PHYS 3313 – Section 001
Lecture #17

Wednesday, Mar. 26, 2014
Dr. Jaehoon Yu

- Probability of Particle
- Schrodinger Wave Equation and Solutions
- Normalization and Probability
- Time Independent Schrodinger Equation
- Expectation Values
- Momentum Operator

Announcements

- Research paper template has been uploaded onto the class web page link to research
- Special colloquium on April 2, triple extra credit
- Colloquium this Wednesday at 4pm in SH101

Special Project #4

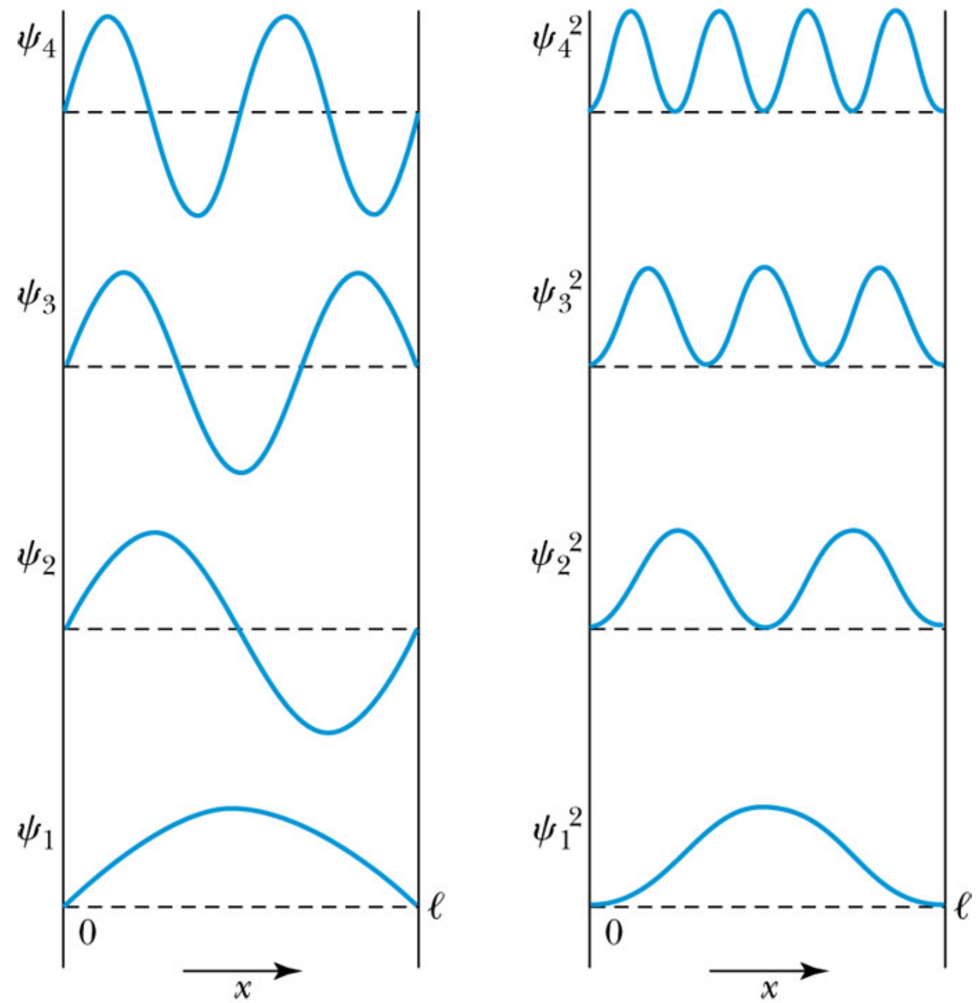
- Prove that the wave function $\Psi = A[\sin(kx-\omega t) + i\cos(kx-\omega t)]$ is a good solution for the time-dependent Schrödinger wave equation. Do NOT use the exponential expression of the wave function. (10 points)
- Determine whether or not the wave function $\Psi = Ae^{-\alpha|x|}$ satisfy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

Probability of the Particle

- The probability of observing the 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 Heinsenberg proposed quantum theory in 1920
  - The two proposed very different forms of equations
  - Heinserberg: 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 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. Prove that the wave function in Schrodinger 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 Schrodinger Eq.

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

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

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

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

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

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

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 Schrodinger wave Eq.

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

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

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

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

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

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

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 Schrodinger Eq.

Ex 6.3: Bad Solution for Wave Equation

Determine $\Psi(x,t)=A\sin(kx-\omega t)$ is an acceptable solution for the time-dependent Schrodinger wave Eq.

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

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

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

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

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

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

This is not true in all x and t. So $\Psi(x,t)=A\sin(kx-\omega t)$ is not an acceptable solution for Schrodinger Eq.

Normalization and Probability

- The probability *P*(*x*) *dx* of a particle being between *x* and *X* + *dx* was given in 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

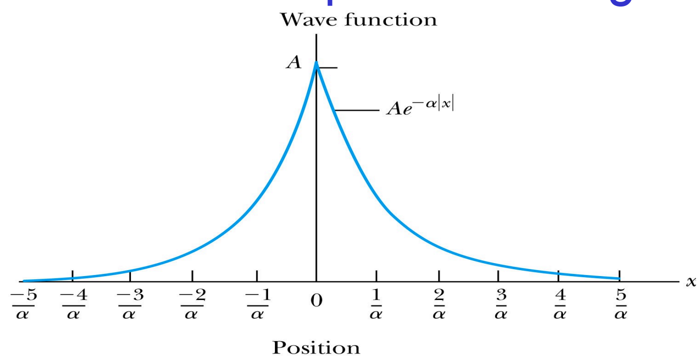
$$P = \int_{x_1}^{x_2} \Psi^*\Psi\, dx$$

- 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

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

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

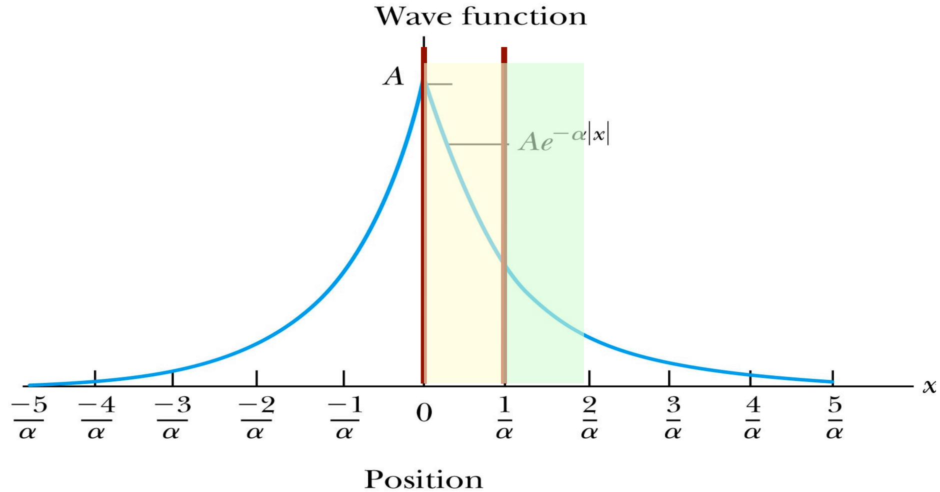
$$A = \sqrt{\alpha}$$

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 with 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 ∞?

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.

Time-Independent Schrödinger Wave Equation

- The potential in many cases will not depend explicitly on time.
- The dependence on time and position can then be separated in the Schrödinger wave equation. Let, $\Psi(x,t) = \psi(x) f(t)$

which yields: $$i\hbar \psi(x) \frac{\partial f(t)}{\partial t} = -\frac{\hbar^2 f(t)}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) f(t)$$

Now divide by the wave function: $$i\hbar \frac{1}{f(t)} \frac{\partial f(t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)$$

- The left side of this last equation depends only on time, and *the right side* depends only on spatial coordinates. Hence each side must be equal to a constant. The time dependent side is

$$i\hbar \frac{1}{f} \frac{df}{dt} = B$$

Time-Independent Schrödinger Wave Equation(con't)

- We integrate both sides and find: $i\hbar\int\frac{df}{f}=\int B\,dt \Rightarrow i\hbar\ln f=Bt+C$

  where *C* is an integration constant that we may choose to be 0. Therefore

$$\ln f=\frac{Bt}{i\hbar}$$

  This determines *f* to be by comparing it to the wave function of a free particle $f(t)=e^{Bt/i\hbar}=e^{-iBt/\hbar}=e^{-i\omega t} \Rightarrow B/\hbar=\omega \Rightarrow B=\hbar\omega=E$

$$i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=E$$

- This is known as the **time-independent Schrödinger wave equation**, and it is a fundamental equation in quantum mechanics.

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

Stationary State

- Recalling the separation of variables: $\Psi(x,t)=\psi(x)f(t)$ and with $f(t) = e^{-i\omega t}$ the wave function can be written as: $\Psi(x,t)=\psi(x)e^{-i\omega t}$
- The probability density becomes:

$$\Psi^*\Psi = \psi^2(x)\left(e^{i\omega t}e^{-i\omega t}\right)=\psi^2(x)$$

- The probability distributions are constant in time. This is a standing wave phenomena that is called the stationary state.

Comparison of Classical and Quantum Mechanics

- Newton’s second law and Schrödinger’s wave equation are both differential equations.
- Newton’s second law can be derived from the Schrödinger wave equation, so the latter is the more fundamental.
- Classical mechanics only appears to be more precise because it deals with macroscopic phenomena. The underlying uncertainties in macroscopic measurements are just too small to be significant due to the small size of the Planck’s constant

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 <*x*>.
- 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 $\dfrac{\partial \Psi}{\partial x} = i\dfrac{p}{\hbar}\Psi$

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 $\hat{p} = -i\hbar\dfrac{\partial}{\partial x}$
- The expectation value of the momentum is

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