Quantum Physics 1
Class 9

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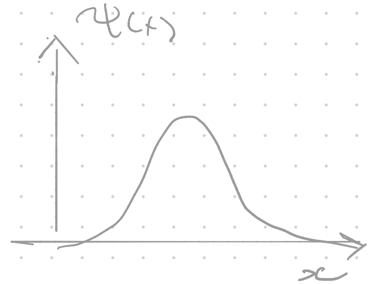
Particle in a box

Last Time:

$$\Psi(x) = \int_{-\infty}^{\infty} A(k)\, e^{i(kx-\omega t)}\, dk$$



where expectation value, $\langle A \rangle = \int \Psi^*(x)\, \hat{A}\, \Psi(x)\, dx$

$$\hat{x} \to x \quad , \quad \hat{x}^2 \to x^2$$

$$\hat{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x} \quad , \quad \hat{p}^2 \to \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2$$

w/ Uncertainty: $\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$

eg) for gaussian: $\Psi(x) = \left(\frac{1}{2\pi}\right)^{1/4} \frac{1}{\sqrt{\sigma}}\, e^{-x^2/4\sigma^2}$

$$\left.\begin{aligned} \Delta x &= \sigma \\ \Delta p &= \frac{\hbar}{2\sigma} \end{aligned}\right\} \quad \boxed{\Delta x\, \Delta p = \frac{\hbar}{2}} \quad **$$

NB Exam 1: Everything up to class #8.

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

Recall Schrödinger Equation:

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

Separation of variables: $\Psi(x,t) = \psi(x) f(t)$

$$\Rightarrow \frac{1}{\psi(x) f(t)}\left[-\frac{\hbar^2}{2m} f(t) \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) f(t)\right] = \left[i\hbar\, \psi(x) \frac{\partial f(t)}{\partial t}\right]\frac{1}{\psi(x) f(t)}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = i\hbar \frac{1}{f(t)} \cdot \frac{\partial f(t)}{\partial t} = \text{const} = E$$

$$\Rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\,\psi(x) \quad \ldots (1) \\ \frac{\partial f(t)}{\partial t} = -\frac{iE}{\hbar} \cdot f(t) \quad \ldots (2) \end{cases}$$

[Time Independent Schrod. Eqn.]

from (2) $\frac{1}{f(t)}\frac{\partial f}{\partial t} = -iE/\hbar$

$$\ln f(t) = -\frac{iE}{\hbar} t + c$$

$$f(t) = e^{-i\frac{E}{\hbar}t + c} = f(0)\, e^{-i\frac{Et}{\hbar}}$$

$\therefore$ Solution: $\boxed{\Psi(x,t) = \psi(x)\, e^{iEt/\hbar}}$

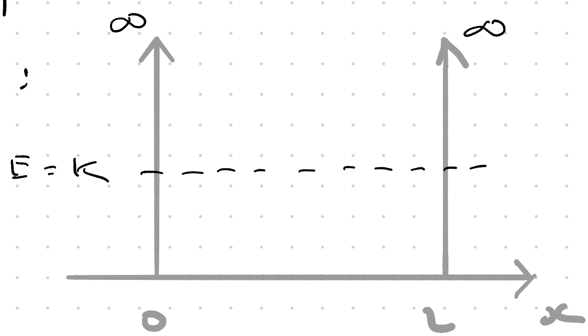
NB: $|\Psi(x,t)|^2 = |\psi(x)|^2$ independent of time.

NB: Now, precise form of solution to the time independent S.E. depends on our choice of $V(x)$.

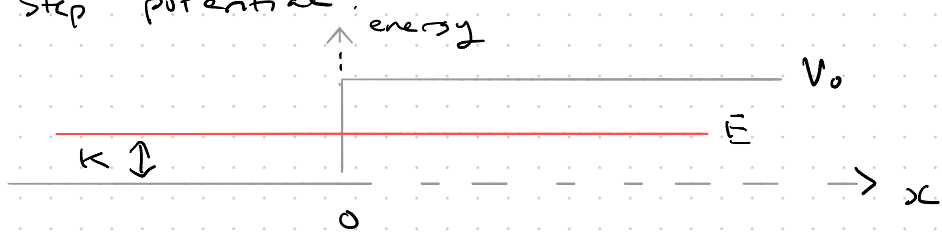
examples of $V(x)$:

(i) $V(x) = 0$ everywhere.

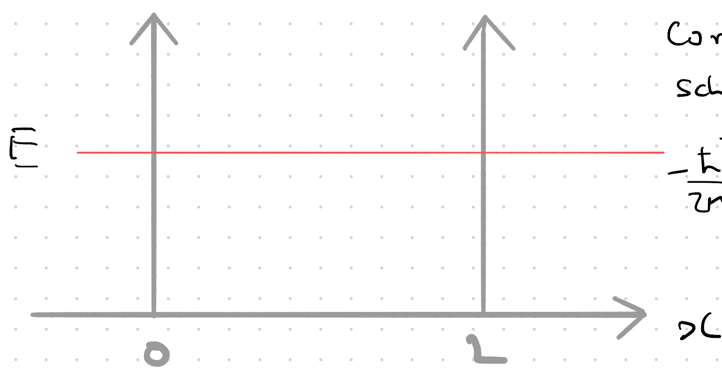
(ii) Particle in a box: (1-D box)



(iii) "step" potential:



Particle in a box



Consider time-indep Schrödinger eqn.

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} = E\,\psi(x) \quad \ldots (3)$$

Recall: $E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} \Rightarrow \boxed{k^2 = \frac{2mE}{\hbar^2}}$

Ansatz: $\psi(x) \sim e^{\pm ikx}$

$$\psi(x) \sim A e^{+ikx} + e^{-ikx}$$

Consider form of ③:

$$\frac{d^2y}{dt^2} = \text{const.}\, y$$

(i) $$\frac{d^2y}{dt^2} = -\frac{k}{m} y$$

Classical Harmonic Oscillator

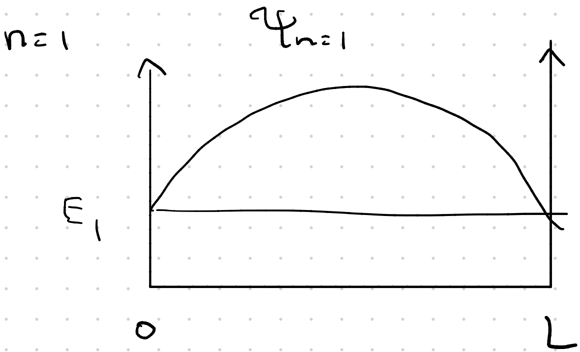
(ii) E.M. waves in a metal box.

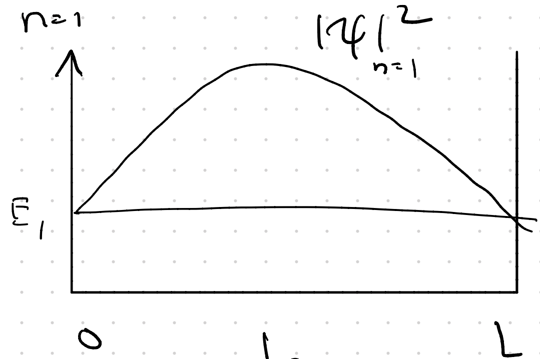
In-class 9-1

From in-class assignment we found:

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2} \; ; \quad \psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

- E is quantized
- $E_n > 0$!!! even at the ground state $n=1$.
- $\exists$ time independence $|\psi_n|^2$





where $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$ (zero point) energy

probability density.

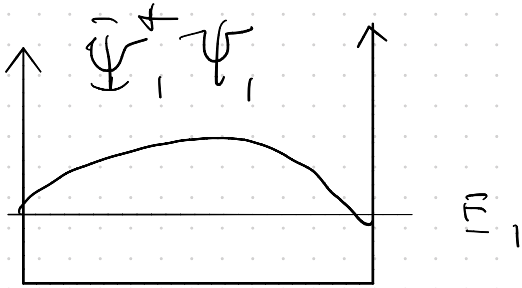
NB:

① Probability density is stationary (not moving). Not like the classical particle of a particle bouncing back and forth.

Even though $E \neq 0$, $p \neq 0$, $\Delta p \neq 0$

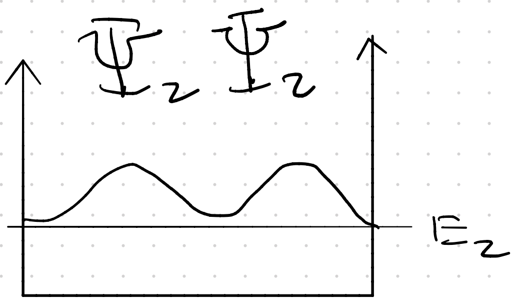
consider:

$|\Psi_1|^2 \quad n=1$



& $|\Psi_2|^2 \quad n=2$

$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L} x\right)$



$$E_2 = \frac{2^2 \pi^2 \hbar^2}{2mL^2}$$

- for $n=2$, still not bouncing back and forth. Does not satisfy our classical notions.
  (NB @ $x = L/2$)

- Consider uncertainty principle, if particle at rest $p=0$ (no uncertainty) then Δx would $\rightarrow \infty$.

Recall: $E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \equiv$ Zero point energy.

- Since particle is confined to box Δx is finite, $\therefore$ Δp must also be finite.

That is, $\Delta p \propto$ Energy (origin of zero point energy)

$\boxed{\text{Inclass 9.2, 9.3, 9.4}}$

Recall that the superposition of waves is possible.

$$\Psi_{n=1} + \Psi_{n=2} = ?$$

last time we defined $\Psi(x) = \int A(k) \sin(kx)\, dk$

So, $A(k) = ?$

In general, $\Psi(x) = \sum c_n \underbrace{\sin\left(\frac{n\pi x}{L}\right)}_{\text{basis}}$

$c_n \sim A(k)$

* Fourier Series Expansion

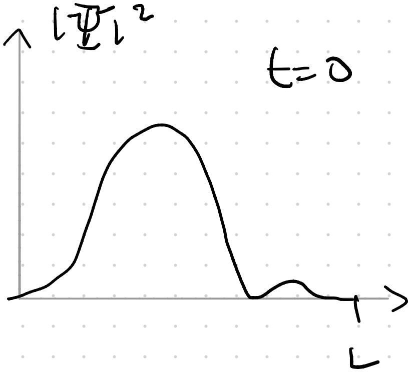
N.B.: $\exists$ wave superposition gives rise to time dependence!

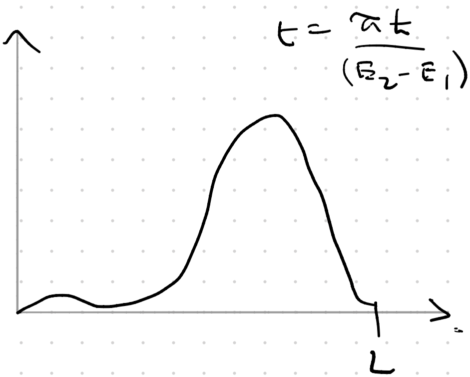
Let's consider: $\Psi(x,t) = \frac{1}{\sqrt{2}}\Psi_1(x,t) + \frac{1}{\sqrt{2}}\Psi_2(x,t)$

$$= \frac{e^{-iE_1t/\hbar}}{\sqrt{2}}\psi_1 + \frac{e^{-iE_2t/\hbar}}{\sqrt{2}}\cdot\psi_2$$

$$= e^{-iE_1t/\hbar}\left[\frac{1}{\sqrt{2}}\psi_1 + \frac{e^{-i(E_2-E_1)t/\hbar}}{\sqrt{2}}\psi_2\right]$$

& $|\Psi(x,t)|^2 = \frac{1}{2}\psi_1^2 + \frac{1}{2}\psi_2^2 + \psi_1\psi_2\cos(E_2-E_1)t/\hbar$





Recall: $\Psi_n(x,t) = \varphi_n(x)e^{-iE_nt/\hbar}$; $\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

General Solution: $\Psi(x,t) = \sum c_n\varphi_n(x)e^{-iE_nt/\hbar}$

@ $t=0$: $\Psi(x,0) = \sum c_n\varphi_n(x) = F(x)$

i.e. Fourier series expansion

$$\Rightarrow \quad \varphi_m^*(x)\,\Psi(x,0) = \sum c_n\, \varphi_m^*(x)\, \varphi_n(x)$$

$$\int \varphi_m^*(x)\,\Psi(x,0)\,dx = \sum_n c_n \underbrace{\int \varphi_m^*(x)\,\varphi_n(x)\,dx}$$

$$\int \varphi_m^*(x)\,\varphi_n(x)\,dx = \int \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)dx$$

$$= \begin{cases} 0, & m \neq n \\ 1, & m = 1 \end{cases}$$

$$= \delta_{m,n}$$ Kronecker Delta

$$\int \varphi_m^*(x)\,\Psi(x,0)\,dx = \sum c_n\, \delta_{m,n}$$

$$\boxed{\int \varphi_m^*(x)\,\Psi(x,0)\,dx = c_m}$$

Fourier Coefficient