PHYS 3313 – Section 001
Lecture #18

Wednesday, Nov. 13, 2013
Dr. Jaehoon Yu

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

Announcements

- Reminder: homework #6
  - CH6 end of chapter problems: 34, 39, 46, 62 and 65
  - Due on Monday, Nov. 18, in class
- Reading assignments
  - CH7.6 and the entire CH8
- Colloquium at 4pm in SH101

Physics Department
The University of Texas at Arlington
COLLOQUIUM

THE SYNTHESIS, OPTICAL PROPERTIES, AND APPLICATIONS OF NOVLE LUMINESCENT PARTICLES IN CANCER TREATMENT AND RADIATION DETECTION

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4:00 pm Wednesday November 13, 2013 room 101 SH

Abstract:

Luminescent materials emit light under external energy excitation. In addition to illuminations and lighting, luminescent materials have also gained increasing attention as versatile fluorescent agents in developing new methods for bio-imaging and cancer treatment due to their unique luminescence and photophysical properties. Comparing to other cancer treatment methods such as surgery, radiotherapy, hormonal therapy and chemotherapy, photodynamic therapy (PDT) has less uncomfortable or side effects and costs less. However, conventional PDT treatments are primarily limited in treating superficial cancers due to the poor tissue penetration ability of light. New light sources or photosensitizers for PDT are in need to be developed to extend PDT for treating tumors deeply sited in tissues. Here, for the first time, we synthesized water soluble afterglow nanoparticles as new PDT light source for deep tumor treatment. Meanwhile, afterglow property enhancement and possible mechanism are also performed and discussed. On the other hand, a new PDT photosensitizer is synthesized which can be efficiently activated by X-ray while the traditional PDT drugs cannot. As X-rays can penetrate tissues deeply, the new PDT modality using the X-ray excited photosensitizer can thus be applied for treating deep tumors. Interesting material properties and results will be talked. Moreover, luminescence is also a sensitive probe for radiation detection. A newly observed light emission from our ZnS doped particles is shown and used to detect radiation doses quantitatively using a fluorescence intensity ratio method. The intense emission not only offers a very sensitive method for radiation detection but also provides a violet light for solid state lighting and color displays.

Refreshments will be s[illegible]n the Physics Lounge

Group Number	Reseasrch Group Members	Research Topic	Presentation Date and Order
1	Z.Citty, S. Lagerson, K. McElvain, J. Vellarreal	Michelson-Morley Experiment	#6, Dec. 2
2	W. Brown, C. Hair, R. Reyes, H. Zapata	The Photo-Electric Effect	#2, Dec. 2
3	R. Clark, M. Kruse, C. Nguyen, B. Watson	The Unification of Electromagnetic and Weak Forces	#3, Dec. 2
4	J. Bolton, J. Day, B. Nuar,	Discovery of Electron	#6, Dec. 4
5	J. Bowerman, C. McNutt, M. Obiang, E. Perez	The property of molecules - the Brownian Motions	#4, Dec. 2
6	N. Boseman, V. Hopkins, S. Moorman, S. Moriaty	Black-body Radiation	#1, Dec. 4
7	E. Bainglass, J. Chavez, K. Izuagbe,	Rutherford Scattering	#3, Dec. 4
8	E. Blomberg, E. Duran, J. Grandinatti, R. Loew	The Discovery of Radioactivity	#1, Dec. 2
9	P. Conlin, J. Guevara, F. Islam, A. Nelson	Special Relativity	#5, Dec. 2
10	G. Brown, G. Collier, B. Ferguson, R. Subramaniam	Compton Effect	#2, Dec. 4
11	K. Brackney, C. Dunn, S. Schroeder, S. Sheladia	Super-Conductivity	#4, Dec. 4
12	A. Farrar, C. Jay, C. Smith, J. Umphress	The discovery of the Higgs particle	#5, Dec. 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

- $e^{im_l\phi}$ 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
- Now, set the remaining equation equal to $-m_\ell^2$ and divide either side with $\sin^2\theta$ and rearrange them as

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

- 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 $\ell(\ell + 1)$.
  - 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 satisfies the appropriate boundary conditions are called *associated Laguerre functions*.
- Assume the ground state has ℓ = 0, and this requires m_ℓ = 0.

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

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

Principal Quantum Number *n*

- The principal quantum number, n, results from the solution of *R*(*r*) in the separate Schrodinger Eq. since *R*(*r*) includes the potential energy *V*(*r*).

  The result for this quantized energy is

$$E_n = -\frac{\mu}{2}\left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2\frac{1}{n^2} = -\frac{E_0}{n^2}$$

- The negative sign of the energy *E* indicates that the electron and proton are bound together.

Quantum Numbers

- The full solution of the radial equation requires an introduction of a quantum number, n, which is a non-zero positive integer.
- The three quantum numbers:
  - n Principal quantum number
  - ℓ Orbital angular momentum quantum number
  - m_ℓ Magnetic quantum number
- The boundary conditions put restrictions on these
  - $n = 1, 2, 3, 4, \ldots$ $(n>0)$ Integer
  - $\ell = 0, 1, 2, 3, \ldots, n-1$ $(\ell < n)$ Integer
  - $m_\ell = -\ell, -\ell+1, \ldots, 0, 1, \ldots, \ell-1, \ell$ $(|m_\ell| \le \ell)$ Integer
- The predicted energy level is $E_n = -\frac{E_0}{n^2}$

Ex 7.3: Quantum Numbers & Degeneracy

What are the possible quantum numbers for the state n=4 in atomic hydrogen? How many degenerate states are there?

n	ℓ	m_ℓ
4	0	0
4	1	-1, 0, +1
4	2	-2, -1, 0, +1, +2
4	3	-3, -2, -1, 0, +1, +2, +3

The energy of a atomic hydrogen state is determined only by the primary quantum number, thus, all these quantum states, 1+3+5+7 = 16, are in the same energy state.

Thus, there are 16 degenerate states for the state n=4.

Hydrogen Atom Radial Wave Functions

- The radial solution is specified by the values of *n* and ℓ
- First few radial wave functions $R_{n\ell}$

Table 7.1 Hydrogen Atom Radial Wave Functions

n	ℓ	$R_{n\ell}(r)$
1	0	$\frac{2}{(a_0)^{3/2}} e^{-r/a_0}$
2	0	$\left(2 - \frac{r}{a_0}\right) \frac{e^{-r/2a_0}}{(2a_0)^{3/2}}$
2	1	$\frac{r}{a_0} \frac{e^{-r/2a_0}}{\sqrt{3}(2a_0)^{3/2}}$
3	0	$\frac{1}{(a_0)^{3/2}} \frac{2}{81\sqrt{3}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0{}^2}\right) e^{-r/3a_0}$
3	1	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{6}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$
3	2	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{30}} \frac{r^2}{a_0{}^2} e^{-r/3a_0}$

Solution of the Angular and Azimuthal Equations

- The solutions for azimuthal eq. are $e^{im_l\phi}$ or $e^{-im_l\phi}$
- Solutions to the angular and azimuthal equations are linked because both have m_ℓ
- Group these solutions together into functions

$$Y(\theta,\phi) = f(\theta)g(\phi)$$

---- spherical harmonics

Normalized Spherical Harmonics

Table 7.2 Normalized Spherical Harmonics $Y(\theta, \phi)$

ℓ	m_ℓ	$Y_{\ell m_\ell}$
0	0	$\frac{1}{2\sqrt{\pi}}$
1	0	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$
1	±1	$\mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{\pm i\phi}$
2	0	$\frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$
2	±1	$\mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$
2	±2	$\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{\pm 2i\phi}$
3	0	$\frac{1}{4}\sqrt{\frac{7}{\pi}}(5\cos^3\theta - 3\cos\theta)$
3	±1	$\mp\frac{1}{8}\sqrt{\frac{21}{\pi}}\sin\theta(5\cos^2\theta - 1)\, e^{\pm i\phi}$
3	±2	$\frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$
3	±3	$\mp\frac{1}{8}\sqrt{\frac{35}{\pi}}\sin^3\theta\, e^{\pm 3i\phi}$

Ex 7.1: Spherical Harmonic Function

Show that the spherical harmonic function Y11(θ,φ) satisfies the angular Schrodinger equation.

$$Y_{11}(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{i\phi} = A\sin\theta$$

Inserting $l = 1$ and $m_l = 1$ into the angular Schrodinger equation, we obtain

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dY_{11}}{d\theta}\right) + \left[1(1+1) - \frac{1}{\sin^2\theta}\right]Y_{11} = \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dY_{11}}{d\theta}\right) + \left(2 - \frac{1}{\sin^2\theta}\right)Y_{11}$$

$$= \frac{A}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\sin\theta}{d\theta}\right) + A\left(2 - \frac{1}{\sin^2\theta}\right)\sin\theta = \frac{A}{\sin\theta}\frac{d}{d\theta}(\sin\theta\cos\theta) + A\left(2 - \frac{1}{\sin^2\theta}\right)\sin\theta$$

$$= \frac{A}{\sin\theta}\frac{d}{d\theta}\left(\frac{1}{2}\sin 2\theta\right) + A\left(2 - \frac{1}{\sin^2\theta}\right)\sin\theta = \frac{A}{\sin\theta}\cos 2\theta + A\left(2 - \frac{1}{\sin^2\theta}\right)\sin\theta$$

$$= \frac{A}{\sin\theta}\left(1 - 2\sin^2\theta\right) + A\left(2 - \frac{1}{\sin^2\theta}\right)\sin\theta = \frac{A}{\sin\theta} - 2A\sin\theta + A\left(2 - \frac{1}{\sin^2\theta}\right)\sin\theta = 0$$

Solution of the Angular and Azimuthal Equations

- The radial wave function *R* and the spherical harmonics *Y* determine the probability density for the various quantum states.
- Thus the total wave function $\psi(r,\theta,\phi)$ depends on *n*, ℓ , and m_ℓ . The wave function can be written as

$$\psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r) Y_{lm_l}(\theta,\phi)$$