PH 451/551
QM

Lecture #2

Review of basic systems

Recall WS #1

$$|\Psi\rangle = \frac{1}{3}|\varphi_1\rangle + \frac{1}{6}|\varphi_2\rangle + \frac{2}{3}|\varphi_3\rangle$$

where $|\varphi_n\rangle$ are eigenstates of $\hat{H}$:

$$\hat{H}|\varphi_n\rangle = n\,\mathcal{E}_0\,|\varphi_n\rangle$$

energy units

(a) measure energy $\Rightarrow$ outcomes?

- outcomes are the eigenvalues $\Rightarrow n\mathcal{E}_0$
  Note: must have the energy units!

- probability to achieve a particular outcome is $\mathcal{P}_{E_n} = \dfrac{|\langle\varphi_n|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}$

- examination of given $|\Psi\rangle \Rightarrow$ only $n = 1, 2, 3$ will yield a nonzero $\mathcal{P}_{E_n}$, so the only possible outcomes are $\mathcal{E}_0,\ 2\mathcal{E}_0,\ 3\mathcal{E}_0$

Now, how does one calculate $\mathcal{P}_n$?

Examine whether $|\Psi\rangle$ is normalised:

$$\langle\Psi|\Psi\rangle = \left(\frac{1}{3}\langle\varphi_1| + \frac{1}{6}\langle\varphi_2| + \frac{2}{3}\langle\varphi_3|\right)\cdot$$

$$\cdot\left(\frac{1}{3}|\varphi_1\rangle + \frac{1}{6}|\varphi_2\rangle + \frac{2}{3}|\varphi_3\rangle\right) = \frac{1}{9} + \frac{1}{36} + \frac{4}{9} =$$

$$= \frac{21}{36} = \frac{7}{12} \leftarrow \text{clearly} \neq 1! \qquad \langle\varphi_n|\varphi_m\rangle = \delta_{nm}$$

Two ways of calculating probabilities:

$$\mathcal{P}_n = \frac{|\langle\varphi_n|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}$$ or first normalise the initial state

$$|\Psi\rangle \Rightarrow |\Psi_{norm}\rangle$$

and then use

$$\mathcal{P}_n = |\langle\varphi_n|\Psi_{norm}\rangle|^2$$

Let's do both:

$$\mathcal{P}_1 = \frac{|\langle\varphi_1|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle} = \frac{1/9}{7/12} = \frac{1}{9}\cdot\frac{12}{7} = \frac{4}{21}$$

Similarly, $\mathcal{P}_2 = \frac{1}{21}$ & $\mathcal{P}_3 = \frac{16}{21}$

Check: $\mathcal{P}_1 + \mathcal{P}_2 + \mathcal{P}_3 = \frac{4}{21} + \frac{1}{21} + \frac{16}{21} = 1$ ✓

Now let's first normalize the state: 3

$$|\Psi_{norm}\rangle = \frac{|\Psi\rangle}{\sqrt{\langle\Psi|\Psi\rangle}}$$

Check: $\langle\Psi_{norm}|\Psi_{norm}\rangle = \frac{\langle\Psi|}{\sqrt{\langle\Psi|\Psi\rangle}} \cdot \frac{|\Psi\rangle}{\sqrt{\langle\Psi|\Psi\rangle}} =$

$= \frac{\langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 1 \leftarrow$ just what we want

$$|\Psi_{norm}\rangle = \frac{\frac{1}{3}|\varphi_1\rangle + \frac{1}{6}|\varphi_2\rangle + \frac{2}{3}|\varphi_3\rangle}{\sqrt{\frac{7}{12}}} =$$

$$= \frac{1}{3}\sqrt{\frac{12}{7}}|\varphi_1\rangle + \frac{1}{6}\sqrt{\frac{12}{7}}|\varphi_2\rangle + \frac{2}{3}\sqrt{\frac{12}{7}}|\varphi_3\rangle =$$

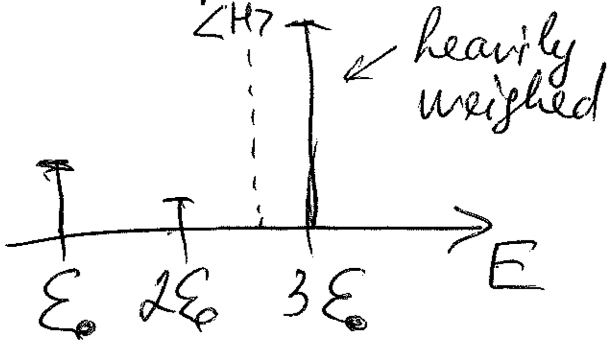
$$= \frac{2}{\sqrt{21}}|\varphi_1\rangle + \frac{1}{\sqrt{21}}|\varphi_2\rangle + \frac{4}{\sqrt{21}}|\varphi_3\rangle$$

Now, $P_n = |\langle\varphi_n|\Psi_{norm}\rangle|^2 \Rightarrow$

$P_1 = \frac{4}{21}$; $P_2 = \frac{1}{21}$; $P_3 = \frac{16}{21}$ as expected

$P_1 + P_2 + P_3 = 1$ ✓

(b) estimate average energy by using the probability histogram



Note: this prediction can be made without having a normalised state (only using relative probabilities)

(c) calculate $\langle H \rangle$

$$\langle H \rangle = P_1 \cdot E_1 + P_2 \cdot E_2 + P_3 \cdot E_3 =$$

$$= \frac{4}{21} \cdot \mathcal{E}_0 + \frac{1}{21} \cdot 2\mathcal{E}_0 + \frac{16}{21} \cdot 3\mathcal{E}_0 = \frac{54}{21}\mathcal{E}_0 =$$

$$= \frac{18}{7}\mathcal{E}_0 \approx 2.6\mathcal{E}_0$$

matches the prediction!

Another way of calculating:

$$\langle \hat{H} \rangle = \langle \Psi_{norm} | \hat{H} | \Psi_{norm} \rangle =$$

$$= \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{1}{7/12} \cdot \left(\frac{1}{3} \left(\langle \varphi_1 | + \frac{1}{2} \langle \varphi_2 | + \right.\right.$$

$$\left. + 2 \langle \varphi_3 | \right) \left(\frac{1}{3} \underbrace{\hat{H} | \varphi_1 \rangle}_{\mathcal{E}_0 | \varphi_1 \rangle} + \frac{1}{6} \underbrace{\hat{H} | \varphi_2 \rangle}_{2\mathcal{E}_0 | \varphi_2 \rangle} + \frac{2}{3} \underbrace{\hat{H} | \varphi_3 \rangle}_{3\mathcal{E}_0 | \varphi_3 \rangle} \right) =$$

$$= \frac{12}{7} \left(\frac{1}{9} \mathcal{E}_0 + \frac{1}{36} \cdot 2\mathcal{E}_0 + \frac{4}{9} \cdot 3\mathcal{E}_0 \right) = \frac{18}{7} \mathcal{E}_0$$

(d) Time evolution of the state ⑤

$$|\Psi_{norm}(t)\rangle = \frac{2}{\sqrt{21}} e^{-\frac{i}{\hbar}\varepsilon_0 t} |\varphi_1\rangle + \frac{1}{\sqrt{21}} e^{-\frac{i}{\hbar}2\varepsilon_0 t} |\varphi_2\rangle + \frac{4}{\sqrt{21}} e^{-\frac{i}{\hbar}3\varepsilon_0 t} |\varphi_3\rangle$$

Systems previously studied:

- free particle
- particle in a box $\nearrow$ infinite well, $\rightarrow$ finite well
- (H)-atom
  - will add harmonic oscillator to this list shortly

like particle-in-a-box but the box is shaped differently

$\Downarrow$

review previously studied systems!

What is common for these? $\Rightarrow$ all were concerned with where the particle is

$\boxed{\text{position space}}$

discrete n, $n = 1, 2, \ldots$

$|n\rangle \Rightarrow |x\rangle$ continuum

$|\Psi\rangle \Rightarrow \langle x|\Psi\rangle \equiv \Psi(x)$ $\boxed{\text{wave function}}$

$\Rightarrow \langle\Psi|x\rangle = \Psi^*(x)$

or: $|\Psi\rangle \doteq \Psi(x)$

"represented by"

$\boxed{\text{Dirac (abstract)}}$ $\boxed{\text{Position space}}$ eigenfunctions

eigenbasis

$|\Psi\rangle = \sum_n C_n |\varphi_n\rangle \Rightarrow \Psi(x) = \sum_n C_n \varphi_n(x)$

$\langle\varphi_n|\varphi_m\rangle = \delta_{nm} \Rightarrow \int_{-\infty}^{+\infty} \varphi_n^*(x)\varphi_m(x)\,dx = \delta_{nm}$

$\langle\Psi|\Psi\rangle = 1 \Rightarrow \int_{-\infty}^{+\infty} \sum_m C_m^* \varphi_m^*(x) \sum_n C_n \varphi_n(x)\,dx$

$= \sum_m \sum_n C_m^* C_n \underbrace{\int_{-\infty}^{+\infty} \varphi_m^*(x)\varphi_n(x)\,dx}_{=\delta_{mn}}$

$= \sum_n |C_n|^2 = 1$

$\left(\sum_m C_m^* \langle\varphi_m|\right)\left(\sum_n C_n|\varphi_n\rangle\right) =$

$= \sum_m \sum_n C_m^* C_n \underbrace{\langle\varphi_m|\varphi_n\rangle}_{=\delta_{mn}} =$

$= \sum_m \sum_n C_m^* C_n \delta_{nm} = \sum_n |C_n|^2 = 1$

(So normalized vector requires $\sum_n |C_n|^2 = 1$)

$\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle \Rightarrow \hat{A}\varphi_n(x) = a_n \varphi_n(x)$

$\langle\hat{A}\rangle = \langle\Psi|\hat{A}|\Psi\rangle \Rightarrow \langle\hat{A}\rangle = \int_{-\infty}^{+\infty} \Psi^*(x)\hat{A}\,\Psi(x)\,dx$

$C_n = \langle\varphi_n|\Psi\rangle \Rightarrow C_n = \int_{-\infty}^{+\infty} \varphi_n^*(x)\Psi(x)\,dx$

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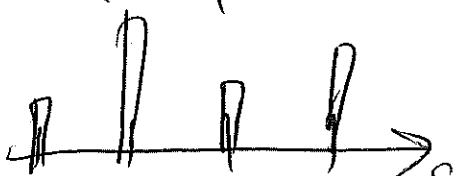
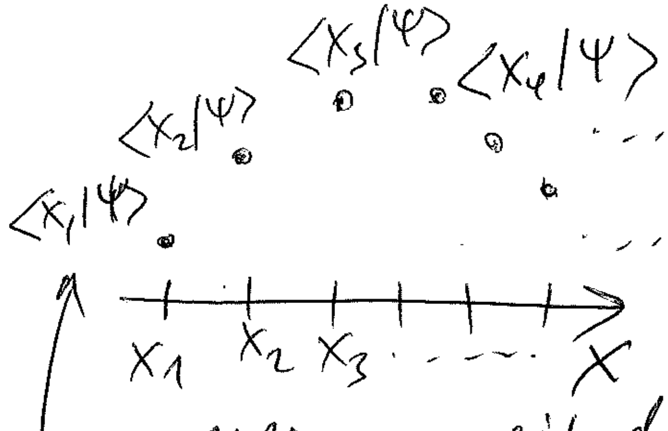
Probability histogram! $\Rightarrow$ wave function

$$P_{E_n} = |\langle \varphi_n | \psi \rangle|^2$$

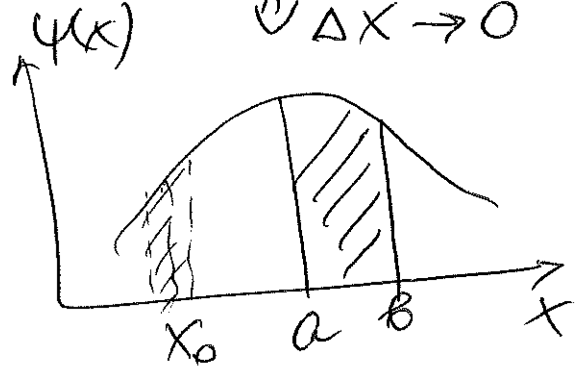


some discrete variable (energy, spin, ...)



probability amplitudes

$\Downarrow \Delta x \to 0$



- what is the probability to find the particle at $x = x_0 \pm \Delta$?

$\uparrow \Delta \to 0$

$$\int_{x_0-\Delta}^{x_0+\Delta} |\psi(x)|^2 dx \underset{\Delta \to 0}{\approx} |\psi(x_0)|^2 \cdot 2\Delta$$

$|\psi(x)|^2$

$\uparrow$ probability density $\leftarrow \frac{1}{[L]}$

- what is the probability to find the particle in the $[a,b]$ region?

$$\underbrace{\int_a^b |\psi(x)|^2 dx}_{\text{probability (dimensionless)}}$$

check: $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$

(8)

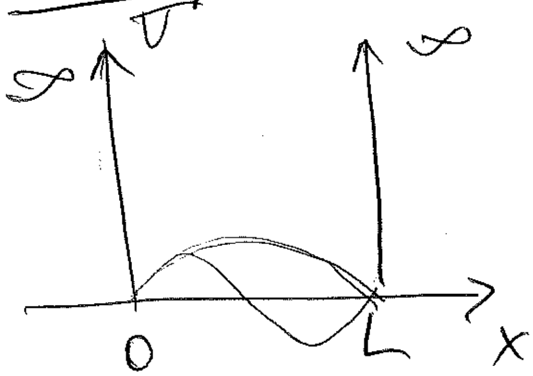
- What if we need the probability of measuring a discrete quantity (e.g. energy),

$$P_{E_n} = |\langle \varphi_n | \psi \rangle|^2 \Rightarrow P_{E_n} = \left| \int dx\, \varphi_n^*(x)\, \psi(x) \right|^2$$

eigen state, initial state (so $|C_n|^2$ in both cases!)

$$\hat{H} |\varphi_n\rangle = E_n |\varphi_n\rangle \qquad \hat{H} \varphi_n(x) = E_n \varphi_n(x)$$

<u>Example</u> particle-in-a-box → infinite well



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

Any $\psi(x)$ can be presented as $\sum_n C_n \varphi_n(x)$

$$\int_0^L \sin \frac{\pi n x}{L} \sin \frac{\pi m x}{L}\, dx = 0 \quad m \neq n \qquad \frac{2}{L} \int_0^L \sin^2 \frac{\pi n x}{L}\, dx = 1$$

$$C_n = \int_0^L \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}\, \psi(x)\, dx$$

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

⇒ if the initial state is $\psi(x)$, the prob. to find the particle in $\varphi_n(x)$ after measuring E_n is $\left| \int_0^L \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}\, \psi(x)\, dx \right|^2$

To find $\Psi(x)$, we need to solve the Schrödinger equation $\Rightarrow$ e.s. eigenvalue problem
time-ind.

$$\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle \Rightarrow \hat{H}(x)\,\varphi_n(x) = E_n\,\varphi_n(x)$$

Convert in a position basis

everything has to be a function of x!

$\boxed{1D}$

$$\frac{\hat{p}^2}{2m} + V(\hat{X})$$

momentum operator

position operator

$$\hat{X} \doteq x$$

$$\hat{p} \doteq -i\hbar\frac{d}{dx}$$

represent in position basis (space)

$$\Rightarrow \hat{H}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Solve $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\varphi_n(x) = E_n\varphi_n(x)$
(or φ_E if continuum)

- free particle $\Rightarrow V = 0$ for any x

$$\varphi_E(x) = Ae^{ikx} + Be^{-ikx} \leftarrow \text{unbound}$$

$$k = \frac{2mE}{\hbar^2}\ ;\ E = \frac{\hbar^2k^2}{2m} \leftarrow \text{continuum}$$

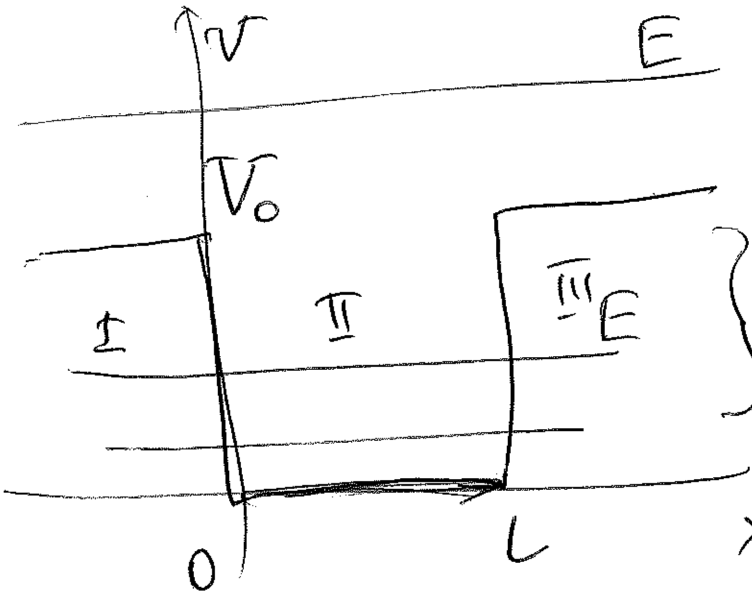
- particle in an infinite well $\Rightarrow$ $V = 0$ for $x \in [0, L]$, $V = \infty$ otherwise

$$\varphi_n = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L} \text{ for } x \in [0, L]$$

0 otherwise

discrete $\nearrow$ $E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$ $(n = 1, 2, \dots)$

- particle in a finite well $\Rightarrow$



scattering states

bound states $\rightarrow$ energies obtained from solving transcendental eqns

general solution

$$\varphi_E(x) = \begin{cases} \text{I} & Ae^{qx} + Be^{-qx} \\ \text{II} & C\sin kx + D\cos kx \\ \text{III} & Fe^{qx} + Ge^{-qx} \end{cases}$$

$E < V_0$:

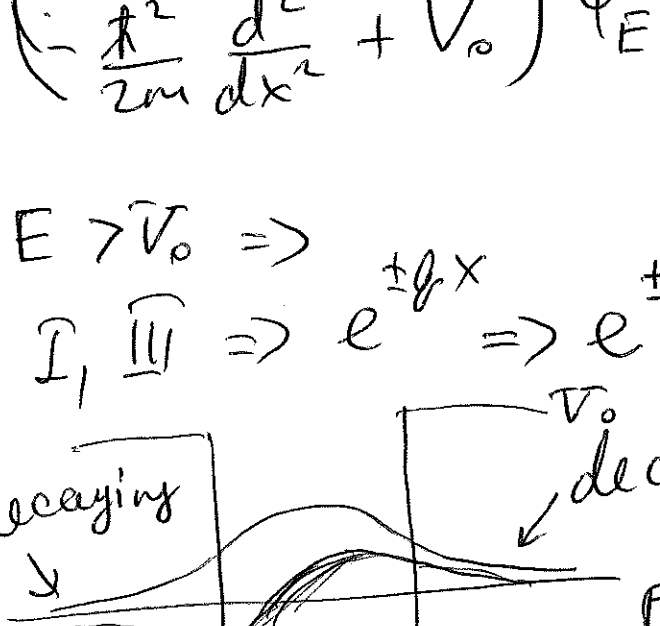
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 0\right)\varphi_E(x) = E\varphi_E(x) \qquad 0 < x < L$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\varphi_E(x) = E\varphi_E(x) \qquad x < 0,\ > L$$

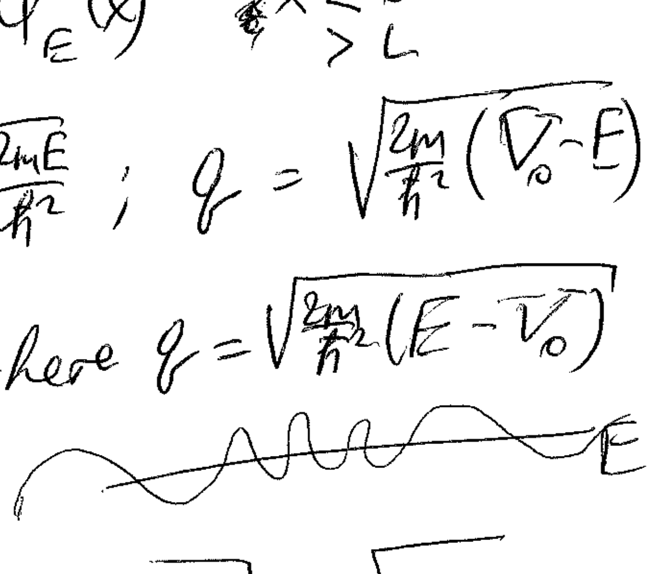
$$k = \sqrt{\frac{2mE}{\hbar^2}}\ ; \quad q = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$E > V_0 \Rightarrow$

I, III $\Rightarrow e^{\pm qx} \Rightarrow e^{\pm iqx}$ where $q = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$



vs



oscillatory everywhere (but different period)

k & q are the spatial frequencies