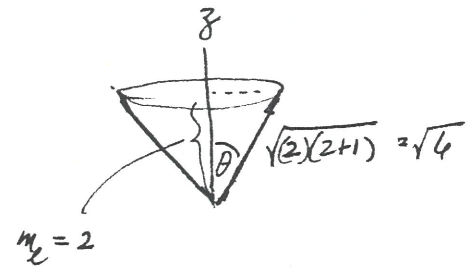
Paramagnetism

d^1 isolated atom or ion

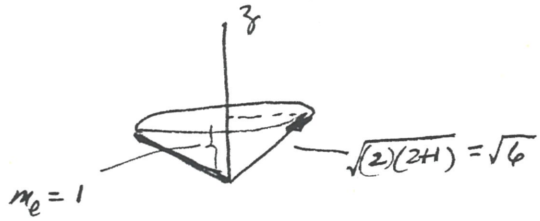
Orbital angular momentum

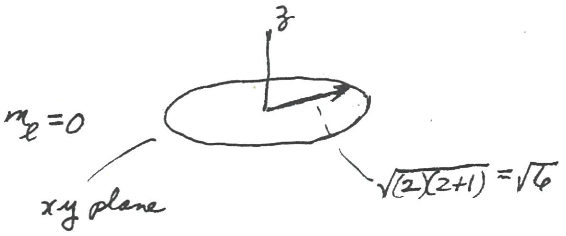
Quantum numbers

$$\begin{cases} L = l = 2 \\ m_l = 0, \pm 1, \pm 2 \end{cases}$$



$$\cos\theta = \frac{m_l}{\sqrt{l(l+1)}}$$

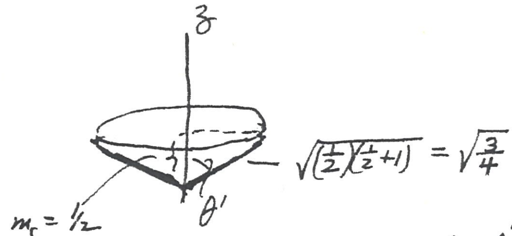




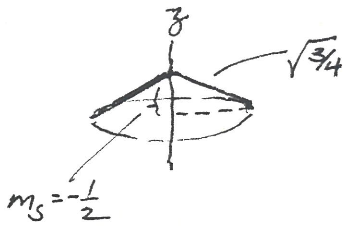
$$\boxed{\begin{aligned} M^2_{orbital} &= L(L+1)\hbar^2 = l(l+1)\hbar^2 \\ &= 6\hbar^2 \end{aligned}}$$

Spin angular momentum

$$\begin{cases} S = s = 1/2 \\ m_s = \pm 1/2 \end{cases}$$

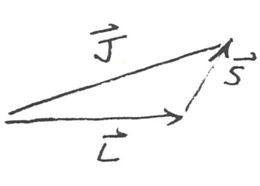


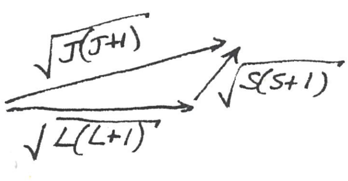
$$\cos\theta' = \frac{\frac{1}{2}}{\sqrt{3/4}}$$



$$\boxed{\begin{aligned} M^2_{spin} &= S(S+1)\hbar^2 = s(s+1)\hbar^2 \\ &= \frac{3}{4}\hbar^2 \end{aligned}}$$

Total angular momentum





J = total angular momentum quantum number

Can only be $L+S$, $L+S-1$, …… $|L-S|$

in units of 1 !

So, for d^1 ion or atom, where $L=2$, $S=1/2$

J can only be $5/2$, $3/2$. In each case $m_J = 0, \pm 1, \ldots \pm J$

and $\boxed{M^2_{total} = J(J+1)\hbar^2 \quad \text{where } J = \tfrac{5}{2} \text{ and } 3/2}$

Accordingly, ion or atom is denoted by S, L, and J as follows:

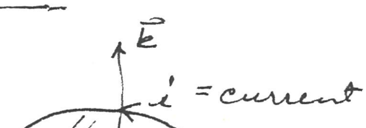
$$^{2S+1}L_J$$

$L=0$,	1,	2,	3	etc
S	P	D	F	etc

So, for d^1 ion or atom, we have

$$^2D_{5/2} \quad \text{and} \quad ^2D_{3/2}$$

<u>Magnetic Moments</u>



A = area of loop

$\vec{\mu} = \vec{k}(iA)$

$\vec{L} = \dfrac{\vec{M}_{orbital}}{\hbar}$

can show in a few steps — $\vec{\mu}_L = \dfrac{(-)e\hbar}{2m_e c}\vec{L}$

for orbiting electrons

Define $\dfrac{e\hbar}{2m_e c} \equiv \beta$ $\qquad \vec{\mu}_L = -\beta\vec{L} = -g_L\beta\vec{L}$

Bohr magneton $\qquad g_L = 1.000$

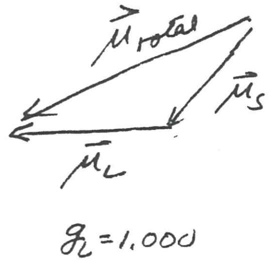
Similar, for spin

$$\vec{\mu}_S = -g_S \beta \vec{S} \quad , \text{ but } g_S = 2.0023$$

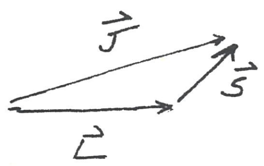
where $\vec{S} = \dfrac{\vec{M}_{spin}}{\hbar}$

<u>Total magnetic momentum</u>

$$\vec{\mu}_{Total} = \vec{\mu}_L + \vec{\mu}_S$$



$g_S = 2.0023$



$\vec{\mu}_{Total}$ not collinear with $\vec{J}$

Only $\vec{\mu}_J$ important!

$$\vec{\mu}_{Total} = \vec{\mu}_L + \vec{\mu}_S = -\beta(g_L \vec{L} + g_S \vec{S})$$

Write $\vec{\mu}_J = g_J \beta \vec{J}$ and define g_J

Then $$g_J \beta \vec{J}\cdot\vec{J} = -\beta(g_L \vec{L}\cdot\vec{J} + g_S \vec{S}\cdot\vec{J})$$

or $$g_J = \frac{1}{J(J+1)}(g_L \vec{L}\cdot\vec{J} + g_S \vec{S}\cdot\vec{J})$$

$$= \frac{1}{J(J+1)}(g_L \vec{J}\cdot\vec{J} + (g_S - g_L)\vec{S}\cdot\vec{J})$$

$$= \frac{1}{J(J+1)}(g_L J(J+1)) + \frac{(g_S - g_L)\vec{S}\cdot\vec{J}}{J(J+1)}$$

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

so $$\vec{S}\cdot\vec{J} = \vec{S}\cdot\vec{L} + S^2$$

and $$J^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S} \quad \text{(cosine law)}$$

or $$\vec{L}\cdot\vec{S} = \frac{1}{2}[J^2 - L^2 - S^2] = \frac{J(J+1) - L(L+1) - S(S+1)}{2}$$

So

$$g_J = g_L + (g_S - g_L)\left[\frac{J(J+1) - L(L+1) + S(S+1)}{2(J)(J+1)}\right]$$

Landé g value!

$$\boxed{\vec{\mu}_J = -g_J \beta \vec{J}}$$