Quantum Mechanics and Atomic Physics

Lecture 19:

Quantized Angular Momentum and Electron Spin

http://www.physics.rutgers.edu/ugrad/361

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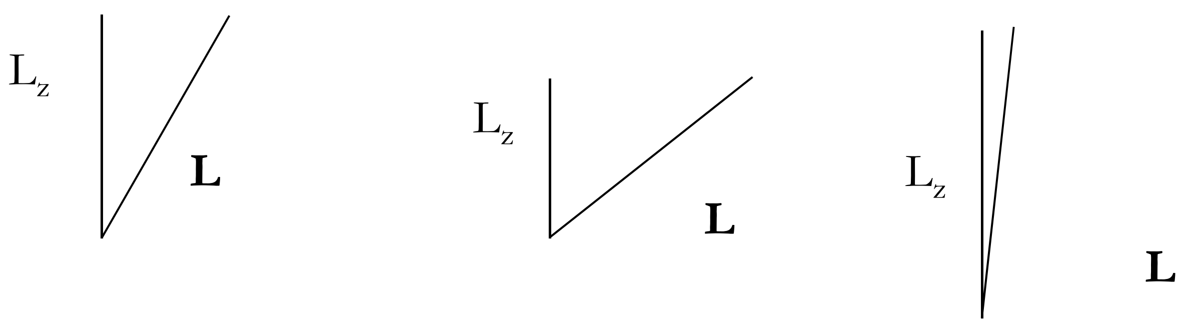
Last time

- Raising/Lowering angular momentum operators:

$$L_z(L_\pm Y_{\ell,m_\ell}) = \hbar(m_\ell \pm 1)(L_\pm Y_{\ell,m_\ell})$$

- L_+ and L_- raise or lower the state of the z component of angular momentum of $Y_{\ell m}$ by one unit in terms of hbar.
- And they have no effect on ℓ or the total angular momentum **L**

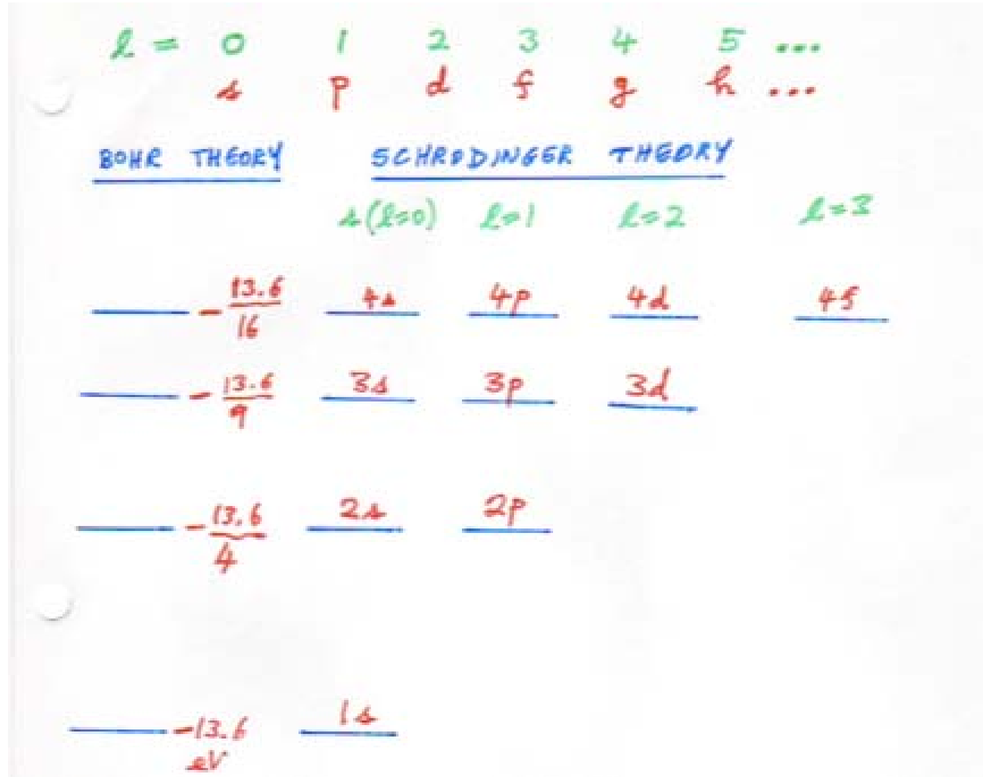


Think of it as also affecting the angle

Recall: Energy level diagram

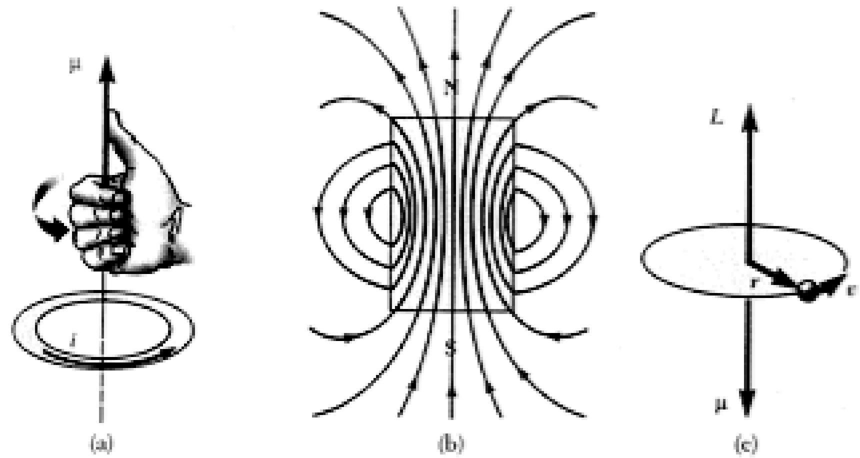
For historical reasons, all states with same quantum number n are said to form a shell.

And states having the same value of both n and ℓ are said to form a subshell (s, p, d, f, …)



- In Schrodinger theory, different ℓ states for same n have same energy
  - Called ℓ-degeneracy
- Energy level diagram omits different m_ℓ states - independent of m_ℓ due to spherical symmetry of the atom.
  - This is for no external magnetic field! - Today we will learn what happens when we apply an external B field

Hydrogen atom in external B field



Magnetic behavior is similar to that of bar magnet (middle figure)

- Electron in circular orbit constitutes a current loop.
- Time it takes to make one orbit = $2\pi r/v$
- Current i = charge/time for one orbit
- So,

$$i = \frac{-e}{2\pi r/v} = -\frac{ev}{2\pi r}$$

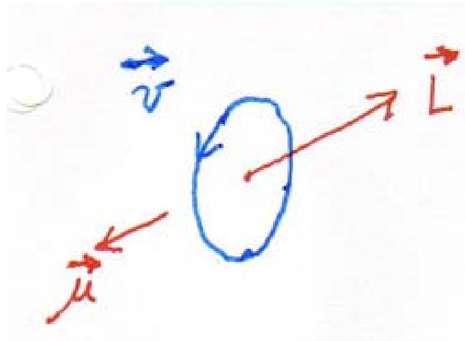
- Area of the current loop $A = \pi r^2$

Magnetic moment

- The magnetic moment μ = (current)(area)

$$\mu = (\text{current})(\text{area}) = iA = \left(-\frac{ev}{2\pi r}\right)(\pi r^2)$$

$$\Rightarrow \mu = \frac{-evr}{2}$$



- But angular momentum
  - L = mvr ⇒ vr = L/m
- So, $\Rightarrow \mu = -\frac{eL}{2m}$
- μ and **L** are vectors so vector relationship:

$$\vec{\mu} = -\frac{e}{2m}\vec{L}$$

- Since magnitude of **L** is quantized

$$|\vec{L}| = \hbar\sqrt{\ell(\ell+1)} \qquad \mu = -\frac{e\hbar}{2m}\sqrt{\ell(\ell+1)}$$

Magnetic moment

$$\vec{\mu} = -g \frac{e}{2m} \vec{L} \qquad g = 1$$

$$\frac{\vec{\mu}}{\vec{L}} = -g \frac{e}{2m}$$

- **μ/L** is called the *gyromagnetic ratio*
- g is called the "g-factor" (first letter of gyromagnetic)

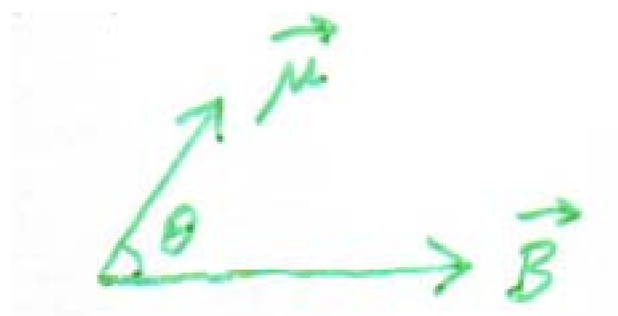
Energy splitting

- Any magnetic moment placed in an external magnetic field produces an interaction potential energy: (Refer to your E&M book.)

$$\Delta E = -\vec{\mu} \cdot \vec{B}$$

- It arises from the torque **τ** that **B** exerts to align **μ** along direction of **B**.

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$



Energy splitting, con't

$$\Delta E = -\left(-g \frac{e}{2m} \vec{L}\right) \cdot \vec{B}$$

$$= g \frac{e}{2m} \vec{L} \cdot \vec{B} = g \frac{e}{2m} B L \cos\theta$$

$$= g \frac{e}{2m} B L_z = g \frac{e}{2m} B m_\ell \hbar$$

- In an external magnetic field, hydrogen energy levels should split.
- Define *Bohr magneton*

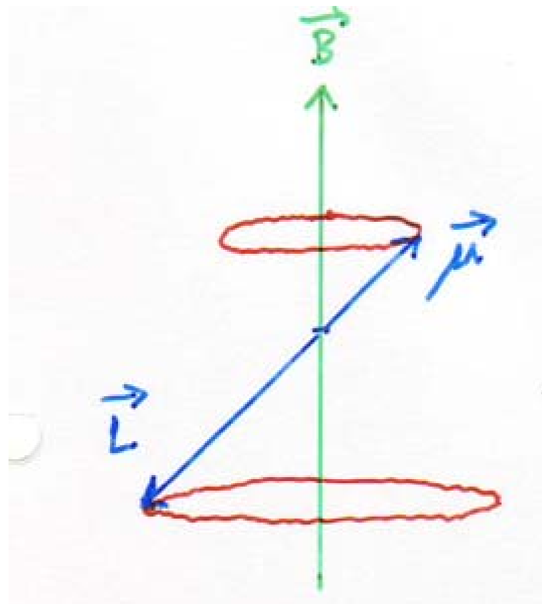
$$\mu_B = \frac{e\hbar}{2m} = 5.8 \times 10^{-5} \frac{eV}{T} = 9.274 \times 10^{-24} A \cdot m^2$$

- So the energy splitting is: $\Delta E = m_\ell g \mu_B B \;, \; g = 1$

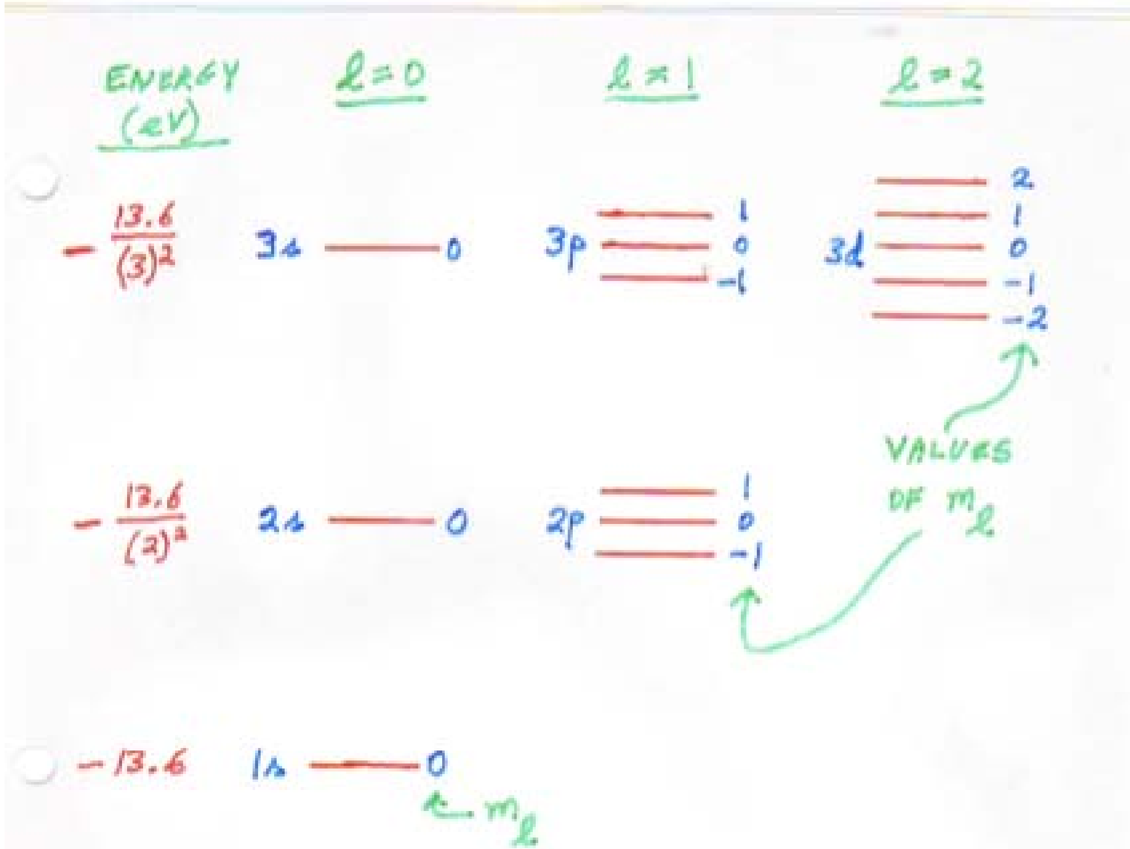
Energy splitting con't

$m_\ell = 0, \pm 1, \pm 2, \ldots \pm \ell$

- There are $(2\ell+1)$ values of m_ℓ for any ℓ.
- Each energy level in hydrogen should split into $(2\ell+1)$ sublevels.
- **L** can precess about **B** which is along the z-axis.
- **μ** is anti-parallel to **L**, so **μ** also precesses about **B**
  - This is called *Larmor precession.*



Energy level diagram, revisited



Compare B field on/off

- For B=0, adjacent energy levels are typically a few eV apart.
  - For example:

$$E(3s) - E(2s) = \frac{-13.6\,eV}{(3)^2} - \left(-\frac{13.6\,eV}{(2)^2}\right) = 1.9\,eV$$

- For B ≠0, magnetic sublevel splittings are:

$$\Delta E = (\Delta m_\ell)\, g\, \mu_B B$$

  - And adjacent sublevels have $\Delta m_\ell=1$
  - Typical B = 0.2T. So,

$$\Delta E = (1)(1)\left(5.8\times 10^{-5}\,\frac{eV}{T}\right)(0.2T) \approx 10^{-5}\,eV$$

- Clearly, the diagram on previous page is exaggerated.

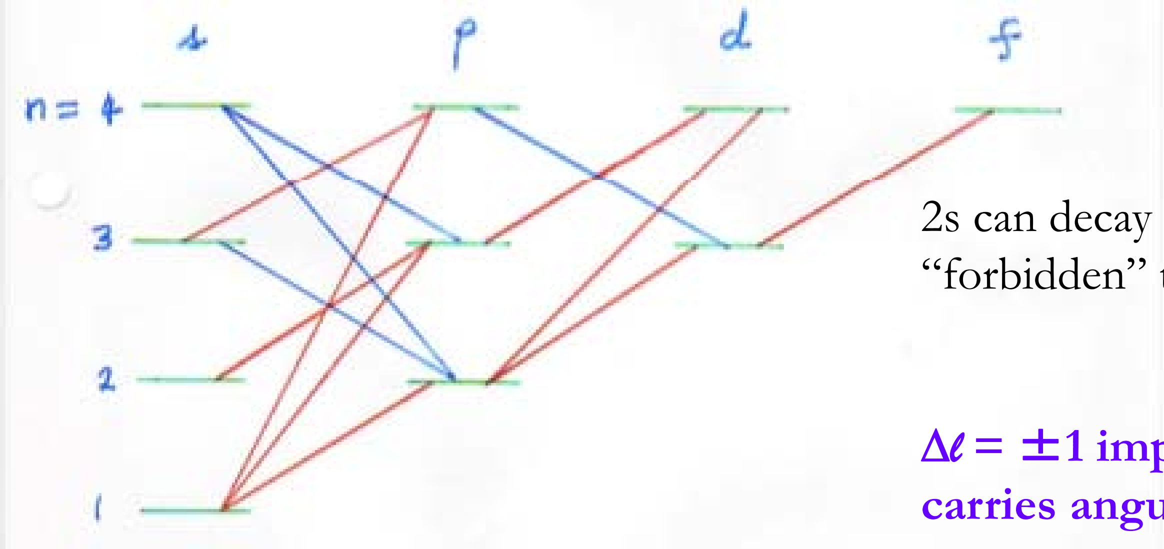
Radiative Transitions (B=0)

- An atom radiates a photon if it make a transition from one state to another of lower n.
- Schrodinger theory provides **selection rules** for "allowed" transitions:

$\Delta \ell = \pm 1 \qquad \Delta m_\ell = 0, \pm 1$

("forbidden" transitions do occur but much less often)

- Allowed transitions for B=0:

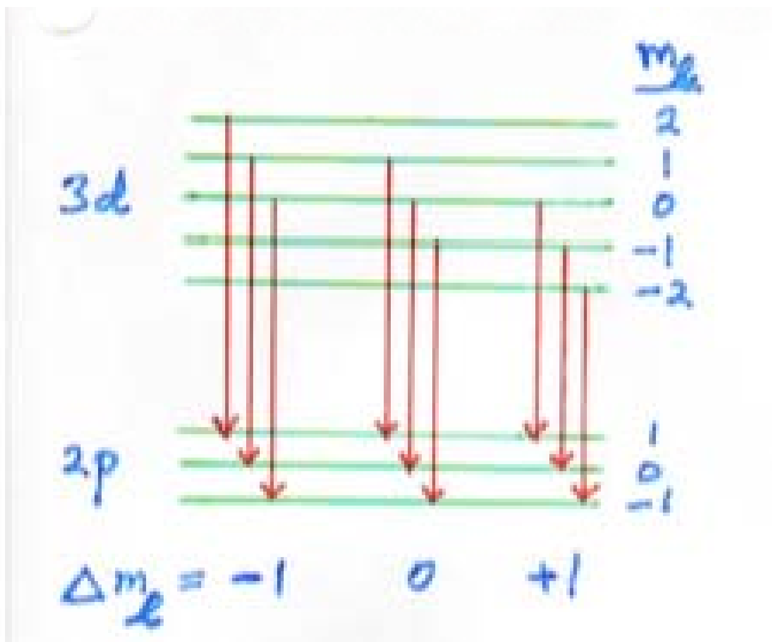


2s can decay to 1s only through "forbidden" transition.

$\Delta \ell = \pm 1$ implies photon carries angular momenum

Radiative Transitions (B ≠0)

- Selection Rules: $\Delta \ell = \pm 1 \quad \Delta m_\ell = 0, \pm 1$
- Let's consider the Balmer series line (3d→ 2p) in an external magnetic field.
- Allowed transitions are:



- Photon energies are:

$$E_\gamma = E_i - E_f = (E_{i\,Bohr} + \Delta E_i) - (E_{f\,Bohr} + \Delta E_f)$$

$$= (E_{i\,Bohr} - E_{f\,Bohr}) + m_{\ell i}\, g\, m_B B - m_{\ell f}\, g\, m_B B$$

$$= E_{\gamma\,Bohr} - \Delta m_\ell\, g\, m_B B$$

$$\Delta m_\ell = m_{\ell f} - m_{\ell i} \qquad \Delta m_\ell = 0, \pm 1 \qquad E_{\gamma\,Bohr} = -13.6\,eV\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

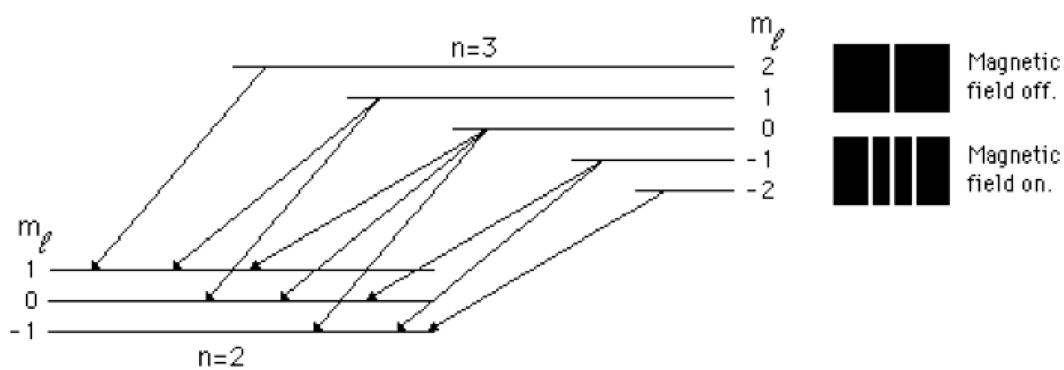
$$\Delta m_\ell = -1 \Rightarrow E_\gamma = E_{\gamma\,Bohr} + g\,\mu_B B$$

$$\Delta m_\ell = 0 \Rightarrow E_\gamma = E_{\gamma\,Bohr}$$

$$\Delta m_\ell = +1 \Rightarrow E_\gamma = E_{\gamma\,Bohr} - g\,\mu_B B$$

What's happening?

- When B≠0, each Bohr model photon line should split into exactly 3 equally spaced lines
  - This is called the (normal) *Zeeman Effect*



(Normal) Zeeman Effect

- In an external B field, every Bohr model photon line should split into exactly 3 equally spaced lines:

  $\Delta E = g\mu_B B$ with $g=1$
- Experimental results:
  - Zeeman effect does occur, and in some atoms it is "normal" (i.e. $\Delta E = g\mu_B B$)
  - In many atoms (including Hydrogen) splitting is not

    $\Delta E = 1\ \mu_B B$. ΔE had right order of magnitude but $g \neq 1$. Zeeman effect is "anomalous" due to spin contribution.
  - Photon lines often split into more than 3 in an external B field
  - More on this next time

Question

- Can a Hydrogen atom in ψ_{421} in a magnetic field emit a photon and end in the following state?

(a) ψ_{511} (b) ψ_{321} (c) ψ_{310} (d) ψ_{31-1}

Electron Spin Angular Momentum

- Electron must have a spin (or intrinsic) angular momentum:

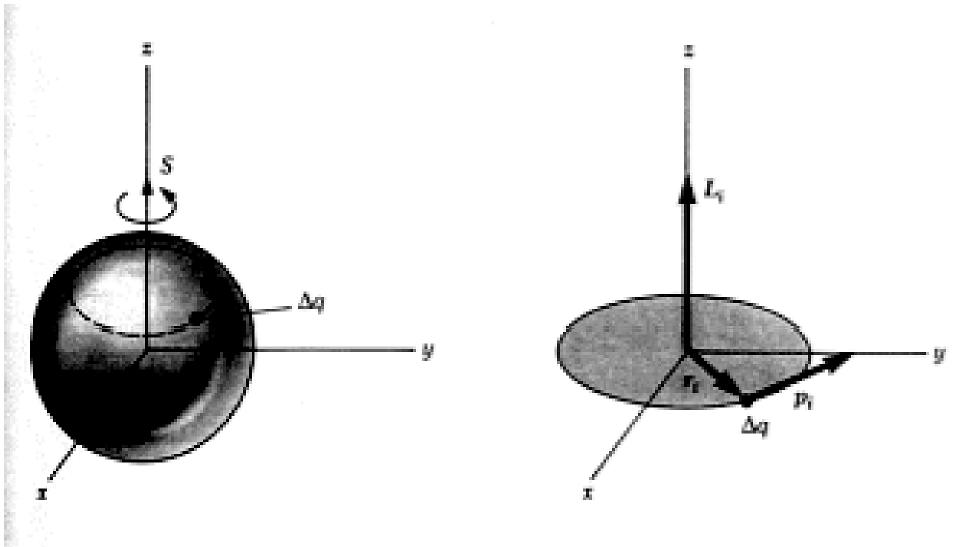


Figure 8.6 A spinning charge q may be viewed as a collection of charge elements Δq orbiting a fixed line, the axis of rotation. The magnetic moments accompanying these orbiting charge elements are summed to give the total magnetic moment of rotation, or spin moment, of the charge q.

$S = \sqrt{s(s+1)}\,\hbar \quad , \quad s = 1/2$

$\Rightarrow S = \sqrt{\left(\tfrac{1}{2}\right)\left(\tfrac{3}{2}\right)}\,\hbar = \frac{\sqrt{3}}{2}\hbar$

Space quantization

$S_z = m_s \hbar$, $m_s = -s, -s+1, \dots +s$

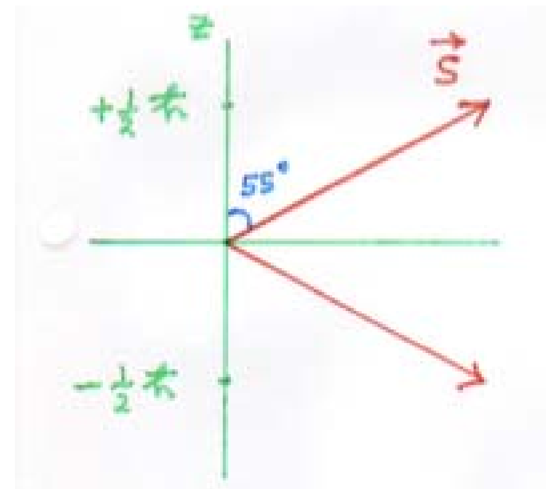
$= \pm 1/2$

(your book : $S_z = s\hbar = \pm 1/2\, \hbar$)

$S_z = \pm \frac{1}{2}\hbar$

$\cos\theta = \frac{S_z}{S} = \frac{\pm\frac{1}{2}\hbar}{\frac{\sqrt{3}}{2}\hbar} = \pm\frac{1}{\sqrt{3}}$

$\Rightarrow \theta = 55^\circ$ or 125°



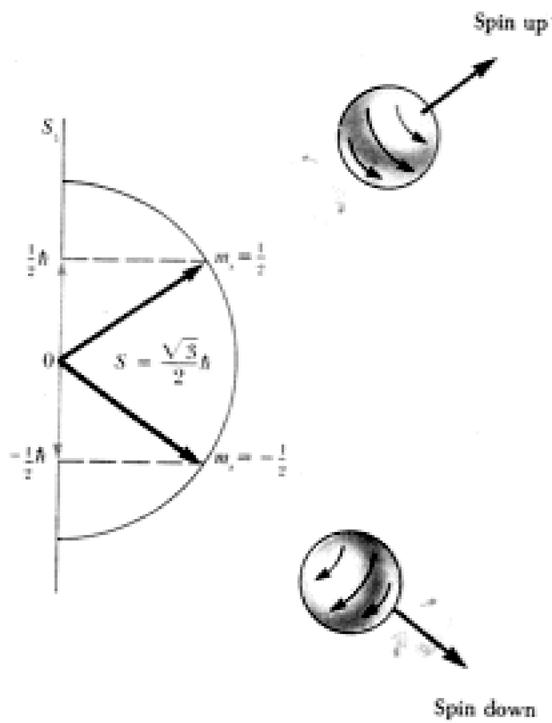


Figure 8.8 The spin angular momentum also exhibits space quantization. This figure shows the two allowed orientations of the spin vector S for a spin $\frac{1}{2}$ particle, such as the electron.

- If $m_s = +1/2$ we say electron is "spin up"
- If $m_s = -1/2$ we say electron is "spin down"
- m_s is called the magnetic spin quantum number
- s is called the spin quantum number

Consequences of electron spin

- Electron spin creates a spin magnetic moment.
- Electron's orbital motion creates an *internal* magnetic field in an atom
- The two interact to cause a splitting of energy levels even if $B_{external} = 0$
  - More on this next time

$$\vec{\mu}_L = -g \frac{e}{2m} \vec{l} \quad , \quad g = 1$$

$$\vec{\mu}_S = -g \frac{e}{2m} \vec{S} \quad , \quad g \approx 2$$

predicted by relativistic QM. (Dirac equation)

Four quantum numbers

- To understand the H atom we need these four quantum numbers:

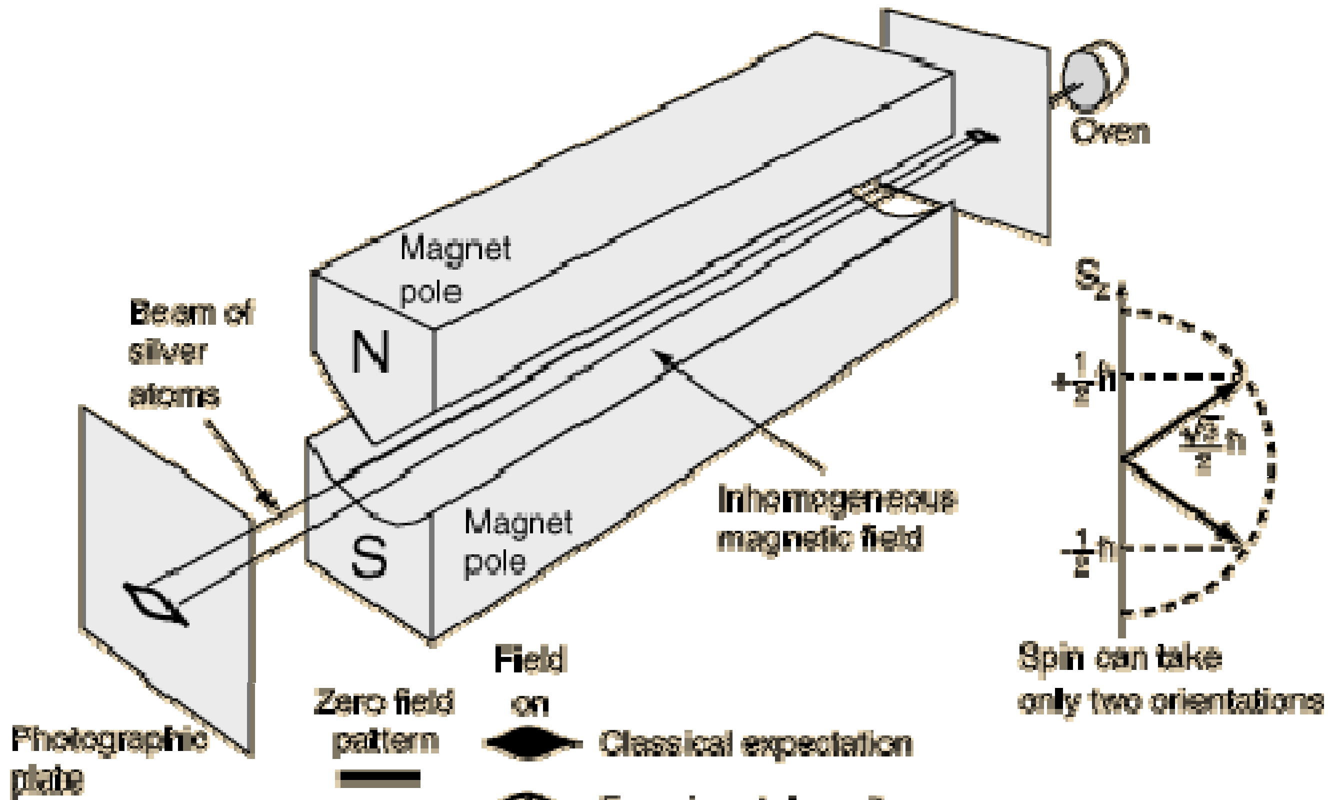
1. n: expresses quantization of energy
2. ℓ: quantizes *magnitude* of **L**
3. m_ℓ: quantizes *direction* of **L**
4. m_s: quantizes *direction* of **S**

- s is left out because it has the single value of s=1/2.
  - It quantizes the *magnitude* of **S**

Stern-Gerlach Experiment (1922)

- Showed the quantization of electron spin into two orientations
- *Electron spin was unknown at the time!*
  - They wanted to demonstrate the space quantization associated with electrons in atoms
- Used a beam of silver atoms from a hot oven directed into a region of non-uniform magnetic field
- The silver atoms allowed Stern and Gerlach to study the magnetic properties of a single electron
  - a single outer electron: 47 protons of the nucleus shielded by the 46 inner electrons: Electron configuration of Ag: $[Kr]^{36}4d^{10}5s^{1}$
  - Expected $2\ell+1$ splittings from space quantization of orbital moments (classically it would be a continuous distribution)
  - Also note: this electron (ground state) has zero orbital angular momentum
    - Therefore, expect there to be no interaction with an external magnetic field.

Schematic of experiment



What they expected/saw

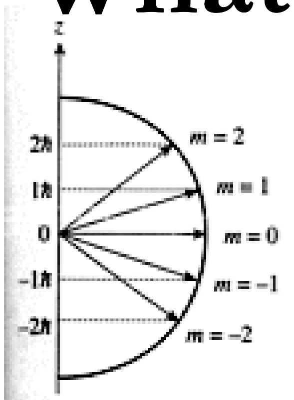
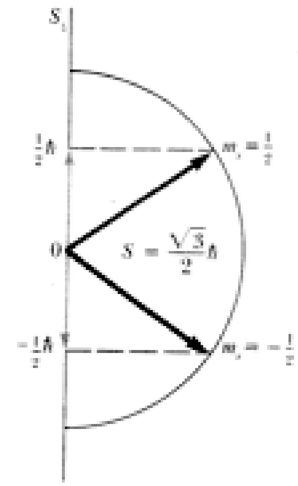


FIGURE 6.5 Possible orientations of **L** for $\ell = 2$, $|\mathbf{L}| = \sqrt{6}\hbar$.



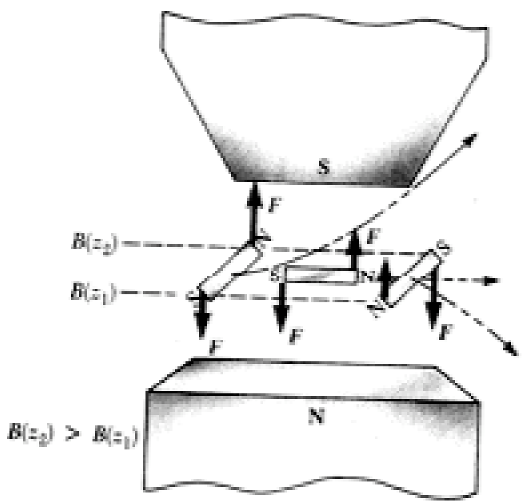
- Expected $2\ell+1$, which is always an odd number, splittings from space quantization of orbital moments
- Classically one would expect all possible orientations of the dipoles so that a continuous smear would be produced on the photographic plate. Even quantum mechanically, they expected odd number of splittings, if at all.
- They found that the field separated the beam into two distinct parts, indicating just two possible orientations of the magnetic moment of the electron!

In external B-field …

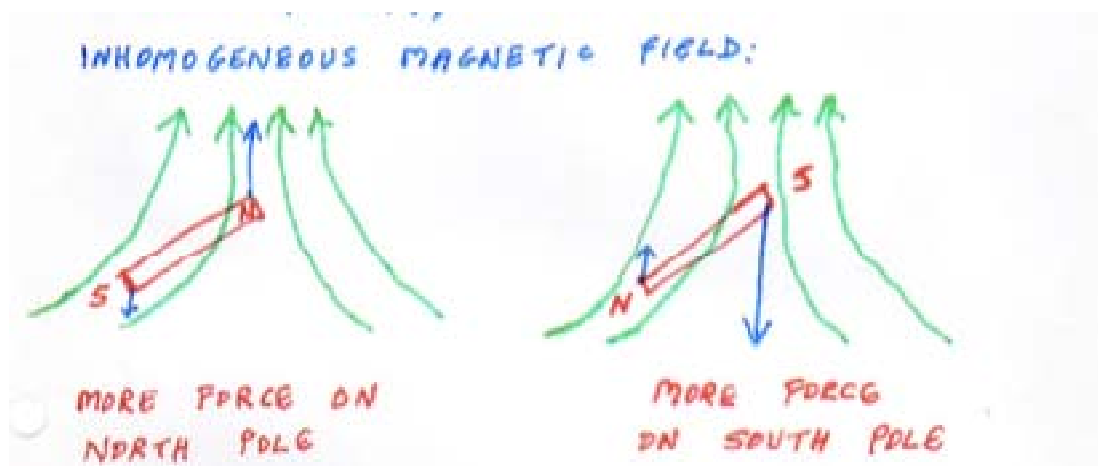
$$\vec{\mu}_s = -g \frac{e}{2m} \vec{S} \quad \text{w/ } g = 2$$

$$\Delta E_s = -\vec{\mu}_s \cdot \vec{B} = +g \frac{e}{2m} B \cdot S_z = m_s g \frac{e\hbar}{2m} B$$

$$\Rightarrow \Delta E_s = (\pm \tfrac{1}{2})(2)\, \mu_B B = \pm \mu_B B$$



(b)



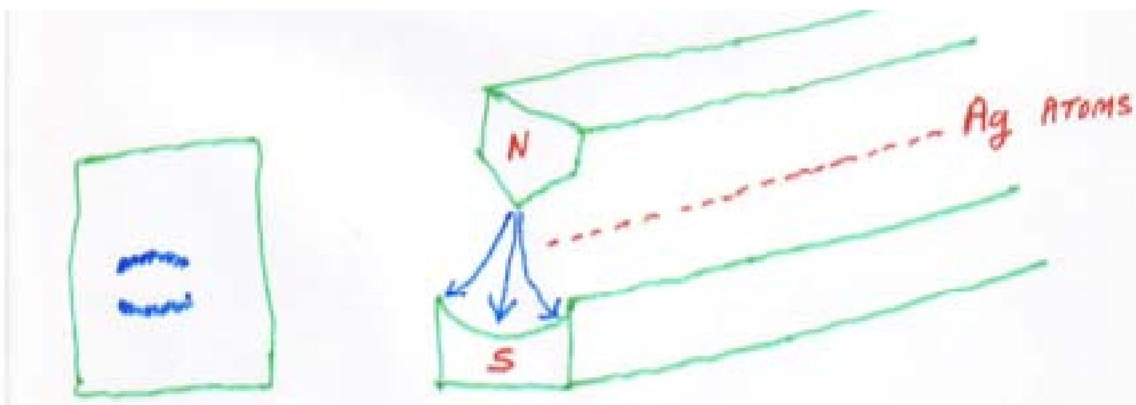
- A magnetic dipole moment will experience a force proportional to the field gradient since the two "poles" will be subject to different fields.

Force

$$F = -\frac{\partial E}{\partial z}$$

$$F = -\frac{\partial}{\partial z}\Delta E_s = \mp \mu_B \frac{dB}{dz}$$

- In inhomogeneous B field, $m_s = +1/2$ is deflected up and $m_s=-1/2$ is deflected down.

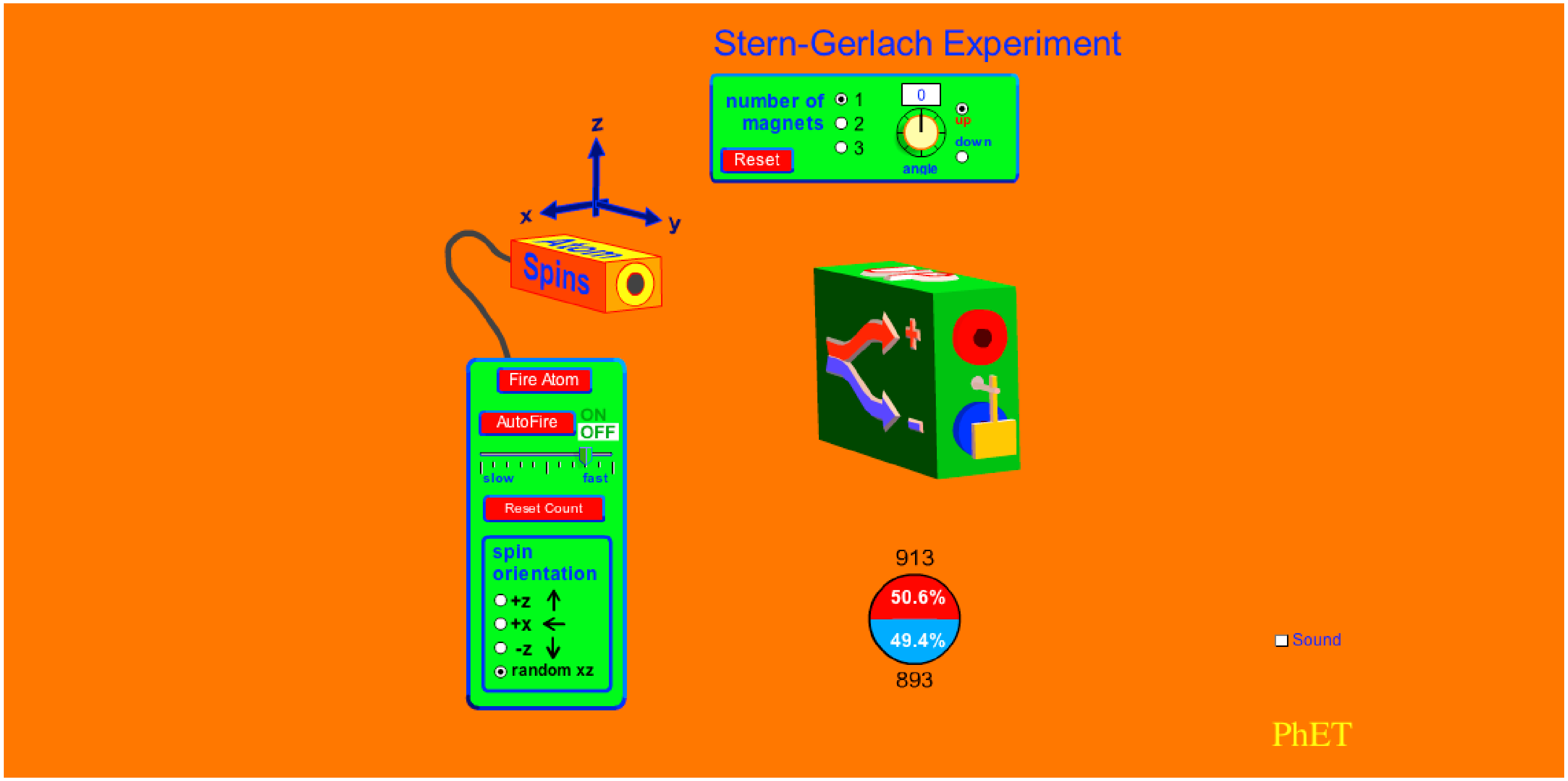


Goudsmit and Uhlenbeck postulate

- How does the electron obtain a magnetic moment if it has zero angular momentum and therefore produces no "current loop" to produce a magnetic moment?
- In 1925, Goudsmit and Uhlenbeck postulated that the electron had an *intrinsic angular momentum*, independent of its orbital characteristics.
- Led to the use of "electron spin" to describe the intrinsic angular momentum.

Interactive simulation

- http://phet.colorado.edu/simulations/sims.php?sim=SternGerlach_Experiment

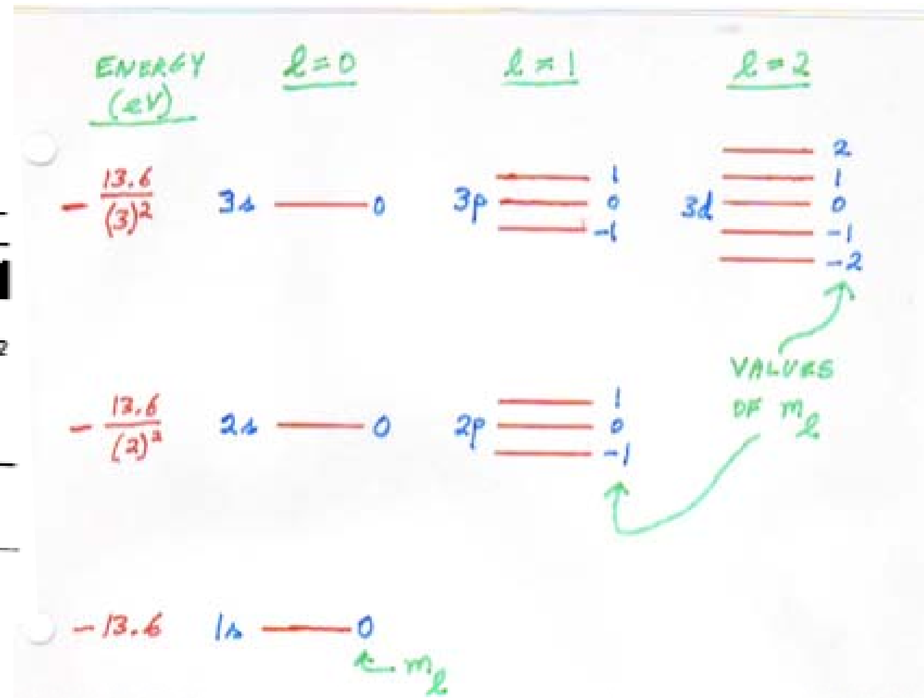


Summary of electron states

Reed: chapter 8

Table 8.1 Electron States.

n	1	2		3		
ℓ	0	0	1	0	1	2
m	0	0	−1 0 1	0	−1 0 1	−2 −1 0 1 2
s	±1/2	±1/2	±1/2	±1/2	±1/2	±1/2
States	2	2	6	2	6	10
Subshell	1s	2s	2p	3s	3p	3d
Shell	K	L		M		
Total states	2	8		18		



Summary/Announcements

Next time: Beyond simple Hydrogen model and Pauli exclusion principle

- *I'm covering more details in lecture on atomic structure than is in your book. If you are interested, refer to:*
  - "Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles" by R. Eisberg and R. Resnick (John Wiley and Sons, 2nd Edition), Chapters 8-10.