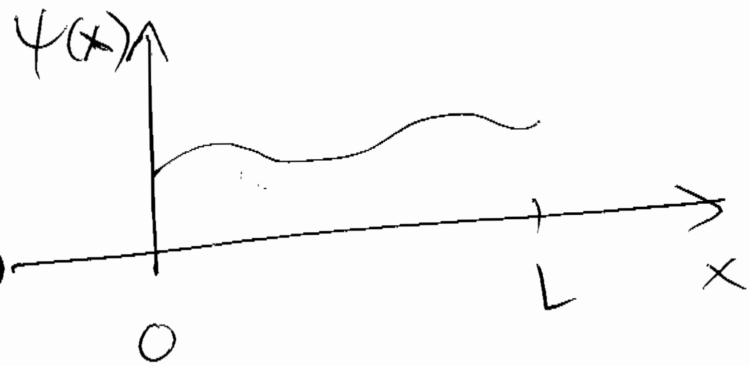
Physics 371 Lecture 7

- Particle in 1D with periodic boundary conditions

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



$$\psi(0) = \psi(L)$$

$$\psi'(0) = \psi'(L)$$

Ansatz: $\psi(x) = A e^{ikx} + B e^{-ikx}$

$$\Rightarrow \quad E = \frac{\hbar^2 k^2}{2m}$$

$$\psi(0) = A + B = \psi(L) = A e^{ikL} + B e^{-ikL}$$

$$\psi'(0) = ik(A - B) = \psi'(L) = ik\left(A e^{ikL} - B e^{-ikL}\right)$$

$$A + B = A e^{ikL} + B e^{-ikL} \qquad (1)$$

$$A - B = A e^{ikL} - B e^{-ikL} \qquad (2)$$

$(1)+(2)$:
$$1 = e^{ikL}$$

A & B free parameters, to be determined by normalization and/or initial conditions.

$$\Rightarrow \quad kL = 2\pi n$$

$$k_n = \frac{2\pi n}{L}, \qquad n = 0, \pm 1, \pm 2, \cdots$$

$$E_n = \frac{h^2 n^2}{2mL^2} \qquad \begin{cases} n=0 & \text{nondegenerate} \\ n\neq 0 & \text{doubly deg.} \end{cases}$$

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{i k_n x}$$

$\psi_n(x)$ is also a momentum

- eigenstate:

$$\hat{p}_x \psi_n(x) = \frac{\hbar}{i}\frac{d}{dx}\psi_n(x) = \hbar k_n \psi_n(x)$$

$$p_x = \hbar k_n$$

<u>Compare to particle in a box:</u>

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

$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}, \quad n = 1, 2, 3, \ldots$$

energy levels are nondegenerate!

$$\psi_n \sim e^{i\tilde{k}_n x} - e^{-i\tilde{k}_n x}$$

- $$\tilde{k}_n = \frac{\pi n}{L}$$

- Q: Is ψ_n also a momentum eigenstate? No.

$$\hat{P}_x \psi_n \sim \frac{\hbar}{i}\frac{d}{dx}\left(e^{i\tilde{k}_n x} - e^{-i\tilde{k}_n x}\right)$$

$$= \hbar\tilde{k}_n\left(e^{i\tilde{k}_n x} + e^{-i\tilde{k}_n x}\right)$$

$$\neq \hbar\tilde{k}_n \, \psi_n(x)$$

- What is $\langle \hat{P}_x \rangle$?

$$\langle \hat{P}_x \rangle = \int_0^L dx \, \psi_n^*(x) \frac{\hbar}{i}\frac{d}{dx} \psi_n(x)$$

$$\sim \hbar\tilde{k}_n \int_0^L dx \, \sin\frac{n\pi x}{L} \cos\frac{n\pi x}{L} \rightarrow 0$$

- $\langle \hat{P}_x \rangle = 0 \qquad \langle P_x^2 \rangle = \hbar^2 \tilde{k}_n^2$

$$\Delta P_x = \hbar\tilde{k}_n = \hbar\pi n / L$$

- Particle-in-a-box eigenstates are standing waves — equal superpositions of k and $-k$. Hence $\langle \hat{p}_x \rangle = 0$.

Back to $\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$.

Note that

- $$\int_0^L dx\, \psi_{n'}^*(x)\, \psi_n(x) = \delta_{nn'}$$

Proof: $$\frac{1}{L}\int_0^L dx\, e^{-ik_{n'}x} e^{ik_n x}$$

$$= \frac{1}{L}\int_0^L dx\, e^{i\frac{2\pi}{L}(n-n')x}$$

- $$= \begin{cases} 1, & n = n' \\ \frac{1}{2\pi i(n-n')}\left(e^{i2\pi(n-n')} - 1\right) \to 0, & n \neq n' \end{cases}$$

Q.E.D.

Dirac Bra-ket notation

- We write integrals such as

$$\int_0^L dx\, \psi_{n'}^*(x)\, \psi_n(x) \equiv \langle n' | n \rangle$$

Expectation values can likewise be written:

- $$\langle \hat{P}_x \rangle = \int dx\, \psi_n^*(x)\, \hat{P}_x\, \psi_n(x)$$

$$= \langle n | \hat{P}_x n \rangle$$

or $\langle n | \hat{P}_x | n \rangle$, assuming $\hat{P}_x$ is a "Hermitian" operator.

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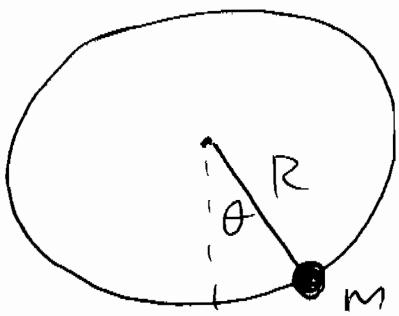
1D Ring

- The problem we have solved w/ PBCs in 1D is equivalent to the motion of a bead on a ring:

$$L = 2\pi R$$



$$E = \frac{1}{2} m R^2 \dot{\theta}^2 = \frac{I}{2} \dot{\theta}^2$$

bead slides without friction

Let $x = R\theta$ $\qquad E = \frac{1}{2} m \dot{x}^2$

Schrödinger equation

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

- $\psi(x) = \psi(R\theta) \equiv C\,\phi(\theta)$

C = normalization constant

$$E\,\phi(\theta) = -\frac{\hbar^2}{2mR^2}\frac{d^2\phi}{d\theta^2}$$

$$= -\frac{\hbar^2}{2I}\frac{d^2\phi}{d\theta^2}$$

Solutions

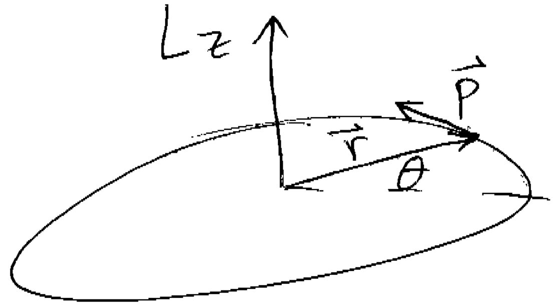
$$\phi = Ae^{ik_n x} = Ae^{i\frac{2\pi n x}{2\pi R}} = Ae^{in\theta}$$

$$\phi_n(\theta) = Ae^{in\theta} = \frac{1}{\sqrt{2\pi}}e^{in\theta}$$

$$1 = \int_0^{2\pi} d\theta\, |\phi_n(\theta)|^2 = 2\pi |A|^2$$

$$A = \frac{1}{\sqrt{2\pi}}$$ normalization

$$E_n = \frac{\hbar^2 n^2}{2I}, \quad n = 0, \pm 1, \pm 2, \ldots$$



Classically,

$$L_z = R P_x = m R^2 \dot{\theta}$$

$$E = \frac{L_z^2}{2I}$$

c.f. Bohr's hypothesis

$$\Rightarrow L_z = n\hbar \qquad n = 0, \pm 1, \pm 2, \ldots$$

At the operator level, we have

$$\hat{L}_z = R\hat{P}_x = R\frac{\hbar}{i}\frac{d}{dx} = \frac{\hbar}{i}\frac{d}{d\theta}$$

$$\hat{L}_z \phi_n(\theta) = \frac{\hbar}{i}\frac{d}{d\theta} A e^{in\theta} = n\hbar\, \phi_n(\theta)$$

$\phi_n(\theta)$ are eigenstates of $\hat{L}_z$ w/ eigenvalue $L_z = n\hbar$.

Uncertainty relation between

- θ & L_z

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

$$\Delta (R\theta) \, \Delta \left(\frac{L_z}{R} \right) \geq \frac{\hbar}{2}$$

$$\boxed{\Delta \theta \, \Delta L_z \geq \frac{\hbar}{2}}$$

- This problem is related to that of an electron moving in a very small metal ring or molecule,

e.g. Benzene :