PHYS 3313 – Section 001 Lecture #13

Wednesday, Oct. 17, 2012 Dr. **Jaehoon** Yu

- Properties of valid wave functions
- Time independent Schrodinger Equation
- Expectation Values
- Operators Position, Momentum and Energy
- Infinite Potential Well
- Finite Potential Well



Announcements

- Reading assignments
 - CH6.1 6.7 + the special topic
- Colloquium this week
 - 4pm, today, Oct. 17, SH101
 - Drs. Musielak and Fry of UTA
- Please mark your calendar for the Weinberg lecture at 7:30pm, coming Wednesday, Oct. 24!!
 - Let all of your family and friends know of this.



Physics Department The University of Texas at Arlington COLLOQUIUM

Fundamental Theories of Physics in Flat and Curved Space-Time

Dr. John Fry and Dr. Zdzislaw Musielak

Department of Physics University of Texas at Arlington 4:00 pm Wednesday October 17, 2012 room 101 SH

Abstract:

As of today, there is no commonly accepted theory that explains the origin and nature of Dark Matter and Dark Energy, and also accounts for the physical effects near the Big Bang singularity. To search for such theory, we developed a novel method that allows us to formulate fundamental theories of elementary particles in flat and curved space-time. In this talk, we shall present our method and use it obtain the original Klein-Gordon equation for scalar state functions as well as its generalization to higher derivatives and to spinor state functions. Possible applications of the generalized Klein-Gordon equations to Dark Matter and Dark Energy will be discussed. We shall also describe our recently developed extension of the method to curved space-time of General Relativity. The corresponding Klein-Gordon equation in space-time of a given curvature will be presented and its possible applications will be discussed. The talk will be concluded with a progress report on our attempts to formulate a new physical theory that is required to be valid in the vicinity of the Big Bang singularity.

Refreshments will be served at 3:30p.m in the Physics Lounge

Special project #4

- Show that the wave function Ψ=A[sin(kx-ωt) +icos(kx-ωt)] is a good solution for the timedependent Schrödinger wave equation. Do NOT use the exponential expression of the wave function. (10 points)
- Determine whether or not the wave function $\Psi = Ae^{-\alpha|x|}$ satisfies the time-dependent Schrödinger wave equation. (10 points)
- Due for this special project is Monday, Oct. 22.
- You MUST have your own answers!



Special project #5

Show that the Schrodinger equation becomes Newton's second law. (15 points)

Deadline Monday, Oct. 29, 2012

■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 derivative 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: $i\hbar \int \frac{df}{f} = \int B \, dt \implies i\hbar \ln f = Bt + C$

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
- 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

$$\bar{x} = \frac{N_1 x_1 + N_2 x_2 + N_3 x_3 + N_4 x_4 + \dots}{N_1 + N_2 + N_3 + N_4 + \dots} = \frac{\sum_{i} N_i x_i}{\sum_{i} N_i}$$



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*.
- Using the wave function, the expectation value is:
- The expectation value of any function *g*(*x*) for a normalized wave function:

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

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

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



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 $E[\Psi(x,t)] = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$

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



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 Schrödinger wave equation becomes $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$ where $k = \sqrt{2mE/\hbar^2}$
- The general solution is $\psi(x) = A \sin kx + B \cos kx$.



0

L

Position

Quantization

- Since the wave function must be continuous, the boundary conditions of the potential dictate that the wave function must be zero at x = 0and *x* = *L*. This yields valid solutions for B=0 and for **integer values** of *n* such that $kL = n\pi \rightarrow k=n\pi/L$
- $\psi_n(x) = A \sin\!\left(\frac{n\pi x}{L}\right)$ • The wave function is now
- We normalize the wave function

$$\int_{-\infty}^{+\infty} \boldsymbol{\psi}_{n}^{*}(x) \boldsymbol{\psi}_{n}(x) dx = 1 \qquad A^{2} \int_{0}^{L} \sin \theta dx$$

$$\int_{0}^{L} \sin^{2}\left(\frac{n\pi x}{L}\right) dx = 1$$

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. PHYS 3313-001, Fall 2012 Wednesday, Oct. 17, 2012 16

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