PHYS 3313 – Section 001
Lecture # 19

Monday, April 13, 2015
Dr. Jaehoon Yu

- Refresher: Infinite Square-well Potential
  - Energy quantization
  - Expectation value computations
- Finite Square Well Potential
- Penetration Depth

Announcements

- Quiz #4 at the beginning of the class this Wednesday, Apr. 15
  – The class web site was down so I will give you an extension..
  – Covers CH 5.4 through what we finish today
  – BFOF
- Colloquium 4pm Wednesday, SH101

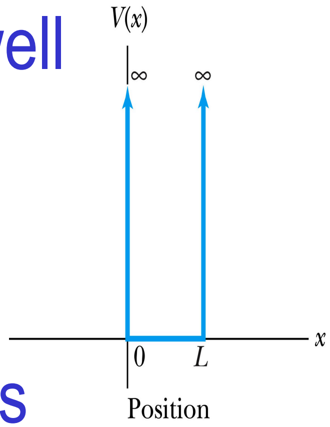
Reminder: Special project #5

- Show that the Schrodinger equation becomes Newton's second law in the classical limit. (15 points)
- Deadline this Wednesday, Apr. 15, 2015
- You MUST have your own answers!

Infinite Square-Well Potential

- The simplest such system is that of a particle trapped in a box with infinitely hard walls that the particle cannot penetrate. This potential is called an infinite square well and is given by

$$V(x)=\begin{cases}\infty & x\le 0, x\ge L\\ 0 & 0<x<L\end{cases}$$



- The wave function must be zero where the potential is infinite.
- Where the potential is zero inside the box, the time independent Schrödinger wave equation $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$ becomes $\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi \quad =-k^2\psi$ where $k=\sqrt{2mE/\hbar^2}$.
- The general solution is $\psi(x)=A\sin kx+B\cos kx$.

Quantization

- Since the wave function must be continuous, the boundary conditions of the potential dictate that the wave function must be zero at $x = 0$ and $x = L$. These yield valid solutions for B=0, and for **integer values** of n such that $kL = n\pi$ ➔ $k=n\pi/L$
- The wave function is now $$\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$$
- We normalize the wave function $\int_{-\infty}^{+\infty}\psi_n^*(x)\psi_n(x)dx = 1$

$$A^2\int_{-\infty}^{+\infty}\sin^2\left(\frac{n\pi x}{L}\right)dx = A^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx = 1$$

- The normalized wave function becomes

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

- These functions are identical to those obtained for a vibrating string with fixed ends.

Quantized Energy

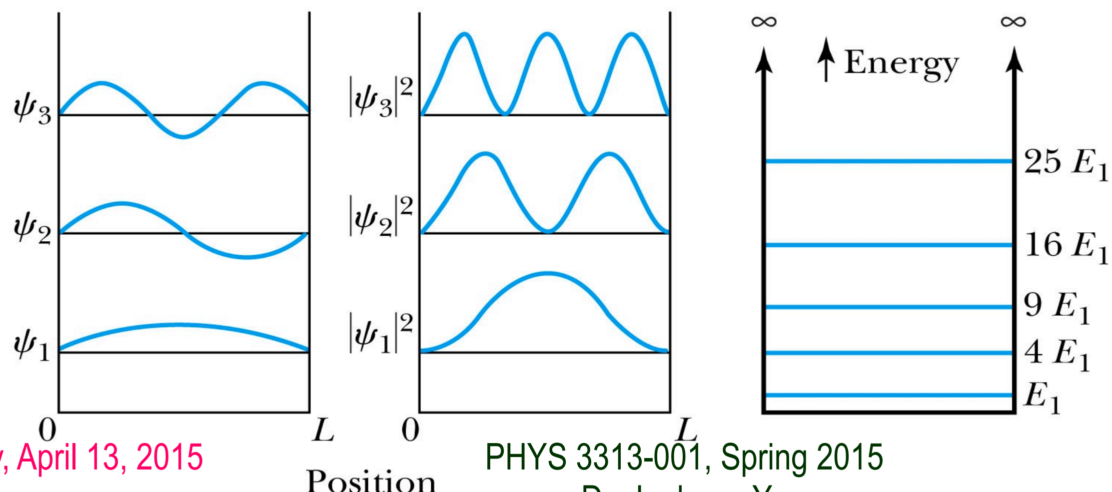
- The quantized wave number now becomes $k_n(x) = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$
- Solving for the energy yields

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

- Note that the energy depends on the integer values of *n*. Hence the energy is quantized and nonzero.
- The special case of *n* = 1 is called the **ground state energy**.

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

$\psi_n^* \psi_n = |\psi_n|^2 = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right)$



$$E_3 = \frac{9\pi^2\hbar^2}{2mL^2} = 9E_1$$

$$E_2 = \frac{2\pi^2\hbar^2}{mL^2} = 4E_1$$

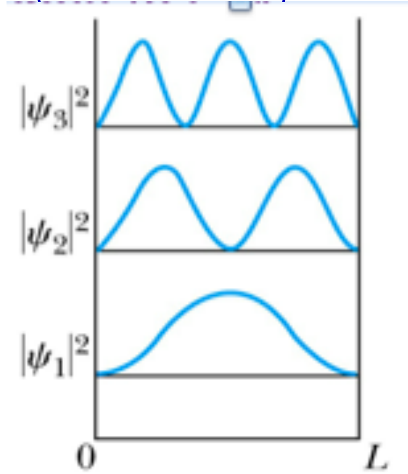
$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

How does this correspond to Classical Mech.?

- What is the probability of finding a particle in a box of length L? $\frac{1}{L}$
- Bohr's **correspondence principle** says that QM and CM must correspond to each other! When?
  - When n becomes large, the QM approaches to CM
- So when n→∞, the probability of finding a particle in a box of length L is

$$P(x) = \psi_n^*(x)\psi_n(x) = \left|\psi_n(x)\right|^2 = \frac{2}{L}\lim_{n\to\infty}\sin^2\left(\frac{n\pi x}{L}\right) \approx \frac{2}{L}\left\langle \sin^2\left(\frac{n\pi x}{L}\right)\right\rangle = \frac{2}{L}\cdot\frac{1}{2} = \frac{1}{L}$$

- Which is identical to the CM probability!!
- One can also see this from the plot of P!



Expectation Value & Operators

- Expectation value for any function g(x)

$$\langle g(x) \rangle = \int_{-\infty}^{+\infty} \Psi(x,t)^* g(x) \Psi(x,t) dx$$

- Position operator is the same as itself, x
- Momentum Operator

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

- Energy Operator

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

Ex 6.8: Expectation values inside a box

Determine the expectation values for x, x^2, p and p^2 of a particle in an infinite square well for the first excited state.

What is the wave function of the first excited state? n=? 2

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

$$\langle x \rangle_{n=2} = \int_{-\infty}^{+\infty} \psi^*_{n=2}(x) x \psi_{n=2}(x) = \frac{2}{L}\int_0^L x \sin^2\left(\frac{2\pi x}{L}\right) dx = \frac{L}{2}$$

$$\langle x^2 \rangle_{n=2} = \frac{2}{L}\int_0^L x^2 \sin^2\left(\frac{2\pi x}{L}\right) dx = 0.32L^2$$

$$\langle p \rangle_{n=2} = \frac{2}{L}\int_0^L \sin\left(\frac{2\pi x}{L}\right)(-i\hbar)\frac{\partial}{\partial x}\left[\sin\left(\frac{n\pi x}{L}\right)\right] dx = -i\hbar \frac{2}{L}\frac{2\pi}{L}\int_0^L \sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right) dx = 0$$

$$\langle p^2 \rangle_{n=2} = \frac{2}{L}\int_0^L \sin\left(\frac{2\pi x}{L}\right)(-i\hbar)^2\frac{\partial^2}{\partial x^2}\left[\sin\left(\frac{2\pi x}{L}\right)\right] dx = \hbar^2 \frac{2}{L}\left(\frac{2\pi}{L}\right)^2 \int_0^L \sin^2\left(\frac{2\pi x}{L}\right) dx = \frac{4\pi^2\hbar^2}{L^2}$$

$$E_2 = \frac{4\pi^2\hbar^2}{2mL^2} = \frac{\langle p^2 \rangle_{n=2}}{2m}$$

Ex 6.9: Proton Transition Energy

A typical diameter of a nucleus is about 10^{-14}m. Use the infinite square-well potential to calculate the transition energy from the first excited state to the ground state for a proton confined to the nucleus.

The energy of the state n is $E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$

What is n for the ground state? n=1

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} = \frac{\pi^2 \hbar^2 c^2}{2mc^2 L^2} = \frac{1}{mc^2} \frac{\pi^2 \cdot (197.3 eV \cdot nm)^2}{2 \cdot \left(10^{-5} nm\right)} = \frac{1.92 \times 10^{15} eV^2}{938.3 \times 10^6 eV} = 2.0 MeV$$

What is n for the 1st excited state? n=2

$$E_2 = 2^2 \frac{\pi^2 \hbar^2}{2mL^2} = 8.0 MeV$$

So the proton transition energy is

$$\Delta E = E_2 - E_1 = 6.0 MeV$$