Angular Magnetic Dipole Moment

Quantized L means quantized magnetic dipole moment, μ

current, I $= e/T$ (associated w/moving e^-)

$$\mu = IA = \frac{e}{T}\pi r^2$$

$$= \frac{e}{2\pi r/v}\pi r^2 = \frac{e}{2m_e}\underbrace{(m_e v r)}_{=L}$$

$$\boxed{\vec{\mu}_L = \frac{-e}{2m_e}\vec{L}}$$

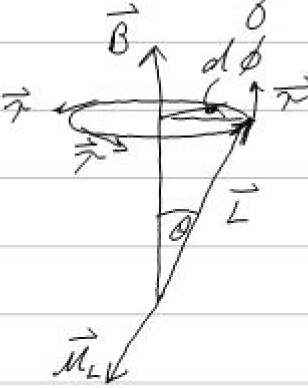
classical, but valid in Quantum

As we will see, the interaction of $\vec{\mu}_L$ with a present $\vec{B}$ suggests a convention.

- Whatever $\vec{B}$ direction becomes a prefferred axis
  - Take it as z-axis by convention

i.e. $\vec{B}$ allows sensitivity to $\vec{L}$, so make it so L_z is what we measure

In a $\vec{B}$ field, a $\vec{\mu}$ causes a torque, $\vec{\tau}$, to be felt



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

Causes a precession of $\vec{L}$ around $\vec{B}$.

$$|\vec{\tau}| = \left|\frac{d\vec{L}}{dt}\right| = |\vec{\mu}_L \times \vec{B}|$$

$$\frac{L \sin\theta \, d\phi}{dt} = \frac{-e}{2m_e} \vec{L} \times \vec{B}$$

$$" = \frac{e}{2m_e} LB \sin\theta$$

$$\boxed{\frac{d\phi}{dt} = \frac{eB}{2m_e}}$$

<u>Larmor frequency</u>: rate of precession

Stern-Gerlach Experiment

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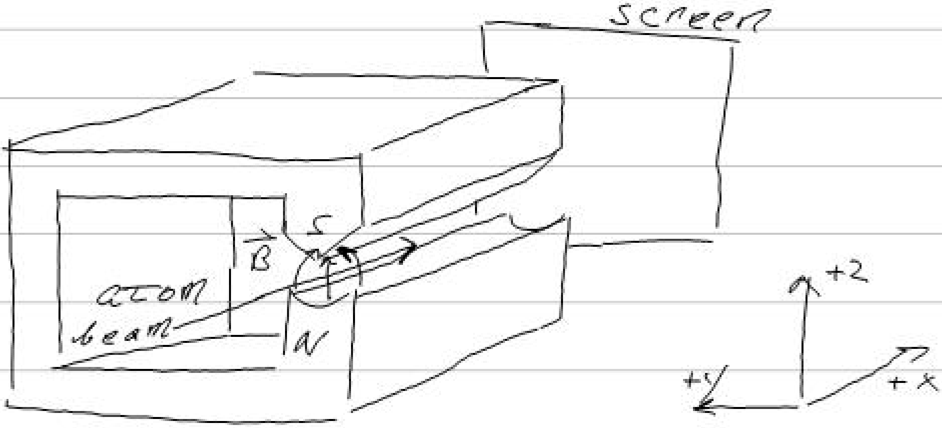


Potential energy of a dipole thru $\vec{B}$ field: $\underline{U = -\vec{\mu} \cdot \vec{B}}$

For H atom, $U = -\vec{\mu}_L \cdot \vec{B}$

Force on the atom

$$\underline{\underline{\vec{F}}} = -\nabla(-\vec{\mu}_L \cdot \vec{B}) = \nabla(\vec{\mu}_L \cdot \vec{B})$$

$$= \mu_z \frac{\partial B_z}{\partial z} \hat{z} = \frac{-e}{2m_e} L_z \frac{\partial B_z}{\partial z} \hat{z}$$

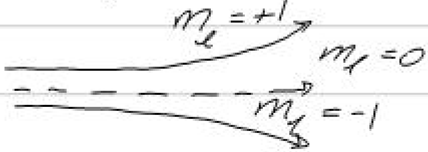
$$= \boxed{\frac{-e m_l \hbar}{2m_e} \frac{\partial B_z}{\partial z} \hat{z}}$$

You only get a force if field non-uniform.

$\Rightarrow$ Deflection expected to vary as m_l

Results of Stern-Gerlach Experiment

We expect for each value of $m_l \Rightarrow$ different deflection of atom



- if $l = 1$:
  - then $m_l = -1, 0, +1$
  - so should see 3 deflections

Only 2 were seen!

- if $l = 0$:

  $m_l = 0$ + only one deflection expected

  2 deflections observed!

What is going on?

Spin:

It turns out particles have another intrinsic property (i.e. like mass + charge) which gives particle:

- intrinsic magnetic dipole moment
- intrinsic angular momentum

this is a natural result of the relativistic treatment of Quantum Mechanics (recall Schrödinger Eq. is non-relativistic)

$\vec{S}$ is the angular momentum associated with spin.

1) $\boxed{|S| = \sqrt{s(s+1)}\,\hbar}$: 's' is a particular value for types of particle

2) $\boxed{S_z = m_s \hbar}$: $m_s = -s, -s+1, \ldots, s-1, s$

Similarly to orbital angular momentum, there is a spin magnetic moment:

3) $\boxed{\vec{\mu}_s = g \frac{q}{2m} \vec{S}}$ $\quad g_e = \sim 2$

$\quad g \to$ "gyromagnetic ratio" $\quad g_p \sim 5.6$

→ since $m_p \gg m_e$, $\vec{\mu}_{s, proton}$ is tiny

For an electron, $s = 1/2$.

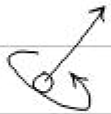
With the Stern-Gerlach experiment, force on atom must include:

$$\vec{F} = \frac{-e}{m_e} S_z \frac{\partial B_z}{\partial z} \hat{z}$$

Explains $l=0$ S-G result
- there are 2 values of force due to $m_s = \pm \frac{1}{2}$

Also explains why get a deflection for $l=1$, $m_l=0$.
→ but a more complicated case

What is Spin?



Classical picture

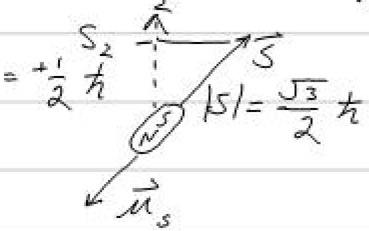
We do not actually have a small sphere with a magnetic moment

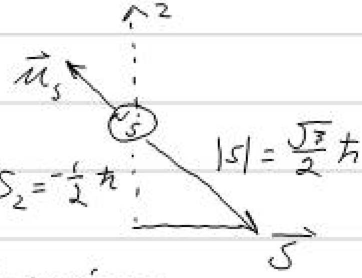
→ no 'radius', r
→ no mass or charge density

we have a (relativistic) wave function
- yields observables corresponding to spin upon appropriate measurements (operators)

Spatial state: n, l, m_l
Spin state: m_s

$$\psi \rightarrow \psi_{n,l,m_l,m_s}(r, \theta, \phi)$$





space quantization

Spins of Particles

Two general categories:
each has very different
properties

Fermions: half-integer spins

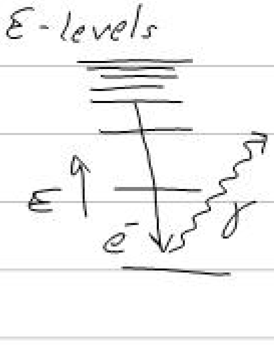
e, p, ν : $s = 1/2$

Ω : $s = 3/2$

Bosons:

α, π^0 : $s = 0$

W, γ : $s = 1$



Photons can only have
$L_z = m_s \hbar$ ($m_s = \pm 1, 0$)

When atom deexcites,
- emits a γ
- only $\pm \hbar$ angular momentum can be carried away

"selection rules" in spectroscopy

Exclusion Principle

Consider two identical fermions occupying states n & n'.

Need following assumption

"Probability density must be unchanged if labels of indistinguishable particles are switched."

i.e. you cannot distinguish such cases

When use this with 2-particle Schrödinger Eq., need either

$$\psi_S = \psi_n(1)\,\psi_{n'}(2) + \psi_{n'}(1)\,\psi_n(2)$$

symmetric

-and-

$$\psi_A = \psi_n(1)\,\psi_{n'}(2) - \psi_{n'}(1)\,\psi_n(2)$$

antisymmetric

combinations of wave functions to completely describe system.

Fermions (the antisymmetric case)

Consider case where $n = n'$

$$\psi_A = \psi_n(1)\psi_n(2) - \psi_n(1)\psi_n(2) = 0$$

We take this to mean $n = n'$ isn't allowed.

"No two indistinguishable fermions may occupy the same individual particle state."

↳ this means quantum #s must be different.

Bosons: the symmetric case

$$\psi_S = \psi_n(1)\psi_n(2) + \psi_n(1)\psi_n(2) \neq 0$$

so exclusion does not apply.

Many Electron Atoms

Going past Hydrogen → add e^-'s
- even 1 more e^- is a huge complication
→ $e^- \leftrightarrow e^-$ interactions render Schrödinger Eq. insoluble.

Exclusion principle permits progress ⇒ rules for atomic structure

1) e^-'s in an atom tend to occupy the lowest energy levels available to them.

2) only one e^- can be in a state with a given complete set of quantum #'s

	n	l	m_l	m_s
H	1	0	0	$\pm 1/2$
He → e#1	1	0	0	$+1/2$
→ e#2	1	0	0	$-1/2$

Experiment: He e^-'s are anti-aligned

Shells + Subshells

Shells → correspond to values of principle quantum #, n

Each shell has a subshell!

$n=1$ → "1s" : $1s^1$ / $1s^2$

H → $1s^1$; He → $1s^2$; superscript: # e^- in subshell

$n=2$ → "2s" : $2s^1$ (Li)

State of e^- for lithium (Li):

	n	l	m_l	m_s
Li →	2	0	0	$\pm 1/2$

Since 1s subshell is full

→ 1s e^-'s feel all 3 proton charges

→ 2s e^- only sensitive to net charge inside its orbit

Gauss's Law → all that contribute to E-field

∴ 2s e^- less tightly bound

What about >3 electrons?

for ea. l : $2l+1$ values of m_l
for ea. m_l : 2 values of m_s

$\therefore$ each subshell has $2(2l+1)$ e^-'s

s subshells : $l=0$; $m_l=0$; $m_s=\pm\frac{1}{2}$
$\rightarrow$ $\underline{\underline{2}}$ states
p subshells : $l=1$; $m_l=-1,0,+1$; $m_s=\pm\frac{1}{2}$
$\rightarrow$ $\underline{\underline{6}}$ states
d subshells : $2(2\cdot2+1)=\underline{\underline{10}}$
f subshells : $\underline{\underline{14}}$ states

So as fill atoms up with electrons:

$\underline{\underline{n=1}}$: $l=0$, 2 states — H, $\underline{He}$ Noble gas

$\underline{\underline{n=2}}$: 2 $l=0$ states — Li, Be
6 $l=1$ states — B, C, N, O, F, $\underline{Ne}$ Noble gas

These are what observed in 1st 2 rows of periodic table.

Screening & Heavier Elements

Within a given shell
- orbits more 'spherical' as l increases
- so they spend less time inside the nucleus

$\therefore$ sometimes sub-shells with higher l fill later than lower l subshells with a higher quantum #

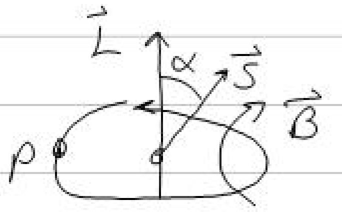
$\boxed{\text{minimize } n+l}$

Example:
- energy levels for 4s lower than for 3d electrons

			$n+l$
$n=3$:	2 $l=0$ states	'3s'	3
	6 $l=1$ states	'3p'	4
	10 $l=2$ " "	'3d'	5
$n=4$:	2 $l=0$ (before '3d')	'4s'	4
	6 $l=1$	'4p'	5
	10 $l=2$ (fill between 5s + 5p)	'4d'	6
	14 $l=3$	'4f'	7

Gets more complicated as get more e^-s

Spin-orbit Coupling



in e^- rest frame

Proton appears to orbit e^-

$$d\vec{B} = \frac{\mu_0}{4\pi} \frac{I\, d\vec{s} \times \hat{r}}{r^2}$$

(Biot-Savart Law)

So there is a $\vec{B}$ from orbital motion, and $\vec{\mu}_s$ from spin

$$\underline{V_{S\ell} = -\vec{\mu}_s \cdot \vec{B}}$$ (a component coupling these two)

$$= \frac{\mu_0 e^2}{4\pi m_e^2 r^2} \vec{S} \cdot \vec{L}$$

$$\propto \underline{SL \cos \alpha}$$

When $m_s = -1/2$: energy level lower than for $m_s = +1/2$.

So spin orbit coupling splits $2P$ into $\underline{2P_{1/2}}$ & $2P_{3/2}$

$\downarrow$

@ lower energy

Total Angular Momentum

Combination of orbital + spin angular momentum

$$\boxed{\vec{J} = \vec{L} + \vec{S}}$$

By analogy w/ S + L:

$$\boxed{|J| = \sqrt{j(j+1)}\,\hbar}$$

$$\boxed{J_z = m_j\,\hbar} \qquad m_j = -j \ldots +j$$

half-integer steps because $m_s = \pm 1/2$

Since $s = 1/2$,

$$\boxed{j = l \pm s} \qquad l + 1/2 \text{ or } l - 1/2$$

Notation

$$n\,L_j$$

n: principal quantum #

L: indicates orbital angular momentum quantum #, l (an upper case letter S, P, D, ...)

j: total angular momentum

Single Electron Atoms - Selection Rules

Δn = any integer $\qquad \Delta l = \pm 1$

$\Delta m_j = 0, \pm 1 \qquad \Delta j = 0, \pm 1$

So in H, going from $n=3 \rightarrow n=2$

can do: $3S_{1/2} \rightarrow 3P_{1/2}$ ($\Delta l = -1$, $\Delta j = 0$)

can't do: $3S_{1/2} \rightarrow 2S_{1/2}$ ($\Delta l = 0$ ×, $\Delta j = 0$)

Many e^- Atoms:

- 2 rules of thumb

Hund's Rule

1) S should be maximized to extent possible without violating Pauli exclusion Principle

2) L should be maximized without violating 1)

Example: first $5e^-$'s of 'd' subshell same m_s, different m_l's ($-2, -1, 0, +1, +2$)

Spectroscopic Notation

For many e^- atoms, use

$$\boxed{n^{2S+1}L_J}$$

S: sum of m_s values for e^-'s

eg. $S = 0, 1$ for $2e^-$'s
(anti-aligned or aligned)

L: is sum of l values

L>S case - for a given $L \rightarrow 2S+1$ values of $J = L-S$ to $L+S$

L<S case - J has $< 2S+1$ possible values

Example Carbon has 2p e^-'s outside closed $2s^2$ subshell

Both e^-'s have $l = 1$

$\rightarrow L = 0, 1, 2$

$S = 0, 1$

S	L	J	
0	0	0	2^1S_0
0	2	2	2^1D_2