PHYS 3313 – Section 001
Lecture #20

Monday, Apr. 7, 2014
Dr. Jaehoon Yu

- 3D Infinite Potential Well
- Degeneracy
- Simple Harmonic Oscillator
- Barriers and Tunneling

Announcements

- Research paper deadline is Monday, Apr. 28
- Research presentation deadline is Sunday, Apr. 27
- Reminder: Homework #4
  - End of chapter problems on CH5: 8, 10, 16, 24, 26, 36 and 47
  - Due this Wednesday, Apr. 9
- Bring out special project #4 at the end of class

Reminder: Special project #5

- Show that the Schrodinger equation becomes Newton’s second law in the classical limit. (15 points)
- Deadline Monday, Apr. 21, 2014
- You MUST have your own answers!

Three-Dimensional Infinite-Potential Well

- The wave function must be a function of all three spatial coordinates.
- We begin with the conservation of energy $E = K + V = \dfrac{p^2}{2m} + V$
- Multiply this by the wave function to get

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

- Now consider momentum as an operator acting on the wave function. In this case, the operator must act twice on each dimension. Given:

$$p^2 = p_x^2 + p_y^2 + p_z^2 \qquad \hat{p}_x\psi = -i\hbar\frac{\partial\psi}{\partial x} \quad \hat{p}_y\psi = -i\hbar\frac{\partial\psi}{\partial y} \quad \hat{p}_z\psi = -i\hbar\frac{\partial\psi}{\partial z}$$

- The three dimensional Schrödinger wave equation is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi = E\psi \quad \xrightarrow{\text{Rewrite}} \quad -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Ex 6.10: Expectation values inside a box

Consider a free particle inside a box with lengths L_1, L_2 and L_3 along the x, y, and z axes, respectively, as shown in the Figure. The particle is constrained to be inside the box. Find the wave functions and energies. Then find the ground energy and wave function and the energy of the first excited state for a cube of sides L.

What are the boundary conditions for this situation?

Particle is free, so x, y and z wave functions are independent from each other!

Each wave function must be 0 at the wall! Inside the box, potential V is 0.

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

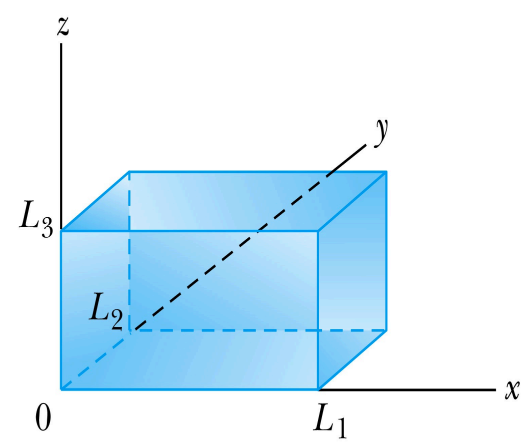
A reasonable solution is

$$\psi(x,y,z) = A\sin(k_1x)\sin(k_2y)\sin(k_3z)$$

Using the boundary condition

$$\psi = 0 \text{ at } x = L_1 \Rightarrow k_1L_1 = n_1\pi \Rightarrow k_1 = n_1\pi/L_1$$

So the wave numbers are $k_1 = \frac{n_1\pi}{L_1}$ $k_2 = \frac{n_2\pi}{L_2}$ $k_3 = \frac{n_3\pi}{L_3}$



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The energy can be obtained through the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

$$\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}\left(A\sin(k_1x)\sin(k_2y)\sin(k_3z)\right) = k_1A\cos(k_1x)\sin(k_2y)\sin(k_3z)$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2}{\partial x^2}\left(A\sin(k_1x)\sin(k_2y)\sin(k_3z)\right) = -k_1^2A\sin(k_1x)\sin(k_2y)\sin(k_3z) = -k_1^2\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = \frac{\hbar^2}{2m}\left(k_1^2+k_2^2+k_3^2\right)\psi = E\psi$$

$$E = \frac{\hbar^2}{2m}\left(k_1^2+k_2^2+k_3^2\right) = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2}+\frac{n_2^2}{L_2^2}+\frac{n_3^2}{L_3^2}\right)$$

What is the ground state energy?

$E_{1,1,1}$ when $n_1=n_2=n_3=1$, how much?

When are the energies the same for different combinations of n_i?

Degeneracy*

- Analysis of the Schrödinger wave equation in three dimensions introduces three quantum numbers that quantize the energy.
- A quantum state is degenerate when there is more than one wave function for a given energy.
- Degeneracy results from particular properties of the potential energy function that describes the system. A perturbation of the potential energy, such as the spin under a B field, can remove the degeneracy.

***Mirriam-webster: having two or more states or subdivisions**