PHYS 3313 – Section 001
Lecture #17

Wednesday, Nov. 7, 2012
Dr. Jaehoon Yu

- Solutions for Schrodinger Equation for Hydrogen Atom
- Quantum Numbers
- Principal Quantum Number
- Orbital Angular Momentum Quantum Number
- Magnetic Quantum Number

Announcements

- Research team member list have been updated on the web!
  - Remember the deadline for your research paper is Monday, Nov. 26!!
- Reminder: homework #6
  - CH6 end of chapter problems: 34, 39, 46, 62 and 65
  - Due on Monday, Nov. 12, in class
- Reading assignments
  - CH7.6 and the entire CH8
- Colloquium today
  - At 4pm, Wednesday, Nov. 7, in SH101
  - Dr. Nick White of Goddard Space Center, NASA

Physics Department
The University of Texas at Arlington
COLLOQUIUM

Science at the Goddard Space Flight Center

Dr. Nick White

Goddard Space Flight Center

4:00 pm Wednesday November 7, 2012 room 101 SH

Abstract:

The Sciences and Exploration Directorate of the NASA Goddard Space Flight Center (GSFC) is the largest Earth and space science research organization in the world. Its scientists advance understanding of the Earth and its life-sustaining environment, the Sun, the solar system, and the wider universe beyond. Researchers in the Sciences and Exploration Directorate work with engineers, computer programmers, technologists, and other team members to develop the cutting-edge technology needed for space-based research. Instruments are also deployed on aircraft, balloons, and Earth's surface. I will give an overview of the current research activities and programs at GSFC including the James Web Space Telescope (JWST), future Earth Observing programs, experiments that are exploring our solar system and studying the interaction of the Sun with the Earth's magnetosphere.

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

Group – Research Topic Association

Research Group	Research Topic	Presentation Date
1	6	12/5-4
2	5	12/5-5
3	7	12/5-1
4	2	12/3-2
5	1	12/3-3
6	9	12/3-5
7	10	12/3-1
8	4	12/5-3
9	3	12/5-2
10	8	12/3-4

Solution of the Schrödinger Equation for Hydrogen

- Substitute ψ into the polar Schrodinger equation and separate the resulting equation into three equations: *R*(*r*), *f*(*θ*), and *g*(φ).

Separation of Variables

- The derivatives in Schrodinger eq. can be written as

$$\frac{\partial \psi}{\partial r} = fg\frac{\partial R}{\partial r} \qquad \frac{\partial \psi}{\partial \theta} = Rg\frac{\partial f}{\partial \theta} \qquad \frac{\partial^2 \psi}{\partial \phi^2} = Rf\frac{\partial^2 g}{\partial \phi^2}$$

- Substituting them into the polar coord. Schrodinger Eq.

$$\frac{fg}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{Rg}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{Rf}{r^2\sin^2\theta}\frac{\partial^2 g}{\partial \phi^2} + \frac{2\mu}{\hbar^2}(E-V)Rgf = 0$$

- Multiply both sides by $r^2 \sin^2 \theta / Rfg$

$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{\sin\theta}{f}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{g}\frac{\partial^2 g}{\partial \phi^2} + \frac{2\mu}{\hbar^2}r^2\sin^2\theta(E-V) = 0$$

Reorganize

$$-\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2\mu}{\hbar^2}r^2\sin^2\theta(E-V) - \frac{\sin\theta}{f}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) = \frac{1}{g}\frac{\partial^2 g}{\partial \phi^2}$$

Solution of the Schrödinger Equation

- Only r and θ appear on the left-hand side and only ϕ appears on the right-hand side of the equation
- The left-hand side of the equation cannot change as ϕ changes.
- The right-hand side cannot change with either r or θ.
- Each side needs to be equal to a constant for the equation to be true in all cases. Set the constant $-m_\ell^2$ equal to the right-hand side of the reorganized equation

$$\frac{d^2 g}{d\phi^2} = -m_l^2 g$$ -------- **azimuthal equation**

- It is convenient to choose a solution to be $e^{im_l\phi}$.

Solution of the Schrödinger Equation

- $e^{im_l\phi}$ satisfies the previous equation for any value of m_ℓ.
- The solution be single valued in order to have a valid solution for any ϕ, which requires $g(\phi) = g(\phi + 2\pi)$

$$g(\phi = 0) = g(\phi = 2\pi) \Rightarrow e^0 = e^{2\pi i m_l}$$

- m_ℓ must be zero or an integer (positive or negative) for this to work
- If the sign were positive, the solution would not be normalized.
- Now, set the remaining equation equal to $-m_\ell^2$ and divide either side with $\sin^2\theta$ and rearrange it.

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{2\mu r^2}{\hbar^2}(E - V) = \frac{m_l^2}{\sin^2\theta} - \frac{1}{f\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right)$$

- Everything depends on r on the left side and θ on the right side of the equation.

Solution of the Schrödinger Equation

- Set each side of the equation equal to constant ℓ(ℓ + 1).
  - Radial Equation

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2\mu r^2}{\hbar^2}(E-V)=l(l+1)\Rightarrow\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}\left[E-V-\frac{\hbar^2}{2\mu}l(l+1)\right]R=0$$

  - Angular Equation

$$\frac{m_l^2}{\sin^2\theta}-\frac{1}{f\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right)=l(l+1)\Rightarrow\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{df}{d\theta}\right)+\left[l(l+1)-\frac{m_l^2}{\sin^2\theta}\right]f=0$$

- Schrödinger equation has been separated into three ordinary second-order differential equations, each containing only one variable.

Solution of the Radial Equation

- The radial equation is called the **associated Laguerre equation,** and the *solutions R* that satisfy the appropriate boundary conditions are called *associated Laguerre functions*.
- Assume the ground state has $\ell = 0$, and this requires $m_\ell = 0$.

  We obtain
$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}\left[E-V\right]R=0$$

- The derivative of $r^2\frac{dR}{dr}$ yields two terms, we obtain

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\frac{2\mu}{\hbar^2}\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)R=0$$

Solution of the Radial Equation

- Let's try a solution $R = Ae^{-r/a_0}$ where *A* is a normalization constant, a_0 is a constant with the dimension of length.
- Take derivatives of *R*, we obtain.

$$\left(\frac{1}{a_0^2}+\frac{2\mu}{\hbar^2}E\right)+\left(\frac{2\mu e^2}{4\pi\varepsilon_0\hbar^2}-\frac{2}{a_0}\right)\frac{1}{r}=0$$

- To satisfy this equation for any *r*, each of the two expressions in parentheses must be zero.
- Set the second parentheses equal to zero and solve for a_0.

$$a_0=\frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}$$

Bohr's radius

- Set the first parentheses equal to zero and solve for *E*.

$$E=-\frac{\hbar^2}{2\mu a_0^2}=-E_0=-13.6eV$$

Ground state energy of the hydrogen atom

- Both equal to the Bohr's results