PHYS 3313 – Section 001
Lecture #22

Monday, April 17, 2017
Dr. Jaehoon Yu

- Hydrogen Atom Wave Functions
- Solution for Angular and Azimuthal Equations
- Angular Momentum Quantum Numbers
- Magnetic Quantum Numbers
- Zeeman Effects

Announcements

- Homework #5
  - CH6 end of chapter problems: 34, 46 and 65
  - CH7 end of chapter problems: 7, 9, 17 and 29
  - Due Monday, Apr. 22
- Reading assignments
  - CH7.6 and the entire CH8
- Research presentation deadline is 8pm, Sunday, April 20
- Research paper deadline is Wednesday, April 24
- Quiz 4 this Wednesday
  - At the beginning of the class this Wednesday
  - Covers CH6.2 to what we finish today
  - BYOF
- Reminder: Quadruple extra credit
  - Colloquium this Wednesday, April 19, in UH108
  - Speaker: Dr. Nigel Lockyer, Director of Fermilab

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

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

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

- Group these solutions together into functions

$$Y_{lm_l}(\theta,\phi)=f(\theta)g(\phi)$$

---- **spherical harmonics**

Normalized Spherical Harmonics

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

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

Ex 7.1: Spherical Harmonic Function

Show that the spherical harmonic function $Y_{11}(\theta,\phi)$ satisfies the angular Schrodinger equation.

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

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 for 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

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

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 $E_n = -\dfrac{E_0}{n^2}$

Orbital Angular Momentum Quantum Number ℓ

- It is associated with the $R(r)$ and $f(\theta)$ parts of the wave function.
- Classically, the orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$ with $L = mv_{orbital}r$.
- ℓ is related to the magnitude of L by $L = \sqrt{l(l+1)}\hbar$
- In an ℓ = 0 state, $L = \sqrt{0(1)}\hbar = 0$.

It disagrees with Bohr's semi-classical "planetary" model of electrons orbiting a nucleus $L = n\hbar$.

Orbital Angular Momentum Quantum Number ℓ

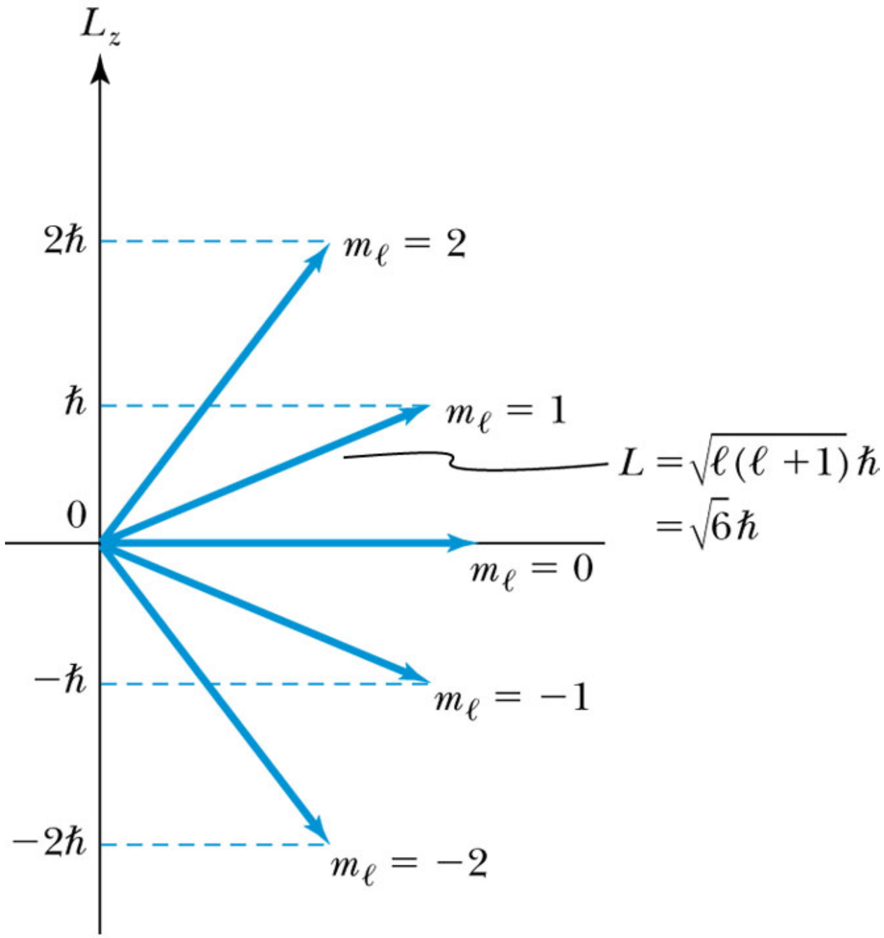
- Certain energy level is **degenerate** with respect to ℓ when the energy is independent of ℓ.
- Use letter names for the various ℓ values
  - ℓ = 0 1 2 3 4 5 . . .
  - Letter = *s* *p* *d* *f* *g* *h* . . .
- Atomic states are referred by their *n* and ℓ
  - **s**=**s**harp, **p**=**p**rincipal, **d**=**d**iffuse, **f** =**f**undamental, then in alphabetical order afterward
- A state with $n = 2$ and $\ell = 1$ is called the 2*p* state
  - Is 2d state possible?
- The boundary conditions require $n > \ell$

Magnetic Quantum Number m_ℓ

- The angle ϕ is a measure of the rotation about the z axis.
- The solution for $g(\phi)$ specifies that m_ℓ is an integer and related to the z component of L.

$$L_z = m_l \hbar$$

- The relationship of L, L_z, ℓ, and m_ℓ for $\ell = 2$.
- $L = \sqrt{l(l+1)}\hbar = \sqrt{6}\hbar$ is fixed.
- Because L_z is quantized, only certain orientations of $\vec{L}$ are possible and this is called **space quantization**.
- m_ℓ is called the magnetic moment since z axis is chosen customarily along the direction of magnetic field.



Magnetic Quantum Number m_ℓ

- Quantum mechanics allows $\vec{L}$ to be quantized along only one direction in space and because of the relationship $L^2 = L_x^2 + L_y^2 + L_z^2$, once a second component is known, the third component will also be known. ➔ violation of uncertainty principle
  - One of the three components, such as L_z, can be known clearly but the other components will not be precisely known
- Now, since we know there is no preferred direction,

$$\langle L_x^2 \rangle = \langle L_y^2 \rangle = \langle L_z^2 \rangle$$

- We expect the average of the angular momentum components squared to be: $\langle L^2 \rangle = 3\langle L_z^2 \rangle = \dfrac{3}{2l+1}\sum_{m_l=-l}^{+l} m_l^2\hbar^2 = l(l+1)\hbar^2$

Magnetic Effects on Atomic Spectra—The Normal Zeeman Effect

- A Dutch physicist Pieter Zeeman showed as early as 1896 that the spectral lines emitted by atoms in a magnetic field split into multiple energy levels. It is called the **Zeeman effect**.

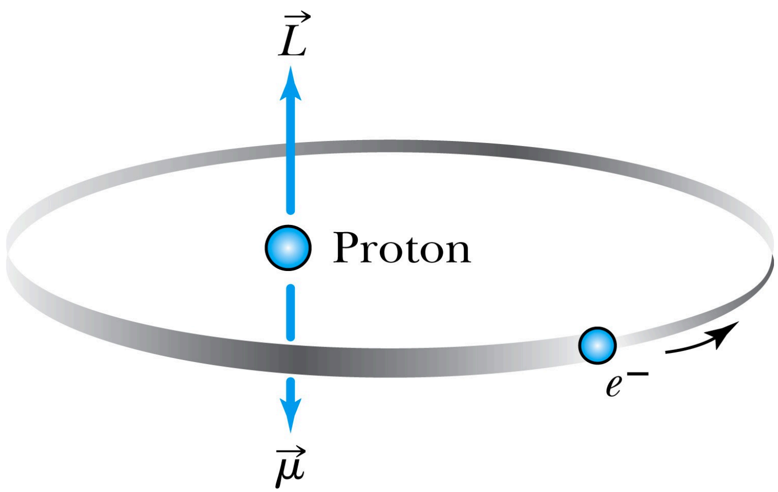
The Normal Zeeman effect:

- A spectral line of an atom is split into **three** lines.
- Consider the atom to behave like a small magnet.
- The current loop has a magnetic moment $\mu = IA$ and the period $T = 2\pi r / v$. If an electron can be considered as orbiting a circular current loop of $I = dq / dt$ around the nucleus, we obtain

$$\mu = IA = qA/T = \pi r^2 (-e)/(2\pi r/v) = -erv/2 = -\frac{e}{2m} mrv = -\frac{e}{2m} L$$

- $\vec{\mu} = -\frac{e}{2m}\vec{L}$ where $L = mvr$ is the magnitude of the orbital angular momentum

The Normal Zeeman Effect



- Since there is no magnetic field to align them, $\vec{\mu}$ points in random directions.
- The dipole has a potential energy

$$V_B = -\vec{\mu} \cdot \vec{B}$$

- The angular momentum is aligned with the magnetic moment, and the torque between $\vec{\mu}$ and $\vec{B}$ causes a precession of $\vec{\mu}$.

$$\mu_z = \frac{e}{2m} L_z = \frac{e\hbar}{2m} m_l = -\mu_B m_l$$

Where **$\mu_B = e\hbar / 2m$** is called the **Bohr magneton**.

- $\vec{\mu}$ cannot align exactly in the z direction and has only certain allowed quantized orientations.

$$\vec{\mu} = -\frac{\mu_B \vec{L}}{\hbar}$$

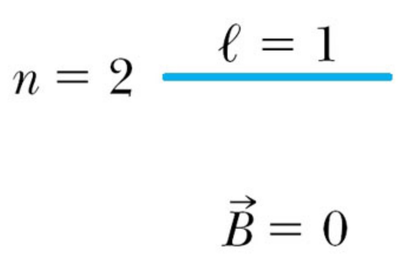
The Normal Zeeman Effect

- The potential energy is quantized due to the magnetic quantum number m_ℓ.

$$V_B = -\mu_z B = +\mu_B m_l B$$

- When a magnetic field is applied, the 2*p* level of atomic hydrogen is split into three different energy states with the electron energy difference of $\Delta E = \mu_B B\, \Delta m_\ell$.

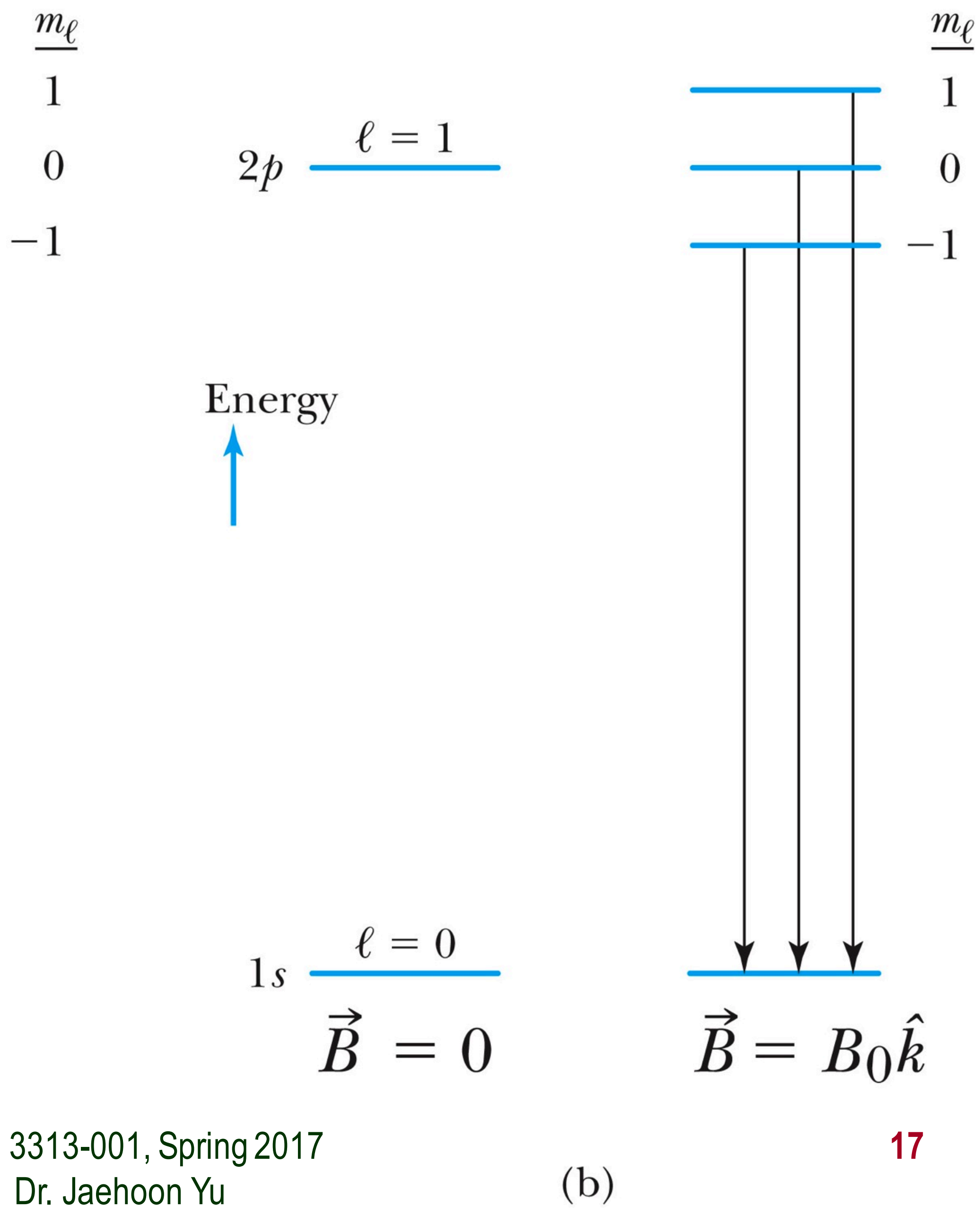
m_ℓ	**Energy**
1	$E_0 + \mu_B B$
0	E_0
−1	$E_0 - \mu_B B$



- So split is into a total of $2\ell+1$ energy states

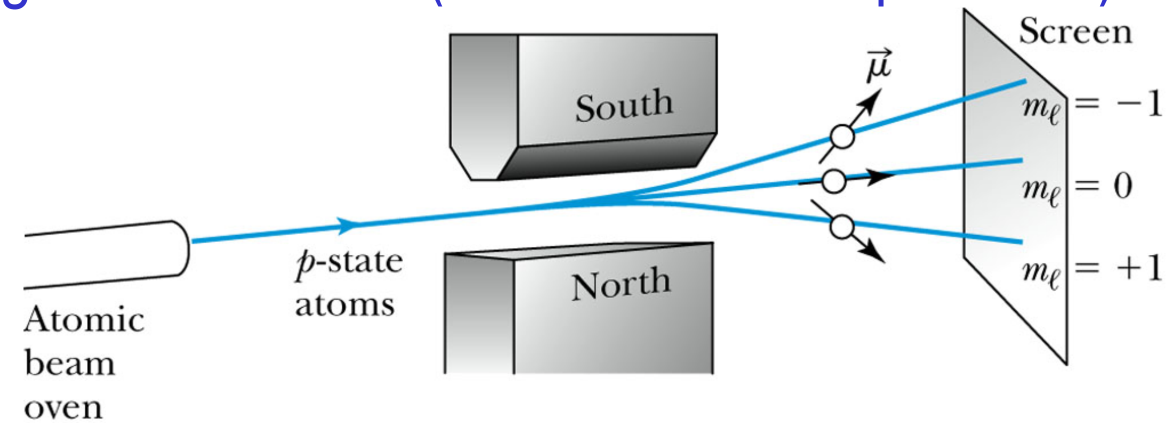
The Normal Zeeman Effect

- A transition from 1s to 2p
- A transition from 2*p* to 1*s*



The Normal Zeeman Effect

- An atomic beam of particles in the $\ell = 1$ state pass through a magnetic field along the *z* direction. (Stern-Gerlach experiment)



- $$V_B = -\mu_z B$$
- $$F_z = -\left(dV_B/dz\right) = \mu_z\left(dB/dz\right)$$
- The $m_\ell = +1$ state will be deflected down, the $m_\ell = -1$ state up, and the $m_\ell = 0$ state will be undeflected. ➔ saw only 2 with silver atom
- If the space quantization were due to the magnetic quantum number m_ℓ, the number of m_ℓ states is always odd at $(2\ell + 1)$ and should have produced an odd number of lines.