PHYS 3313 – Section 001
Lecture #13

Wednesday, Oct. 23, 2013
Dr. Jaehoon Yu

- Wave Function Normalization
- Time-Independent Schrödinger Wave Equation
- Expectation Values
- Operators – Position, Momentum and Energy
- Infinite Square Well Potential

Announcements

- Mid-term grade discussion Monday, Oct. 28
  - In Dr. Yu's office, CPB 342
  - Last name begins with A – C: 12:50 – 1:20pm
  - Last name begins with D – L: 1:20 – 1:50pm
  - Last name begins with M – Z: 1:50 – 2:20pm
- Colloquium today
  - 4pm today, SH101, Dr. X. Chu, U. of Colorado
  - Double extra credit for this colloquium

Physics Department
The University of Texas at Arlington

COLLOQUIUM

Dr. Xinzhao Chu

The University of Colorado at Boulder

Candidate for Faculty Position:
The Richard N. Claytor
Distinguished Professorship in Optics

Wednesday October 23 at 4:00 pm in Room 101 SH

Photons from Atomic World to the Space

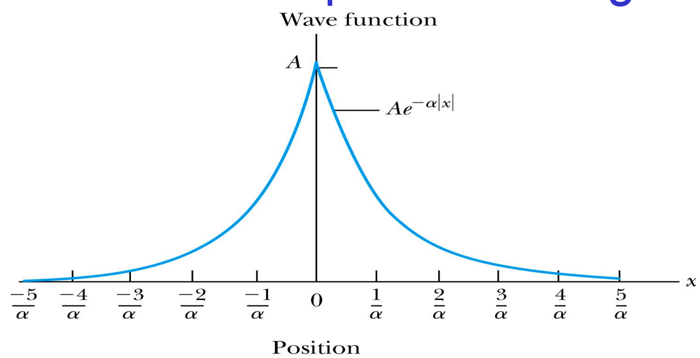
Abstract:

Living and working with photons every day, I do believe that photons are a key element to human society and scientific research. Photons have allowed people to explore the detailed structures of a single atom and its interaction with radiation fields; photons have enabled many fancy technologies and products used in our daily life; and photons have extended human's eyes to peek into the Universe – just a few examples among millions of photon "fairy tales". In this colloquium I will share my experience of using photons to explore the unknowns from atomic dimension to the space, and discuss the future of optics and photonics – how this very active science branch could bring prosperity to our world. In particular, I would like to tell the stories of how we use photons to unlock the secrets of Antarctica – the last frontier on Earth!

Refreshments will be served at 3:30p.m in the Physics lounge room 106 SH

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

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

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

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

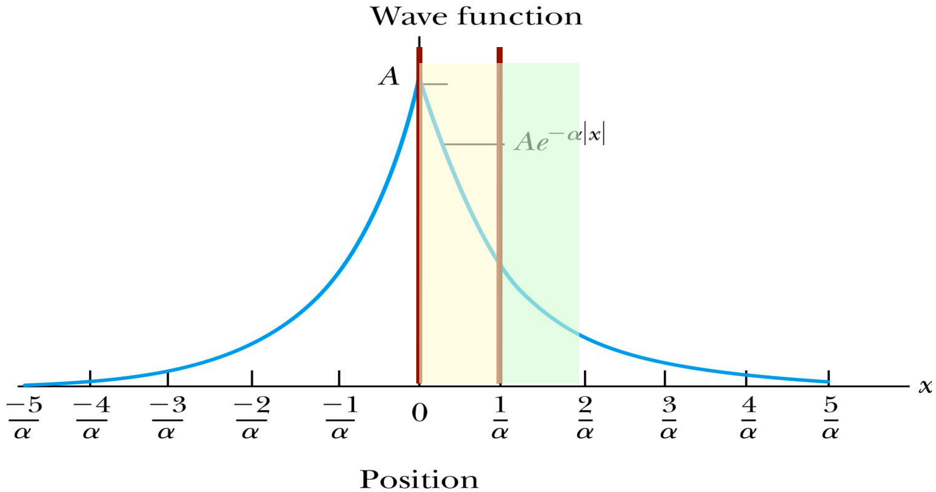
Normalized Wave Function

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

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 $1/\alpha$ 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 $2/\alpha$: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 $\frac{\partial \Psi}{\partial x} = i\frac{p}{\hbar}\Psi$

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

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

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