PHYS 3313 – Section 001
Lecture #18

Monday, April 3, 2017
Dr. Jaehoon Yu

- Probability of Particle
- Time Independent Schrodinger Equation
- Normalization and Probability
- Expectation Values
- Momentum, Position and Energy Operators

Announcements

- Quiz this Wednesday, April 5
  - At the beginning of the class
  - Covers CH5.1 through what we finish today
  - BYOF with the same rule as before
- Reminder: Quadruple extra credit
  - Colloquium on April 19, 2017
  - Speaker: Dr. Nigel Lockyer, Director of Fermilab
  - Make your arrangements to take advantage of this opportunity

Reminder: Special Project #4

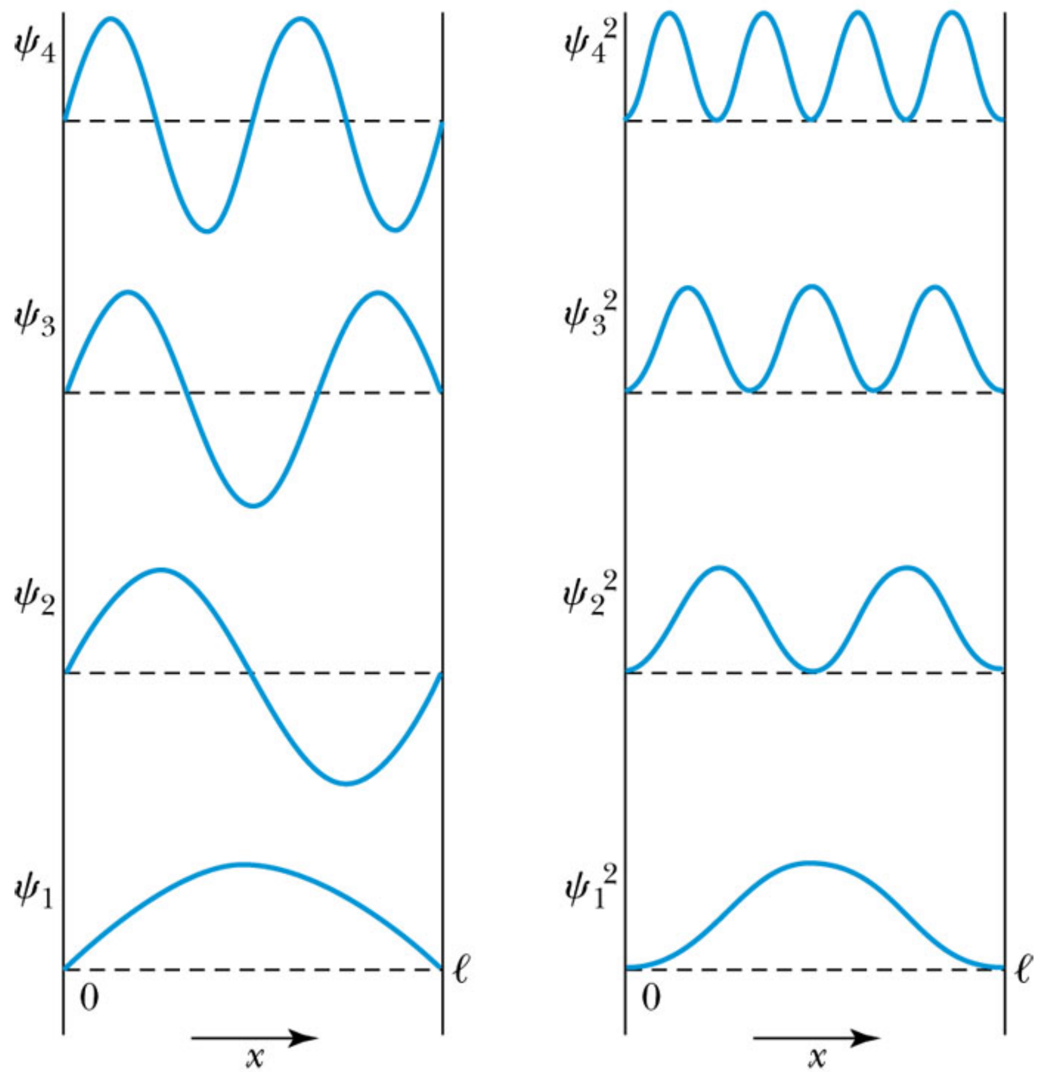
- Prove that the wave function $A\left[\cos(kx-\omega t)+i\sin(kx-\omega t)\right]$ is a good solution for the time-dependent Schrödinger wave equation. Do NOT use the exponential expression of the wave function. (10 points)
- Determine whether or not the wave function $\Psi = Ae^{-\alpha|x|}$ satisfy the time-dependent Schrödinger wave equation. (10 points)
- Due for this special project is this Wednesday, Apr. 5.
- You MUST have your own answers!

Probability of the Particle

- The probability of observing a particle between *x* and *x* + *dx* in each state is

$$P_n dx \propto \left|\Psi_n(x)\right|^2 dx$$

- Note that $E_0 = 0$ is not a possible energy level.
- The concept of energy levels, as first discussed in the Bohr model, has surfaced in a natural way by using waves.



The Schrödinger Wave Equation

- Erwin Schrödinger and Werner Heisenberg proposed quantum theory in 1920
  - The two proposed very different forms of equations
  - Heisenberg: Matrix based framework
  - Schrödinger: Wave mechanics, similar to the classical wave equation
- Paul Dirac and Schrödinger later on proved that the two give identical results
- The probabilistic nature of quantum theory is contradictory to the direct cause and effect seen in classical physics and makes it difficult to grasp!

The Time-dependent Schrödinger Wave Equation

- The Schrödinger wave equation in its **time-dependent** form for a particle of energy *E* moving in a potential *V* in one dimension is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V\Psi(x,t)$$

- The extension into three dimensions is

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+V\Psi(x,y,z,t)$$

- where $i=\sqrt{-1}$ is an imaginary number

Ex 6.1: Wave equation and Superposition

The wave equation must be linear so that we can use the superposition principle to form a wave packet. Prove that the wave function in Schrödinger equation is linear by showing that it is satisfied for the wave equation $\Psi(x,t)=a\Psi_1(x,t)+b\Psi_2(x,t)$ where a and b are constants and $\Psi_1(x,t)$ and $\Psi_2(x,t)$ describe two waves each satisfying the Schrödinger Eq.

$$\Psi = a\Psi_1 + b\Psi_2 \qquad i\hbar\frac{\partial \Psi_1}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi_1}{\partial x^2} + V\Psi_1 \qquad i\hbar\frac{\partial \Psi_2}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi_2}{\partial x^2} + V\Psi_2$$

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left(a\Psi_1 + b\Psi_2\right) = a\frac{\partial \Psi_1}{\partial t} + b\frac{\partial \Psi_2}{\partial t}$$

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x}\left(a\Psi_1 + b\Psi_2\right) = a\frac{\partial \Psi_1}{\partial x} + b\frac{\partial \Psi_2}{\partial x} \Rightarrow \frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial}{\partial x}\left(a\frac{\partial \Psi_1}{\partial x} + b\frac{\partial \Psi_2}{\partial x}\right) = a\frac{\partial^2 \Psi_1}{\partial x^2} + b\frac{\partial^2 \Psi_2}{\partial x^2}$$

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

Rearrange terms

$$i\hbar\frac{\partial \Psi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - V\Psi = \left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V\right)\Psi = 0$$

$$i\hbar\frac{\partial \Psi}{\partial t} = i\hbar\left(a\frac{\partial \Psi_1}{\partial t} + b\frac{\partial \Psi_2}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(a\frac{\partial^2 \Psi_1}{\partial x^2} + b\frac{\partial^2 \Psi_2}{\partial x^2}\right) + V\left(a\Psi_1 + b\Psi_2\right)$$

$$a\left(i\hbar\frac{\partial \Psi_1}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2 \Psi_1}{\partial x^2} - V\Psi_1\right) = -b\left(i\hbar\frac{\partial \Psi_2}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2 \Psi_2}{\partial x^2} - V\Psi_2\right) = 0$$

General Solution of the Schrödinger Wave Equation

- The general form of the solution of the Schrödinger wave equation is given by:

$$\Psi(x,t) = Ae^{i(kx-\omega t)} = A\left[\cos(kx-\omega t) + i\sin(kx-\omega t)\right]$$

- which also describes a wave propagating in the *x* direction. In general the amplitude may also be complex. *This is called the* ***wave function of the particle***.
- The wave function is also **not** restricted to being real. Only the physically measurable quantities (or **observables**) must be real. These include the probability, momentum and energy.

Ex 6.2: Solution for Wave Equation

Show that $Ae^{i(kx-\omega t)}$ satisfies the time-dependent Schrödinger wave Eq.

$$\Psi = Ae^{i(kx-\omega t)} \Rightarrow \frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left(Ae^{i(kx-\omega t)}\right) = -iA\omega e^{i(kx-\omega t)} = -i\omega\Psi$$

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x}\left(Ae^{i(kx-\omega t)}\right) = iAke^{i(kx-\omega t)} = ik\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial}{\partial x}(ik\Psi) = ik\frac{\partial}{\partial x}(\Psi) = ik\left(iAke^{i(kx-\omega t)}\right) = -Ak^2e^{i(kx-\omega t)} = -k^2\Psi$$

$$i\hbar\frac{\partial \Psi}{\partial t} = i\hbar(-i\omega\Psi) = \hbar\omega\Psi = -\frac{\hbar^2}{2m}\left(-k^2\Psi\right) + V\Psi$$

$$\left(\hbar\omega - \frac{\hbar^2 k^2}{2m} - V\right)\Psi = 0$$

$$= \left(E - \frac{p^2}{2m} - V\right) = 0$$

The Energy: $E = hf = h\left(\frac{\omega}{2\pi}\right) = \hbar\omega$

The wave number: $k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{2\pi p}{h} = \frac{p}{\hbar}$ $\Rightarrow$ The momentum: $p = \hbar k$

From the energy conservation: $E = K + V = \frac{p^2}{2m} + V$ $\Rightarrow$ $E - \frac{p^2}{2m} - V = 0$

So $Ae^{i(kx-\omega t)}$ is a good solution and satisfies Schrödinger Eq.

Ex 6.3: Bad Solution for Wave Equation

Determine whether Ψ (x,t)=Asin(kx-ωt) is an acceptable solution for the time-dependent Schrödinger wave Eq.

$$\Psi = A\sin(kx-\omega t) \Rightarrow \frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left(A\sin(kx-\omega t)\right) = -A\omega\cos(kx-\omega t)$$

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x}\left(A\sin(kx-\omega t)\right) = kA\cos(kx-\omega t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial}{\partial x}\left(kA\cos(kx-\omega t)\right) = -k^2 A\sin(kx-\omega t) = -k^2\Psi$$

$$i\hbar\left(-\omega\cos(kx-\omega t)\right) = -\frac{\hbar^2}{2m}\left(-k^2\sin(kx-\omega t)\right) + V\sin(kx-\omega t)$$

$$-i\hbar\omega\cos(kx-\omega t) = \left(\frac{\hbar^2 k^2}{2m} + V\right)\sin(kx-\omega t)$$

$$\Rightarrow -iE\cos(kx-\omega t) = \left(\frac{p^2}{2m} + V\right)\sin(kx-\omega t)$$

This is not true in all x and t. So Ψ (x,t)=Asin(kx-ωt) is not an acceptable solution for the Schrödinger Eq. Is it for the classical wave eq: $\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \Psi(x,t)}{\partial t^2}$

Normalization and Probability

- The probability $P(x)\ dx$ of a particle being between x and $X + dx$ was given by the equation

$$P(x)dx = \Psi^*(x,t)\Psi(x,t)dx$$

- Here Ψ^* denotes the complex conjugate of Ψ
- The probability of the particle being between x_1 and x_2 is given by

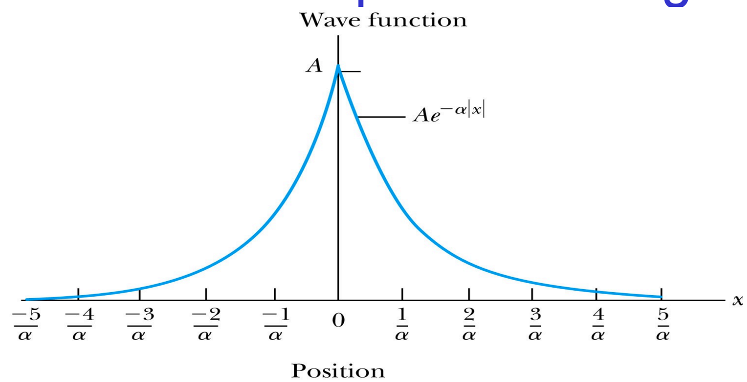
$$P = \int_{x_1}^{x_2} \Psi^* \Psi \, dx$$

- The wave function must also be normalized so that the probability of the particle being somewhere on the x axis is 1.

$$\int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)dx = 1$$

Ex 6.4: Normalization

Consider a wave packet formed by using the wave function that $Ae^{-\alpha|x|}$, where A is a constant to be determined by normalization. Normalize this wave function and find the probabilities of the particle being between 0 and $1/\alpha$, and between $1/\alpha$ and $2/\alpha$.



$$\Psi = Ae^{-\alpha|x|}$$

Probability density

$$\int_{-\infty}^{+\infty} \Psi^* \Psi dx = \int_{-\infty}^{+\infty} \left(Ae^{-\alpha|x|}\right)^* \left(Ae^{-\alpha|x|}\right) dx = \int_{-\infty}^{+\infty} \left(A^* e^{-\alpha|x|}\right)\left(Ae^{-\alpha|x|}\right) dx =$$

$$= \int_{-\infty}^{+\infty} A^2 e^{-2\alpha|x|} dx = 2\int_{0}^{+\infty} A^2 e^{-2\alpha x} dx = \frac{2A^2}{-2\alpha} e^{-2\alpha x}\Big|_0^{+\infty} = 0 + \frac{A^2}{\alpha} = 1$$

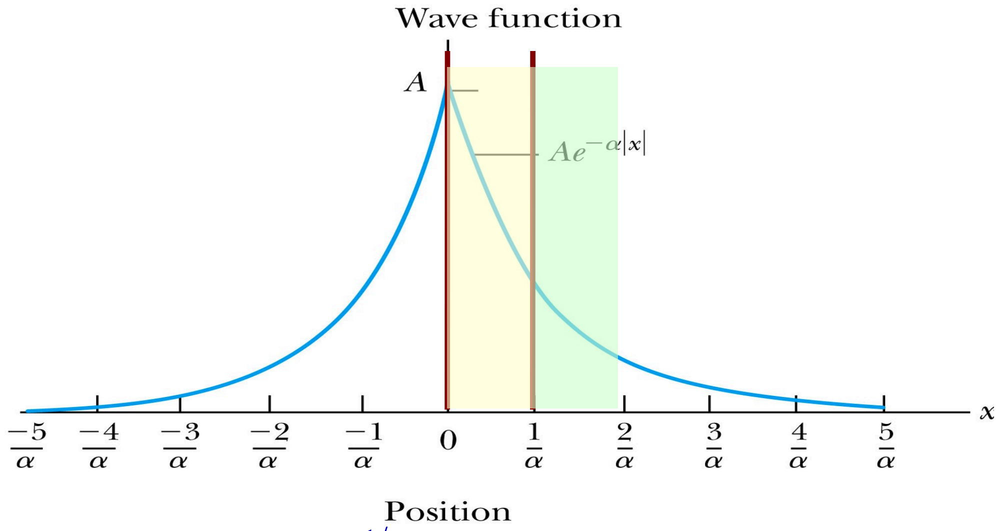
$$A = \sqrt{\alpha}$$

Normalized Wave Function

$$\Psi = \sqrt{\alpha}\, e^{-\alpha|x|}$$

Ex 6.4: Normalization, cont'd

Using the wave function, we can compute the probability for a particle to be in 0 to 1/α and 1/α to 2/α.



$$\Psi = \sqrt{\alpha}e^{-\alpha|x|}$$

For 0 to 1/α:

$$P = \int_0^{1/\alpha} \Psi^*\Psi dx = \int_0^{1/\alpha} \alpha e^{-2\alpha x} dx = \frac{\alpha}{-2\alpha} e^{-2\alpha x}\Big|_0^{1/\alpha} = -\frac{1}{2}\left(e^{-2} - 1\right) \approx 0.432$$

For 1/α to 2/α:

$$P = \int_{1/\alpha}^{2/\alpha} \Psi^*\Psi dx = \int_{1/\alpha}^{2/\alpha} \alpha e^{-2\alpha x} dx = \frac{\alpha}{-2\alpha} e^{-2\alpha x}\Big|_{1/\alpha}^{2/\alpha} = -\frac{1}{2}\left(e^{-4} - e^{-2}\right) \approx 0.059$$

How about 2/α:to ∞?