Announcements

- Homework 5 is due next Wednesday, March 1.
- After today, Exam 1 will be returned to you on April 5 (Exam 2 day)

Last time

- Schrödinger Equation

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

- Recipes for solving Schrödinger Equation
  - find a mathematical function
  - boundary condition, normalization condition

- Expectation values, operator

Today's class

- Particle in an infinite well

in-class quiz (3 min)

The probability that a particle is in a given small region of space is proportional to:

(A) Its energy

(B) Its momentum

(C) The frequency of its wave function

(D) The wavelength of its wave function

(E) The absolute square of its wave function

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Solutions for constant potential energy

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi(x) = E\psi(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E-U_0)\psi(x) \Rightarrow \frac{d^2\psi}{dx^2} = -\underbrace{\frac{2m(E-U_0)}{\hbar^2}}_{k^2}\psi(x)$$

when $E>U_0$

$$\boxed{\frac{d^2\psi}{dx^2} = -k^2\psi(x)} \qquad k^2 = \frac{2m(E-U_0)}{\hbar^2} \text{ or } k = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$$

$$\psi(x) = A\sin kx + B\cos kx$$

$$\psi(x) = Ce^{kx}$$

because
$$\frac{d\psi(x)}{dx} = kA\cos kx - kB\sin kx$$

$$\frac{d^2\psi(x)}{dx^2} = -k^2A\sin kx - k^2B\cos kx = -k^2\psi(x)$$

Solutions for constant potential energy

when $E < U_0$ Penetration of a particle into a forbidden region

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi(x) = E\psi(x)$$

$$U_0\psi(x) - E\psi(x) = \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \Rightarrow \frac{2m(U_0 - E)}{\hbar^2}\psi(x) = \frac{d^2\psi}{dx^2} \Rightarrow \text{let } k' = \sqrt{\frac{2m(U_0-E)}{\hbar^2}}$$

$$\frac{d^2\psi}{dx^2} = k'^2\psi(x)$$

$$\boxed{\psi(x) = Ae^{k'x} + Be^{-k'x}}$$

because $\frac{d\psi(x)}{dx} = k'Ae^{k'x} - k'Be^{-k'x}$

$$\frac{d^2\psi(x)}{dx^2} = k'^2Ae^{k'x} + k'^2Be^{-k'x} = k'^2\psi(x)$$

The free particle

$F = 0$, $F = -\frac{dU}{dx} = 0$, U is constant , set $U_0 = 0$

$\psi(x) = A\sin kx + B\cos kx$ with $k = \sqrt{\frac{2m(E-U_0)}{\hbar^2}} = \sqrt{\frac{2mE}{\hbar^2}}$

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

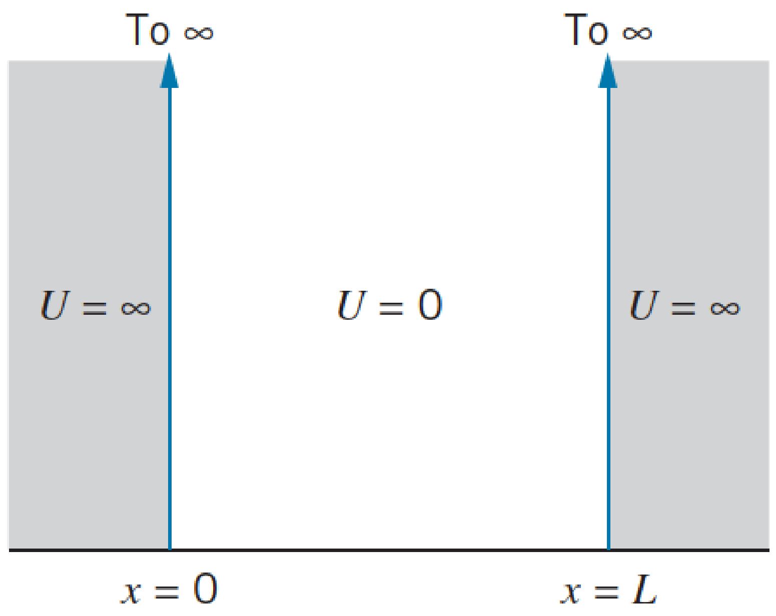
de Broglie relationship $\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda}$, $\lambda = \frac{2\pi}{k}$

$$E = \frac{p^2}{2m} = \frac{(h/\lambda)^2}{2m} = \frac{(h\cdot\frac{k}{2\pi})^2}{2m} = \frac{(\hbar k)^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

any λ , any k , any E not quantized

completely unlocalized (see textbook)

Infinite potential energy well



$$U(x) = 0 \qquad 0 \le x \le L$$
$$= \infty \qquad x < 0, x > L$$

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

trick : find separate solns for different region

Infinite potential energy well

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x) \qquad U(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & x<0,\ x>L \end{cases}$$

$\psi(x) = 0 \quad x<0,\ x>L \qquad$ 0 probability outside the well

$0 \le x \le L \quad \psi(x) = A\sin kx + B\cos kx \ , \quad k = \sqrt{\frac{2mE}{\hbar^2}} \ ,$ mathematically, the same form as the free particle

$$\psi(0) = A\sin 0 + B\cos 0 = 0 \Rightarrow B = 0$$

$$\psi(L) = A\sin kL + \cancel{B\cos kL}^{\,0} = 0 \Rightarrow A\sin kL = 0$$

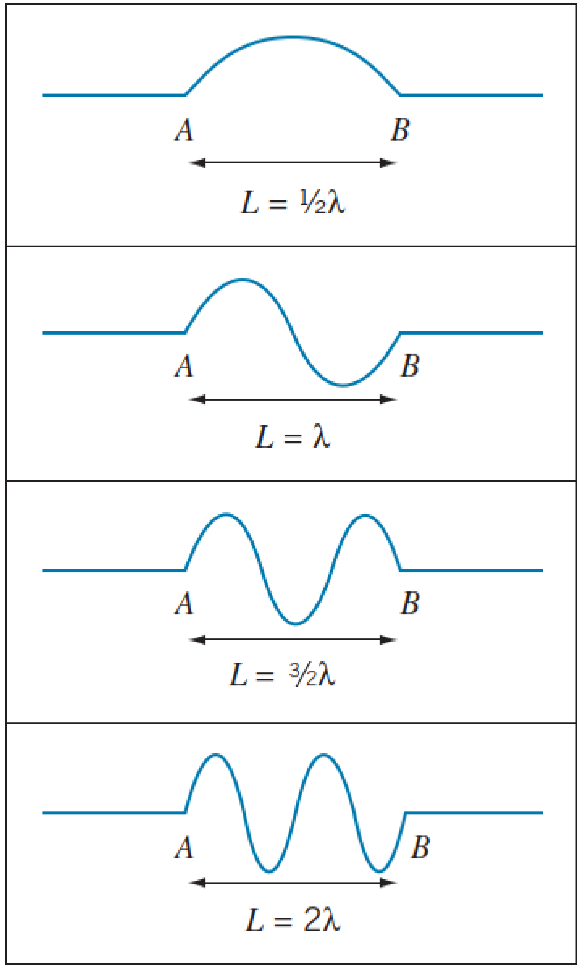
$A = 0$

$\sin kL = 0 \Rightarrow \quad kL = n\pi \qquad n = 1, 2, 3, \ldots$

$$k = \frac{n\pi}{L}$$

$$\psi(x) = A\sin\frac{n\pi}{L}x \qquad n = 1, 2, 3, \ldots$$

Infinite potential energy well



Infinite potential energy well

because $k = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad k = \frac{n\pi}{L}$ $\quad n = 1, 2, 3, \cdots$

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

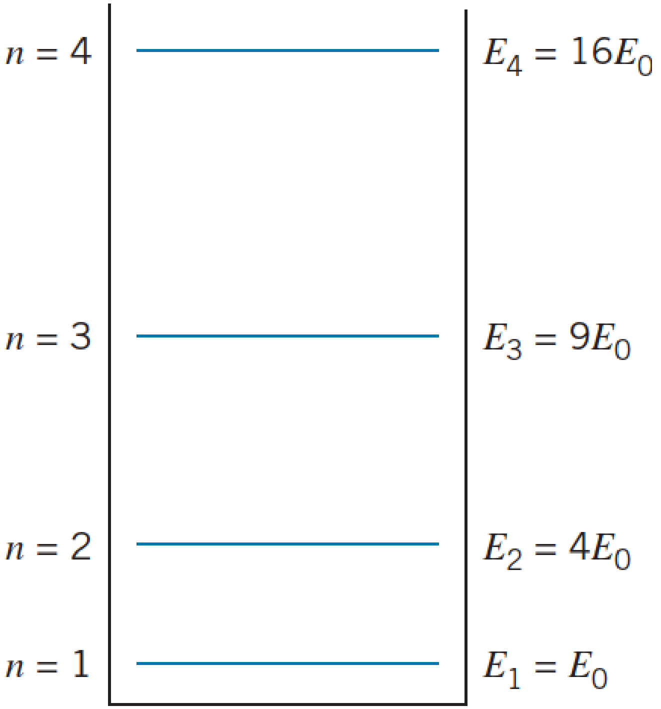
$$= \frac{\hbar^2 \pi^2 n^2}{2mL^2} = \frac{h^2 n^2}{8mL^2} \qquad n = 1, 2, 3, \cdots$$

let $E_0 = E_1 = \frac{h^2}{8mL^2}$

$$E_n = n^2 E_1$$

n : quantum number

Infinite potential energy well



excited state

Can adsorb or release energy to jump between energy states

ground state

In-class exercise (5 min)

Consider an electron confined to a quantum well as infinite potential well. The lowest energy transition produces a photon of 440 nm. What is the approximate width of the well?

$$\Delta E = \frac{hc}{\lambda} = \frac{1240\ eV\cdot nm}{440\ nm} = 2.8\ eV$$

$$\Delta E = E_2 - E_1 = 3E_1 \Rightarrow E_1 = 0.93\ eV$$

$$E_1 = E_0 = \frac{h^2}{8mL^2} \Rightarrow L = \sqrt{\frac{h^2}{8mE_1}} = \frac{hc}{\sqrt{8mc^2E_1}} = 0.63\ nm$$

Infinite potential energy well

Apply normalization conditions to determine constant A

$$\psi(x) = A \sin\frac{n\pi}{L}x \qquad 0 \leq x \leq L$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \quad \Rightarrow \quad \int_0^L A^2 \sin^2\frac{n\pi}{L}x\,dx = 1$$

$$A^2 = \frac{2}{L}, \qquad A = \sqrt{\frac{2}{L}}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots$$