

Constant probability current.

<u>particle in a box</u>

$$V(x) = \begin{cases} 0 & 0<x<a \\ \infty & \text{elsewhere} \end{cases}$$



Since particle energy must be finite
$\psi = 0$ outside box. let $k = \sqrt{2mE}/\hbar$ (real)

$$\psi'' = -k^2 \psi$$

Solution satisfying boundary condition of continuity at $x = 0, a$.

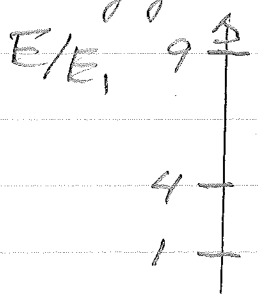
$$\psi_n = \sqrt{\frac{2}{a}} \sin(k_n x)$$

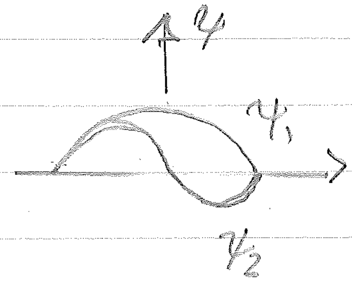
$$k_n a = n\pi \quad \text{where } n = 1, 2, 3, \text{ integer}$$

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

$$\int_0^a |\psi_n|^2 dx = 1$$

Energy level diagram:





Sketch of ground state & 1st excited

Remarks

(i) Ground state ≡ state of lowest energy has non-zero kinetic energy.

$$\lambda \sim \frac{h}{p} \sim a$$

$$\langle E_1 \rangle = \frac{1}{2m} \langle \hat{p}^2 \rangle_1 \sim \frac{1}{2m} \left(\frac{h}{a}\right)^2$$

$$\langle E_n \rangle = \int \Psi_n^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) \Psi_n \, dx$$

$$= \frac{\hbar^2}{2m} k_n^2$$

(ii) Energy of bound state is quantized.

(iii) Energy eigenstates are complete.

Any bound state can be written as a linear combination,

$$\Psi(x,t) = \sum C_n e^{-iE_nt/\hbar} \sqrt{\frac{2}{a}} \sin k_n x$$

linearity of Schrödinger eq. is crucial.

(iv) Energy eigenstates are orthonormal.

$$\phi_n \equiv \sqrt{\frac{2}{a}} \sin k_n x$$

$$\int \phi_n^* \phi_m \, dx = \delta_{nm}$$ Kronecker-delta symbol

then

$$\Psi(x,t) = \sum C_n e^{-iE_nt/\hbar} \phi_n$$

$$\int \phi_m^* \Psi \, dx = \sum_n C_n e^{-iE_nt/\hbar} \int \phi_m^* \phi_n \, dx$$

$$= C_m e^{-iE_mt/\hbar}$$

$$C_m(0) = \int \phi_m^* \Psi \, dx$$

normalization condition,

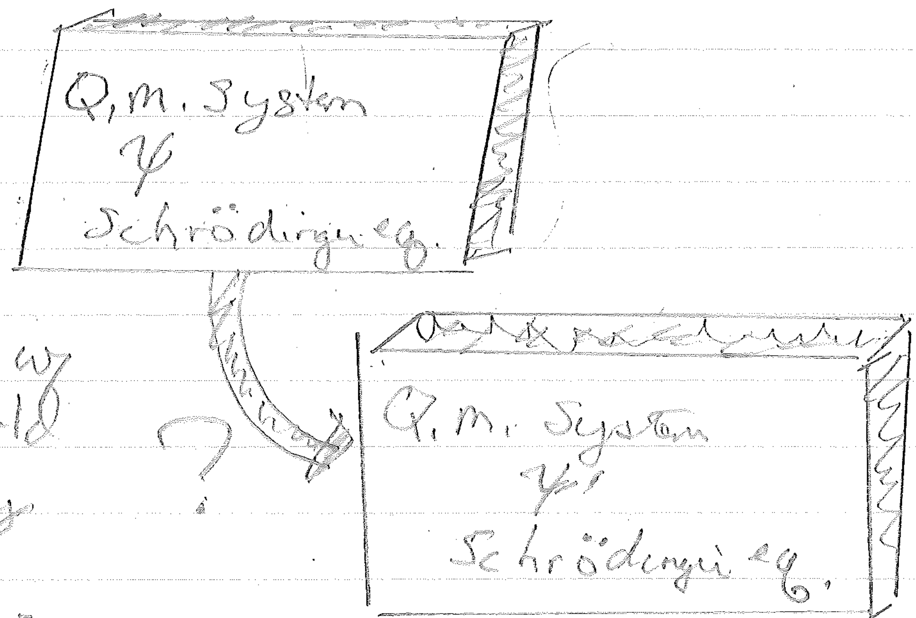
$$\int |\Psi|^2 dx = \sum_n |C_n|^2 = 1$$

(v.) Physical interpretation of C_n

C_n are probability amplitudes to measure E_n.

(vi). Collapse postulate

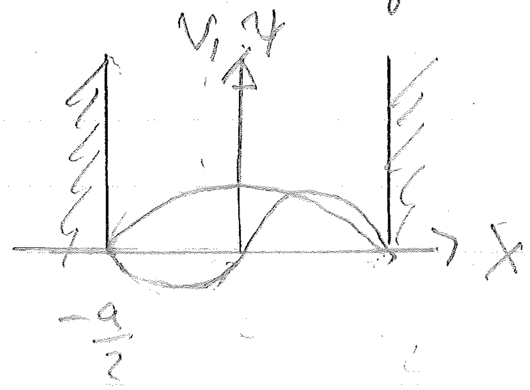
$$\psi(x) \xrightarrow[\text{and get } E_n]{\text{measure } E} \phi_n(x)$$ particle after measurement in energy eigenstate



interaction w/ outside world described by classical physics

(vii) Symmetry

shift x axis by $a/2$:



$V(-x) = V(x)$ reflection symmetry (parity)

$$\psi_n = \begin{cases} \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} & n \text{ odd} \\ \sqrt{\frac{2}{a}} \sin \left(\frac{n\pi x}{a}\right) & n \text{ even} \end{cases}$$

$\psi(-x) = \pm \psi(x)$ even, odd parity solution

physically, PDF $|\psi(-x)|^2 = |\psi(x)|^2$

must have symmetry of V, not ψ.

Ground state is symmetric

Example: An example where the state is a superposition of energy eigenstates.

$$\psi(x) = A\,x(a-x)$$

$$A = \sqrt{\frac{30}{a^5}} \qquad \text{check dimensions.}$$

$$\langle E \rangle = A^2 \int_0^a x(a-x)\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right) x(a-x)\,dx$$

$$= A^2 \frac{\hbar^2}{2m}\frac{a^3}{6} = \left(\frac{\hbar^2}{ma^2}\right)5 > \left(\frac{\hbar^2}{ma^2}\right)\left(\frac{\pi^2}{2}\right)$$

Amplitude to be in the ground state.

$$c_1 = A\sqrt{\frac{2}{a}} \int_0^a x(a-x)\sin\left(\frac{\pi x}{a}\right)dx$$

let $\theta = \pi x/a$

$$c_1 = \sqrt{\frac{30}{a^5}}\sqrt{\frac{2}{a}}\left(\frac{a}{\pi}\right)^3 \int_0^\pi \theta(\pi-\theta)\sin\theta\,d\theta$$

$$= \frac{\sqrt{60}}{\pi^3}\left[\pi\int_0^\pi \theta\sin\theta\,d\theta - \int_0^\pi \theta^2\sin\theta\,d\theta\right]$$

$$= \frac{\sqrt{60}}{\pi^3}\left[\pi(\sin\theta - \theta\cos\theta)\Big|_0^\pi - \left(2\theta\sin\theta - (\theta^2-2)\cos\theta\right)\Big|_0^\pi\right]$$

$$= \sqrt{60}\,\frac{1}{\pi^3}\left[\pi^2 - (\pi^2 - 2 - 2)\right] = \frac{4\sqrt{60}}{\pi^3}$$

$$= \frac{8\sqrt{15}}{\pi^3} = \underline{0.9993}$$

Probability to measure the ground state energy is square = 0.9986

Heisenberg's Uncertainty

Mathematical statement of wave-particle duality. Derived formally later.

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Value of uncertainty product depends on wave function ψ.

Intuitive reason for non-zero ground state energy.

example 1 particle in box $\Delta x \sim a$, $\Delta p \sim \frac{\hbar}{2a}$

$$E_{Ground} \simeq \left(\frac{\hbar}{2a}\right)^2 \frac{1}{2m} \propto \frac{\hbar^2}{ma^2}$$

example 2 H ground state

$$E = \frac{p^2}{2m} - \frac{\alpha \hbar c}{r} \quad \text{let } p \sim \frac{\hbar}{r}$$

$$E(r) = \frac{\hbar^2}{2m}\frac{1}{r^2} - \frac{\alpha \hbar c}{r} \qquad \left.\frac{dE}{dr}\right|_{r_m} = 0 = -\frac{\hbar^2}{mr^3} + \frac{\alpha \hbar c}{r^2}$$

$$r_m = \frac{\hbar}{mc\alpha} = a_0 \text{ Bohr radius} \; ; \; E(r_{min}) = -\frac{1}{2}mc^2\alpha^2$$

example 3 free particle $p = \hbar k$ exactly

so $\Delta p = 0$, $\Delta x \to \infty$.

plane wave is an approximation for wave packet with negligible Δp.

moreover, wave packet is linear superposition of plane waves.