9/28/98

Lecture #12: Change of basis, normalization

Can represent state of a particle with a coordinate space wave function,

$$\psi^*(x)\,\psi(x)\,dx = \text{Prob to be between } x \text{ and } x + dx$$

Normalization

$$\int_{-\infty}^{\infty} dx\, \psi^*(x)\,\psi(x) = 1$$

or could expand in Energy eigenstates

$$\psi(x) = \sum_i c_i\, \psi_i(x)$$

Where the ψ_i are orthonormal

$$\int_{-\infty}^{\infty} dx\, \psi_i^*(x)\,\psi_j(x) = \delta_{ij}$$

Thus
$$\int_{-\infty}^{\infty} dx\, \psi^*(x)\,\psi(x) = \sum_i c_i^* \sum_j c_j \int_{-\infty}^{\infty} dx\, \psi_i^*(x)\,\psi_j(x) = \sum_{i,j} c_i^* c_j\, \delta_{ij}$$
$$= \sum_i c_i^* c_i = 1$$

Can think about representing state of particle with the set

$\{c_i\}$

Where $c_i^* c_i = P_i$ prob. to be in state i

Clearly these c_i are normalized $\sum_i |c_i|^2 = 1$

Alternatively can use a <u>momentum space</u> wave function $\phi(k)$.

Normalization $\int_{-\infty}^{\infty} dk\, \phi^*(k)\, \phi(k) = 1$ (will show)

Prob. interp. $\phi^*(k)\phi(k)dk$ = prob to find particle with momentum between $\hbar k$ and $\hbar(k+dk)$

Remember free particle

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \phi(k)\, e^{ikx}$$

This satisfies S. eq. for $V \equiv 0$ for any $\phi(k)$.

$$\Psi^*(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk'\, \phi^*(k')\, e^{-ik'\cdot x}$$

Compute normalization

$$\int dx\, \Psi^*(x)\,\Psi(x) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk' \int_{-\infty}^{\infty} dk \;\frac{1}{2\pi}\, \phi^*(k')\, e^{-ik'x}$$
$$\phi(k)\, e^{ikx}$$

Do x integral first

$$\int_{-\infty}^{\infty} dx \;\frac{1}{2\pi}\, e^{i(k-k')x} = \delta(k-k')$$

$$\int dx\, \Psi^*(x)\Psi(x) = \int_{-\infty}^{\infty} dk'\, \phi^*(k') \int_{-\infty}^{\infty} dk\, \phi(k)\, \delta(k-k')$$

Do integral over k'

$$\int dk'\, \phi^*(k')\, \delta(k-k') = \phi^*(k)$$

$$\int_{-\infty}^{\infty} dx\, \Psi^*(x)\Psi(x) = \int_{-\infty}^{\infty} dk\, \phi^*(k)\, \phi(k) = 1$$

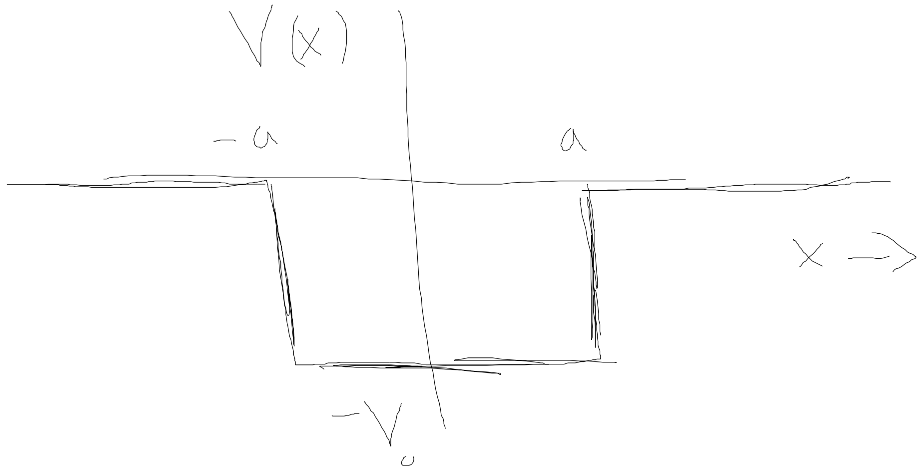
Normalization integral looks the same in x space as in p space

So we have a normalized wave function with a prob. interpretation and we can expand the wave function in any convenient basis.

Finite Square Well

$$V = \begin{cases} -V_0 & -a < x < a \\ 0 & |x| > a \end{cases}$$

with $V_0 > 0$



For $|x| > a$ $\quad V = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

look for bound states $E < 0$

$$\psi = \begin{cases} B e^{\kappa x} & x < -a \\ F e^{-\kappa x} & x > a \end{cases}$$

Want $\psi \to 0$ as $|x| \to \infty$

For $|x| < a$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi$$

or $$\frac{d^2\psi}{dx^2} = -l^2\psi$$

$$l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

want $E + V_0 > 0$ with $E < 0$
$\Rightarrow$ $|E| < V_0$ binding E must be less than V_0

$$\psi = C\sin(lx) + D\cos(lx) \qquad |x| < a$$

Expect ψ to be either even
$\psi(x) = \psi(-x)$
or odd $\psi(x) = -\psi(-x)$ since the pot is even $V(x) = V(-x)$

Look for <u>even</u> solutions $C = 0$

$$\psi = \begin{cases} Fe^{-\kappa x} & x > a \\ D\cos lx & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

Wave function must be cont. at $x = a$

$$F = e^{-\kappa a} = D \cos la$$

also $\frac{d\psi}{dx}$ must be cont. (note V is finite)

$$-\kappa F e^{-\kappa a} = -l D \sin la$$

or $$\boxed{\kappa = l \tan la}$$

This is an eigenvalue equation for the allowed E

$$\kappa = \sqrt{-2mE}/\hbar \qquad l = \sqrt{2m(E+V_0)}/\hbar$$

set $z = la$ and $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$

$$\kappa^2 + l^2 = \frac{2mV_0}{\hbar^2}$$

$$\kappa a = \sqrt{z_0^2 - z^2}$$

$$\sqrt{z_0^2 - z^2} = z \tan z$$

or $$\boxed{\tan z = \sqrt{(z_0/z)^2 - 1}}$$

Can solve numerically

Wide deep well $z_0 \to \infty$

$$\tan z \simeq \infty \quad \Rightarrow \quad \cos z \simeq 0$$

$$z_n \simeq n \frac{\pi}{2} \qquad n \text{ odd}$$

$$E_n + V_0 \simeq \frac{n^2 \pi^2 \hbar^2}{2m \, (2a)^2}$$

Shallow, narrow well.
Let $z_0 \to 0$ expect $z \to z_0 \to 0$

$$\tan z \simeq z = \left(\frac{z_0^2}{z^2} - 1\right)^{1/2}$$

$$\Rightarrow \quad z^2 = \frac{z_0^2}{z^2} - 1$$

$$z^4 + z^2 - z_0^2 = 0$$

$$z^2 = \frac{-1 \pm (1 + 4z_0^2)^{1/2}}{2}$$

$$z^2 = \frac{(1 + 4z_0^2)^{1/2}}{2} - \frac{1}{2}$$

$$z \approx z_0 \quad \Rightarrow \quad E_n \simeq 0$$

In one dim an attractive pot. no matter how weak always has at least one bound state.