PHYS 3313 – Section 001
Lecture #17

Wednesday, March 27, 2019
Dr. Jaehoon Yu

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

Announcements

- Reminder for Homework #4: CH5 end of the chapter problems
  - 8, 10, 16, 24, 26, 37 and 47
  - Due: Monday Apr. 1, 2019
- Quiz #3
  - Beginning of the class, Wednesday, Apr. 3
  - Covers: CH4.8 through what we finish Monday, Apr. 1
  - BYOF: You may bring a one 8.5x11.5 sheet (front and back) of handwritten formulae and values of constants for the exam
  - No derivations, word definitions or setups or solutions of any problems!
    - No Maxwell's equations!
  - No additional formulae or values of constants will be provided!
- Colloquium at 4pm today in SH101
  - Dr. Kevin Pham of National Center for Atmospheric Research

Physics Department
The University of Texas at Arlington
COLLOQUIUM

Modeling the Geospace System at NCAR: A view from the mountaintop

Kevin Pham
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High Altitude Observatory
National Center for Atmospheric Research

Wednesday March 27, 2019
4:00 p.m. Room 101 Science Hall

Abstract

The geospace environment consists of many complex systems that have previously been studied independently. When models for the subsystems are coupled, the dynamics, time scales, and properties of each can influence the dynamics of the whole system. Typically, most consider the solar wind as a main driver and controller of magnetospheric dynamics. However, with the inclusion of more varied models from below (namely better thermospheric and ionospheric models), they become significant and important contributors to magnetospheric dynamics. Here, we model the geospace system via coupled models for the magnetosphere, thermosphere, ionosphere and polar wind. The multi-fluid Lyon-Fedder-Mobarry (LFM) global magnetosphere magnetohydrodynamic model is first coupled to the Thermosphere Ionosphere Electrodynamic General Circulation Model (TIEGCM) to form the coupled Magnetosphere-Ionosphere-Thermosphere (CMIT) model. In this coupling, the impact of the thermosphere on magnetosphere-ionosphere-thermosphere coupling is mainly through its effect on ionospheric conductivity. We improve and expand CMIT with a polar wind model, the Ionosphere Polar Wind Model (IPWM), to form the LFM-IPWM-TIEGCM (LIT) model. The additional of a polar wind model allows for thermospheric properties such as winds, temperature, and composition to feedback and impact the magnetosphere through ionospheric outflow. We find that although the dayside dynamics has not changed too much, the nightside dynamics can be greatly impacted by the thermospheric state. This suggests that an ionospheric polar wind outflow model must be included for other important thermospheric properties to impact the magnetosphere.

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

Special Project #6

- Derive the following using trigonometric identities

$$A\cos\left(k_1 x - \omega_1 t\right) + A\cos\left(k_2 x - \omega_2 t\right) =$$

$$2A\cos\left(\frac{k_1 - k_2}{2}x - \frac{\omega_1 - \omega_2}{2}t\right)\cos\left(\frac{k_1 + k_2}{2}x - \frac{\omega_1 + \omega_2}{2}t\right) =$$

- 10 points total for this derivation
- Due for this special project is Wednesday, Apr. 3.
- You MUST have your own answers!

The Copenhagen Interpretation

- Bohr's interpretation of the wave function consisted of 3 principles:
  1) The uncertainty principle of Heisenberg
  2) The complementarity principle of Bohr
  3) The statistical interpretation of Born, based on probabilities determined by the wave function
- Together, these three concepts form a logical interpretation of the physical meaning of quantum theory. According to the Copenhagen interpretation, physics depends on the outcomes of measurement.

Particle in a Box

- A particle of mass m is trapped in a one-dimensional box of width ℓ.
- The particle is treated as a wave.
- The box puts boundary conditions on the wave. The wave function must be zero at the walls of the box and the outside of the box.
- In order for the probability to vanish at the walls, we must have an integral number of half wavelengths in the box.
  - $$\frac{n\lambda}{2} = \ell \quad \text{or} \quad \lambda_n = \frac{2\ell}{n} \qquad (n = 1,2,3.....)$$
- The energy of the particle is $$E = KE = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$
- The possible wavelengths are quantized and thus yields the energy:

$$E_n = \frac{h^2}{2m\lambda^2} = \frac{h^2}{2m}\left(\frac{n}{2\ell}\right)^2 = n^2\frac{h^2}{8m\ell^2} \qquad (n = 1,2,3.....)$$

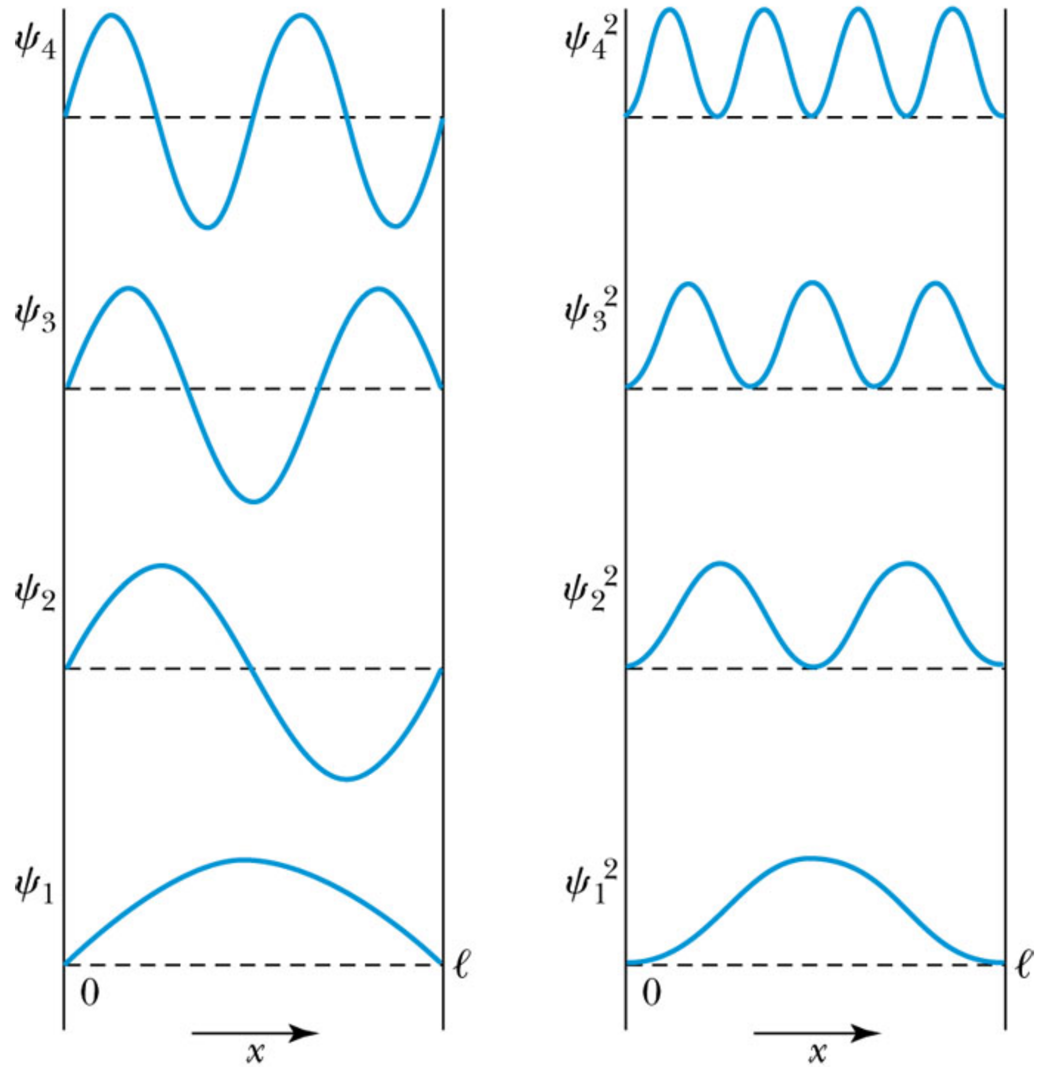
- The possible energies of the particle are quantized.
- Find the quantized energy level of an electron constrained to move in a 1-D atom of size 0.1nm.

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 (1932 Nobel) 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 (1933 Nobel jointly) later 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 the superposition principle can be used to form a wave packet. Prove that the wave function in Schrödinger equation is linear by showing that it is satisfied by 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.

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

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

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

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

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

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

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 the 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

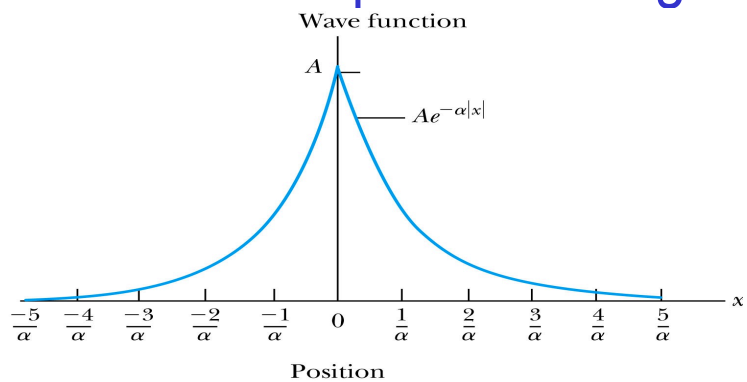
$$P = \int_{x_1}^{x_2} \Psi^* \Psi \, dx$$

- 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

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

$$= \int_{-\infty}^{+\infty} A^2 e^{-2\alpha|x|} dx = 2\int_0^{+\infty} A^2 e^{-2\alpha x} dx = \left. \frac{2A^2}{-2\alpha} e^{-2\alpha x} \right|_0^{+\infty} = 0 + \frac{A^2}{\alpha} = 1$$

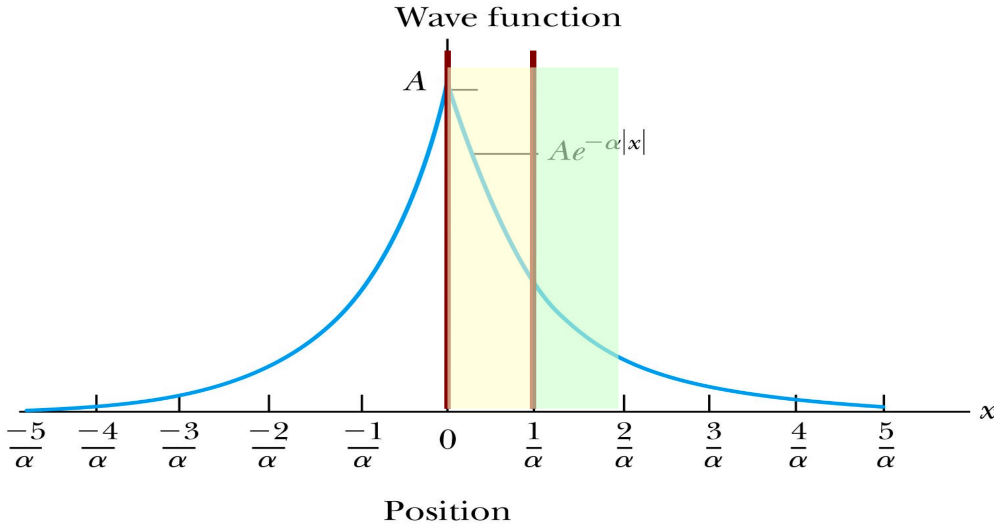
$$A = \sqrt{\alpha}$$

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 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 ∞?