Lecture 8 - more lessons from particle in a box

Thursday, September 8, 2022 1:06 PM

1. Warm-up Quiz
2. HW3 due, HW4 out
3. Today
   - Particle in a box states
   - orthonormality + Fourier
   - expectation values revisited
   - Connection to classical

Reading: Griffiths 2.4

Last time: Particle in a box solutions

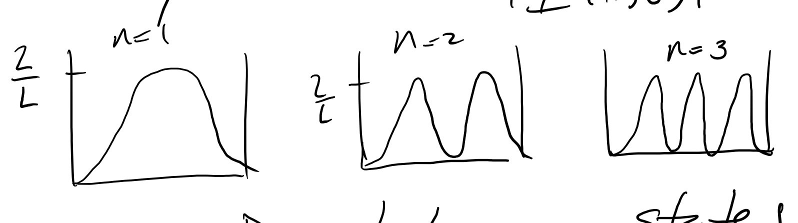
$$\Psi_n(x,t) = \underbrace{\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{n\pi x}{L}\right)}_{\psi(x)} \underbrace{e^{-iEt/\hbar}}_{\phi(t)}$$

① Energy $\Leftrightarrow \dfrac{d^2\psi}{dx^2}$

② $\displaystyle\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{nm}$

These are general features of wavefunctions

Probability function: $|\Psi(x,t)|^2 = \left(\frac{2}{L}\right)\sin^2\left(\frac{n\pi x}{L}\right)$ $\{$Note $\phi^*(t)\phi(t) = 1\}$



.... probability always real, positive

$\Rightarrow$ Stationary states... Eigenstates don't evolve in time.

③ The general Sol$^{\underline{n}}$ is a normalized superposition of the $\Psi_n(x,t)$:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\tfrac{2}{L}} \sin\left(\tfrac{n\pi x}{L}\right) e^{-iE_n t/\hbar}$$

④ The $\psi_n(x)$ are complete $\Rightarrow$ any function $f(x)$ consistent w/ the B.C.'s can be expressed (expanded) in the ψ_n

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\tfrac{2}{L}}\, c_n \sin\left(\tfrac{n\pi x}{L}\right)$$

$\Rightarrow$ Fourier Series!!

$\therefore$ if I know $f(x) \Rightarrow$ can find c_n

multiply by ψ^* on left and integrate

$$\int_{-\infty}^{\infty} \psi_m^*(x) f(x)\, dx = \sum_{n=1}^{\infty} c_n \underbrace{\int \psi_m(x)\psi_n(x)\, dx}_{\delta_{nm}} = c_m$$

Inverse Fourier Series

$\Rightarrow$ These properties are general for sol$^{\underline{ns}}$ of TISE.

General approach.

① solve TISE w/ b.c.'s $\rightarrow$ find Eigenfunctions/Values of $\hat{H}$

② The initial conditions $\Rightarrow f(x)$

$\Rightarrow$ find c_n.

$\Rightarrow$ you know how probability evolves in time.

General Probability: $|\Psi(x,t)|^2 = \left|\sum_n^{\infty} \psi_n e^{-iE_n t/\hbar}\right|^2$

How do I extract "classical" quantities (e.g. $x, p, \ldots$)?

Expectation Values: $|\Psi(x,t)|^2$ is a probability distribution function

Recall: $|\Psi(x,t)|^2 = \Psi^*\Psi$, for any operator $\hat{Q}$

$$\langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi \, dx$$

Example: Suppose $\Psi = \psi_1(x)\, e^{-i\overbrace{E_1 t/\hbar}^{\text{or } \omega_1 t}}$ since $E_n = \hbar\omega_n$ what is p?

$$\langle p \rangle = \int_{-\infty}^{\infty} \sqrt{\tfrac{2}{L}} \sin\left(\tfrac{\pi x}{L}\right) e^{i\omega_1 t} \left(-i\hbar \tfrac{\partial}{\partial x}\right) \sqrt{\tfrac{2}{L}} \sin\left(\tfrac{\pi x}{L}\right) e^{-i\omega_1 t}\, dx$$

$$= -\frac{2i\hbar}{L}\int_0^L \sin\left(\tfrac{\pi x}{L}\right)\left(\tfrac{\pi}{L}\right)\cos\left(\tfrac{\pi x}{L}\right) dx = 0$$

Does $\langle \hat{Q} \rangle = \cancel{\int_{-\infty}^{\infty} \hat{Q}\, \Psi^* \Psi\, dx} = \boxed{\int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi \, dx} = \cancel{\int_{-\infty}^{\infty} \Psi^* \Psi \hat{Q}\, dx}$?

In general?

No $\Rightarrow$ order of operation can matter. More on that later.

what about $\langle KE \rangle$? $\hat{T} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$

$$\langle T \rangle = -\frac{2}{L}\frac{\hbar^2}{2m}\int_0^L \sin\left(\tfrac{\pi x}{L}\right)\frac{\partial^2}{\partial x^2}\left[\sin\left(\tfrac{\pi x}{L}\right)\right] dx$$

$$= \frac{2}{L}\frac{\hbar^2}{2m}\left(\frac{\pi^2}{L^2}\right)\underbrace{\int_0^L \sin\left(\tfrac{\pi x}{L}\right)\sin\left(\tfrac{\pi x}{L}\right) dx}_{L/2} = \frac{\pi^2\hbar^2}{2mL^2} = E_1$$

In the well $\hat{T} = \hat{H}$, so since $\hat{H}\psi = E\psi$

$$\langle \hat{H} \rangle = \int \Psi^* \hat{H} \Psi \, dx = \int \Psi^* E \Psi\, dx = E \quad \text{(in general)}$$

- Note Ψ is an eigenfunction of $\hat{H}$, but not p
  so for $\hat{H} \Rightarrow$ trivial for $\hat{p} \Rightarrow$ have to work it out...

- Also $\langle p \rangle = 0$ $\langle T \rangle \neq 0 \Rightarrow$ superposition of $+p$ and $-p$...

you can see that from $\Psi(x,t)$:

$$\Psi_1(x,t) = \sqrt{\tfrac{2}{L}} \sin(k_1 x)\, e^{-i\omega t} = \sqrt{\tfrac{2}{L}}\left(e^{i(kx-\omega t)} - e^{-i(kx+\omega t)}\right)$$

Wave travels left   wave travels right

e.g. fixed phase:

$kx \mp \omega t = \text{Const}$

$x \mp \underbrace{\tfrac{\omega t}{k}}_{vt} = \text{Const}'$

$$\boxed{\frac{\omega}{k} = \frac{2\pi\nu}{2\pi/\lambda} = \nu\lambda = v \equiv \text{phase velocity}}$$

Quantum $\longrightarrow$ Classical

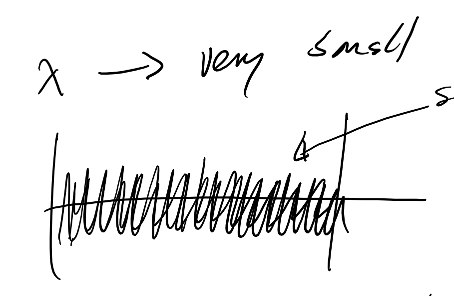
classical – particle bounces back/forth energy E

– Averaged over time, equally likely to be anywhere $x \rightarrow 0 - L$

Quantum – As $E \rightarrow$ classical level $n \rightarrow \infty$

$\lambda \rightarrow$ very small

superposition of many ψ_n



Can describe "classical motion" in terms of $\Psi(x,t)$

Extra interactions w/ uncontrolled environment

$\Rightarrow$ decoherence $\Rightarrow$ lose $\phi(t) \Rightarrow$ Lose wave nature.