If the two lowest energy particle-in-a-box states are $\psi_1(x)$ and $\psi_2(x)$ with energies E_1 and E_2, which of the following statements are correct?

A. $\Psi(x) = \frac{1}{\sqrt{2}}[\psi_1(x) + \psi_2(x)]$ is a possible wave function for the particle at time $t = 0$.

B. $\Psi(x) = \frac{1}{\sqrt{2}}[\psi_1(x) + \psi_2(x)]$ satisfies the ***time-independent*** SE,

$$\hat{H}\Psi(x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(\mathrm{x}) = E\Psi(x)$$

C. $\Psi(x,t) = \frac{1}{\sqrt{2}}[\psi_1(x)e^{\frac{-iE_1t}{\hbar}} + \psi_2(x)e^{\frac{-iE_2t}{\hbar}}]$ satisfies the **full time-dependent** SE:

$$\hat{H}\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

CHM 305 The Quantum World

Lecture 5: Quantum Operators

Reading: McQuarrie Ch. 4

Last lecture we discussed…

Description of the simplest quantum system: the *free particle* in a potential with V(x) = 0

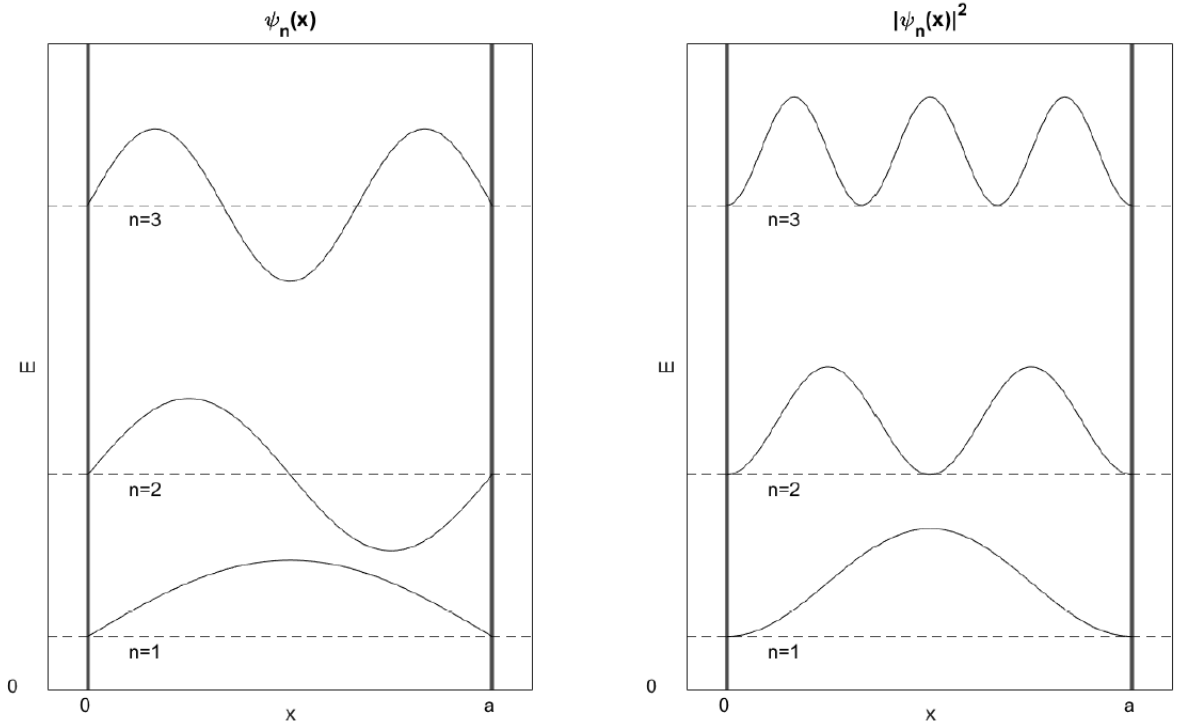
$$\Psi_k(x,t) = \psi_k(x) \cdot e^{-i\omega t} = c_k e^{i(kx-\omega t)}$$

Description of the next simplest quantum system: the particle in a box

- Stationary state wavefunctions & energies for a 1D box
- Boxes of higher dimensions

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{a}\right) \text{ for } n = 1, 2, \ldots$$

$$E_n = \frac{k^2\hbar^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2$$



Road map for today's lecture

$$\hat{A}\psi_n(x) = a_n\psi_n(x)$$

Discuss some rules about how quantum operators and their eigenfunctions behave:

Quantum operators

- are linear
- may or may not commute

Eigenfunctions of an operator

- are normalized
- are mutually orthogonal
- form a complete basis set

Practice problem #1: Eigenvalue problems

Check if $\psi(x) = \sin(kx)$ is an eigenfunction of the following operators:

$$\hat{A} = \frac{d}{dx} \qquad \hat{B} = \frac{d^2}{dx^2}$$

If you find $\psi(x)$ to be an eigenfunction, what is the eigenvalue?

Practice problem #2: Commutation

Do the operators $\hat{A} = \frac{d}{dx}$ and $\hat{B} = x$ commute?

Hint: Evaluate $[\hat{A}, \hat{B}]\psi(x) = (\hat{A}\hat{B} - \hat{B}\hat{A})\psi(x)$

Practice problem #3: Normalizing functions

Normalize the wavefunction

$$\psi(x) = c \cdot (1 - x)$$

over the interval $x = [0, 1]$.

Hint: Solve for c assuming that

$$\int_0^1 |\psi(x)|^2 dx = 1$$

Practice problem #4: Orthonormal basis sets

Show that the set of functions $\psi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}$ is orthonormal over the window $-\pi \leq x \leq \pi$ provided n is an integer.

To do so, you will need to show that the integral

$$\int_{-\pi}^{\pi} \psi_m^*(x)\psi_n(x)dx = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}$$

Practice problem #5: Basis set expansion

Let's again work with the set of orthonormal basis functions

$$\psi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}, \quad n = 1, 2, \ldots$$

defined over the window $-\pi \leq x \leq \pi$.

Say I prepare a wavefunction given by:

$$\rho(x) = \sum_{n=1}^{\infty} b_n \psi_n(x) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$$

Confirm that

$$b_1 = \int_{-\pi}^{\pi} \psi_1^*(x) \rho(x) dx$$

Wrapping up

- **Next week:** the Postulates of Quantum Mechanics
  (e.g. the rules of the game!)

- **Today's reading:** McQuarrie Ch. 4

- **In the last minute or two**: Your muddiest point from today's lecture?