PHYS 3313 – Section 001
Lecture #18

Monday, Mar. 31, 2014
Dr. Jaehoon Yu

- Valid Wave Functions
- Energy and Position Operators
- Infinite Square Well Potential
- Finite Square Well Potential

Announcements

- Research paper template has been uploaded onto the class web page link to research
- Special colloquium at 4pm, this Wednesday, April 2, triple extra credit
- Quiz #3 at the beginning of the class next Monday, Apr. 7
  - Covers CH 5.1 through what we finish this Wednesday

Reminder: Special Project #4

- Prove that the wave function $\Psi = A[\sin(kx-\omega t) + i\cos(kx-\omega t)]$ is a good solution for the time-dependent Schrödinger wave equation. Do NOT use the exponential expression of the wave function. (10 points)
- Determine whether or not the wave function $\Psi = Ae^{-\alpha|x|}$ satisfy the time-dependent Schrödinger wave equation. (10 points)
- Due for this special project is Monday, Apr. 7.
- You MUST have your own answers!

Properties of Valid Wave Functions

Boundary conditions

1) To avoid infinite probabilities, the wave function must be finite everywhere.
2) To avoid multiple values of the probability, the wave function must be single valued.
3) For finite potentials, the wave function and its derivatives must be continuous. This is required because the second-order derivative term in the wave equation must be single valued. (There are exceptions to this rule when *V* is infinite.)
4) In order to normalize the wave functions, they must approach zero as *x* approaches infinity.

Solutions that do not satisfy these properties do not generally correspond to physically realizable circumstances.

Expectation Values

- In quantum mechanics, measurements can only be expressed in terms of average behaviors since precision measurement of each event is impossible (what principle is this?)
- The **expectation value** is the expected result of the average of many measurements of a given quantity. The expectation value of x is denoted by $\langle x \rangle$.
- Any measurable quantity for which we can calculate the expectation value is called a **physical observable**. The expectation values of physical observables (for example, position, linear momentum, angular momentum, and energy) must be real, because the experimental results of measurements are real.
- The average value of x is $$\bar{x} = \frac{N_1 x_1 + N_2 x_2 + N_3 x_3 + N_4 x_4 + \cdots}{N_1 + N_2 + N_3 + N_4 + \cdots} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

Continuous Expectation Values

- We can change from discrete to continuous variables by using the probability $P(x,t)$ of observing the particle at a particular x.

$$\bar{x} = \frac{\int_{-\infty}^{+\infty} xP(x)dx}{\int_{-\infty}^{+\infty} P(x)dx}$$

- Using the wave function, the expectation value is:

$$\bar{x} = \frac{\int_{-\infty}^{+\infty} x\Psi(x,t)^* \Psi(x,t)dx}{\int_{-\infty}^{+\infty} \Psi(x,t)^* \Psi(x,t)dx}$$

- The expectation value of any function $g(x)$ for a normalized wave function:

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

Momentum Operator

- To find the expectation value of p, we first need to represent p in terms of x and t. Consider the derivative of the wave function of a free particle with respect to x:

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x}\left[e^{i(kx-\omega t)}\right] = ike^{i(kx-\omega t)} = ik\Psi$$

With $k = p/\hbar$ we have $\frac{\partial \Psi}{\partial x} = i\frac{p}{\hbar}\Psi$

This yields $p\left[\Psi(x,t)\right] = -i\hbar\frac{\partial \Psi(x,t)}{\partial x}$

- This suggests we define the momentum operator as $\hat{p} = -i\hbar\frac{\partial}{\partial x}$
- The expectation value of the momentum is

$$\langle p\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{p}\Psi(x,t)\,dx = -i\hbar\int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial x}dx$$

Position and Energy Operators

- The position x is its own operator as seen above.
- The time derivative of the free-particle wave function is $$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left[e^{i(kx-\omega t)}\right] = -i\omega e^{i(kx-\omega t)} = -i\omega\Psi$$

  Substituting $\omega = E/\hbar$ yields $E\left[\Psi(x,t)\right] = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$

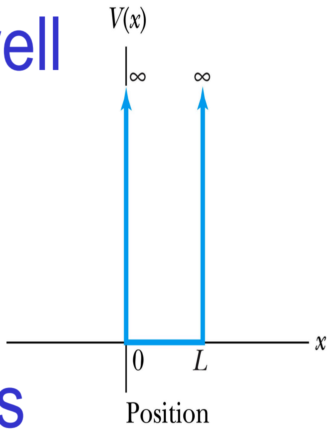
- So the energy operator is $\hat{E} = i\hbar\frac{\partial}{\partial t}$
- The expectation value of the energy is

$$\langle E\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{E}\Psi(x,t)dx = i\hbar\int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial t}dx$$

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

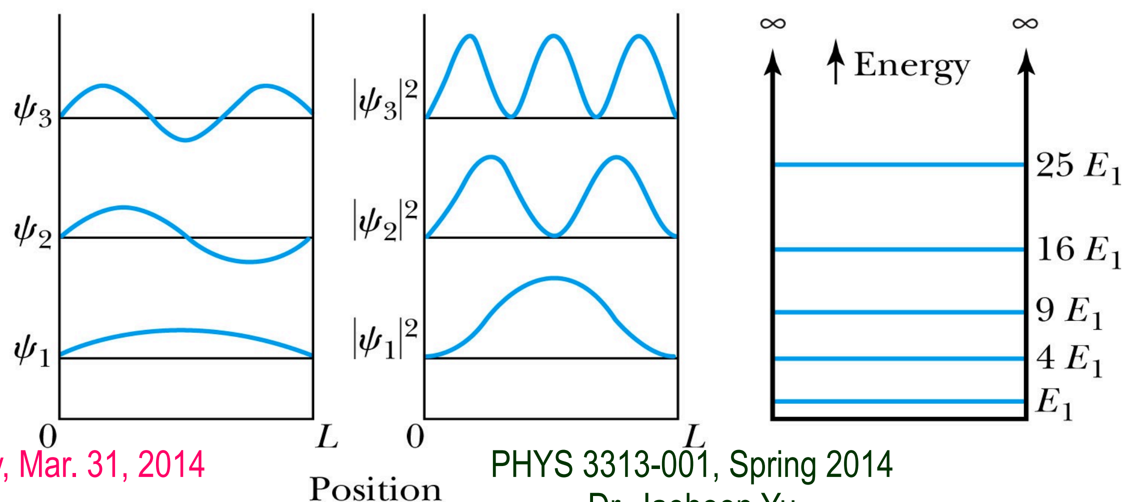
- The quantized wave number now becomes $k_n(x) = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$
- Solving for the energy yields

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

- 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**.

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

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



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

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

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