Interactive Lecture 7: Topics

- Most probable value r vs. expectation value r
- Why orbital angular momentum is not enough?
- Spin angular momentum
- Four quantum numbers
- Total angular momentum
- LS coupling

Most probable vs. expectation value

Expectation Value r $$\langle r \rangle = \int_0^{\infty} r \cdot r^2 R_{n,l}(r)^2 dr$$

Most probable r Value $$\frac{dP(r)}{dr} = \frac{d r^2 R_{n,l}(r)^2}{dr} = 0$$

Most probable vs. expectation value

Expectation Value r $$\langle r \rangle = \int_0^{\infty} r \cdot r^2 R_{n,l}(r)^2 \, dr$$

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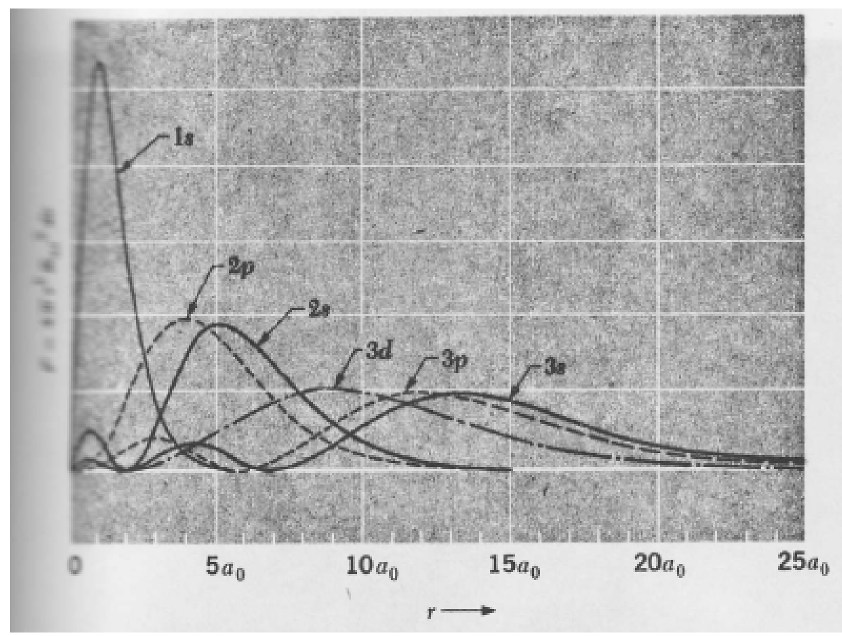
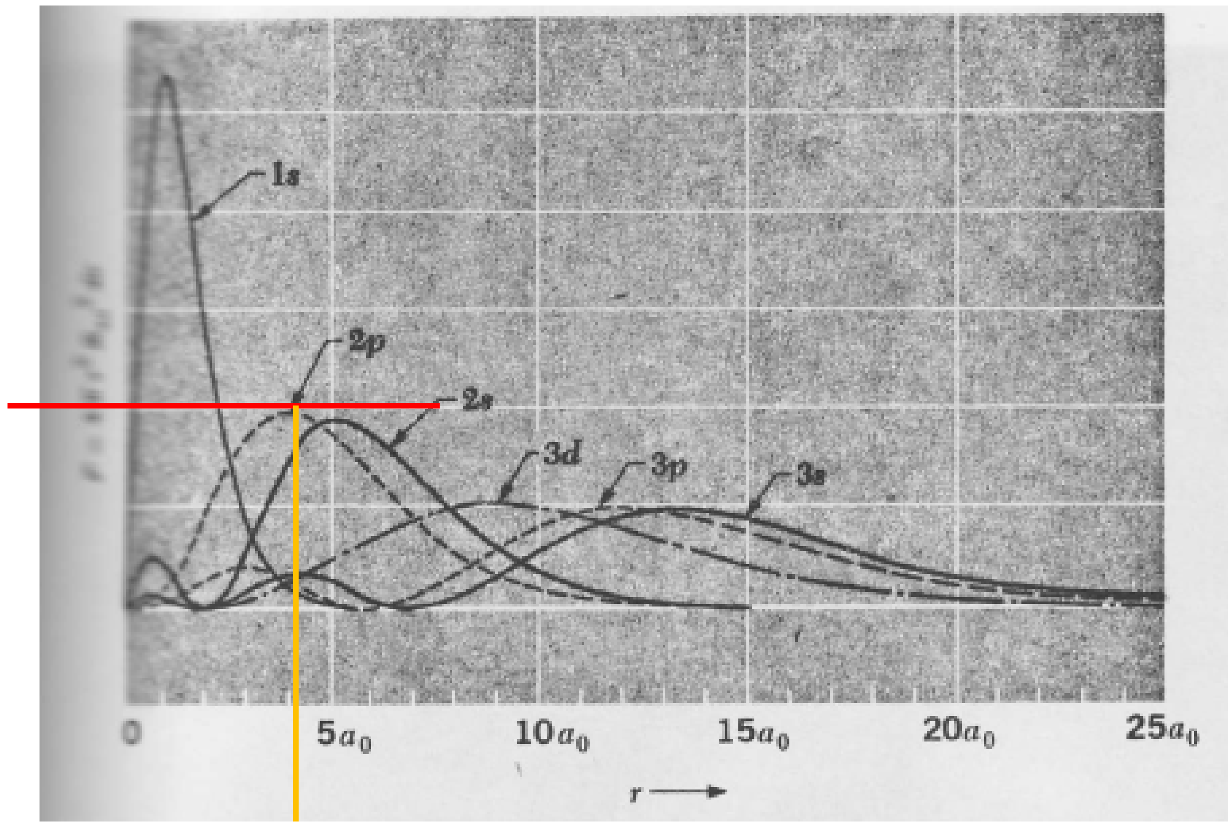


$P(r) \sim r^2 R^2(r)$



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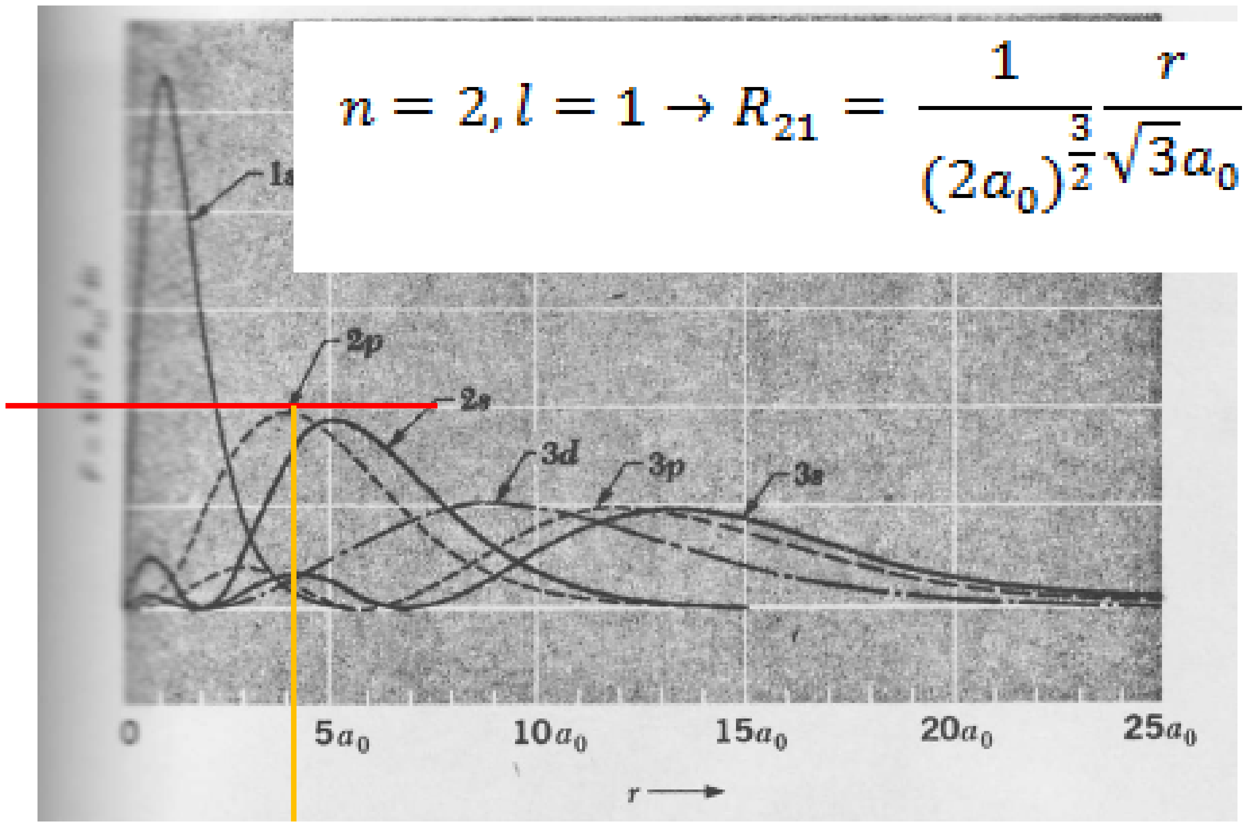


$$n = 2, l = 1 \rightarrow R_{21} = \frac{1}{(2a_0)^{\frac{3}{2}}} \frac{r}{\sqrt{3} a_0} e^{-\frac{r}{2a_0}}$$

Expected value

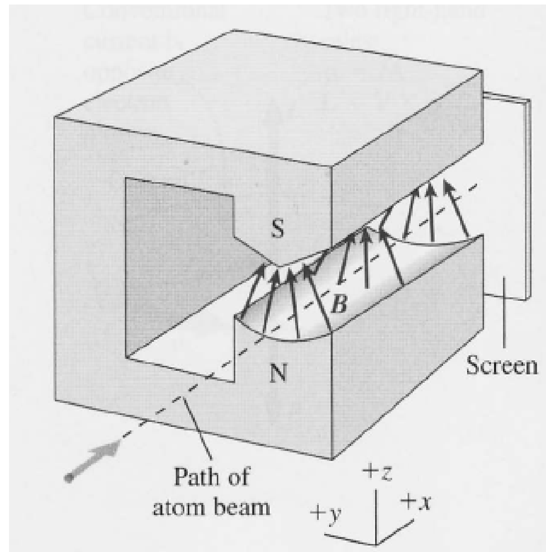
$$\langle r \rangle = \int_0^{\infty} r \cdot r^2 R_{n,l}(r)^2 dr$$

$$\int_0^{\infty} r \cdot r^2 \cdot \frac{1}{(2a_0)^3} \frac{r^2}{3a_0^2} e^{-\frac{r}{a_0}} dr$$

$$\int_0^{\infty} x^m e^{-bx} dr = \frac{m!}{b^{m+1}}$$

$$\frac{1}{3 \cdot 2^3 a_0^5} \int_0^{\infty} r^5 e^{-\frac{r}{a_0}} dr = \frac{1}{3 \cdot 2^3 a_0^5} 5!\, a_0^6 = 5\, a_0$$

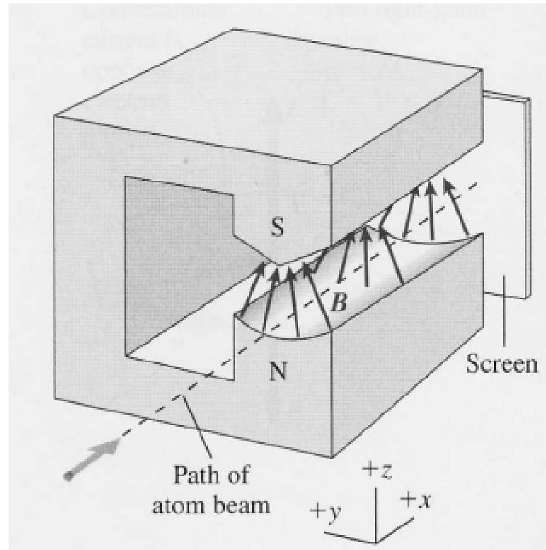
Why not enough?



Why not enough?

$$U = -\vec{\mu} \cdot \vec{B} = \left(\frac{e}{2m}\right) \vec{L} \cdot \vec{B} = \left(\frac{e}{2m}\right) L_z B_z$$

Since $\vec{\mu} = -\left(\frac{e}{2m}\right) \vec{L}$



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$\vec{B} = B_z \hat{z}$ Since $L_z = m_l \hbar$

$$m_l = -l, \dots, +l.$$

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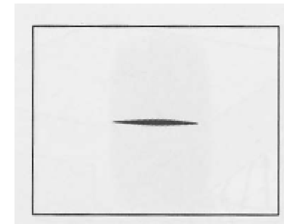

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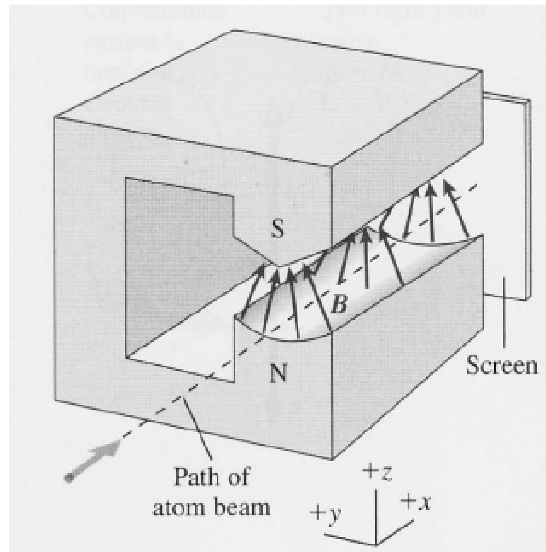

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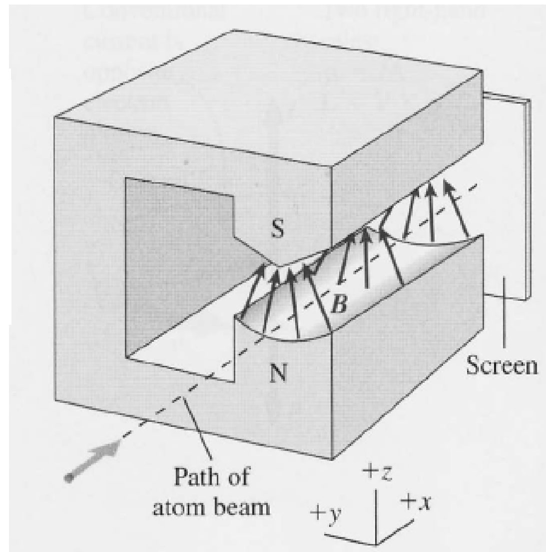

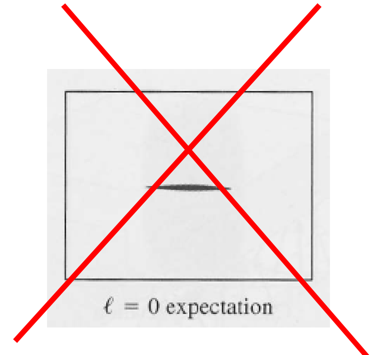

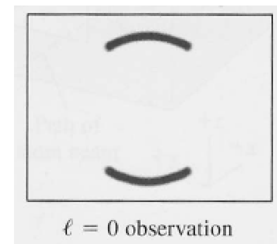

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Since $L_z = m_l \hbar$

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Spin Angular Momentum

- Intrinsic property of a given particle
- Magnitude $|\vec{S}| = \sqrt{s(s+1)}\,\hbar$
- Direction $S_z = m_s \hbar$

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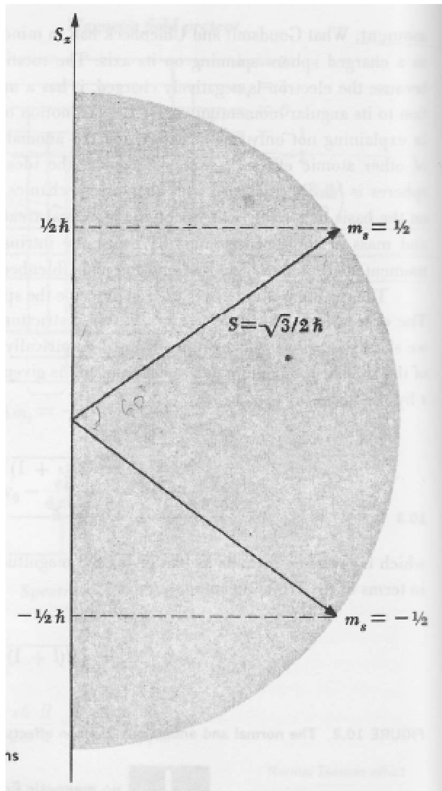
$$m_s = -s, -s+1, \ldots s-1, s$$



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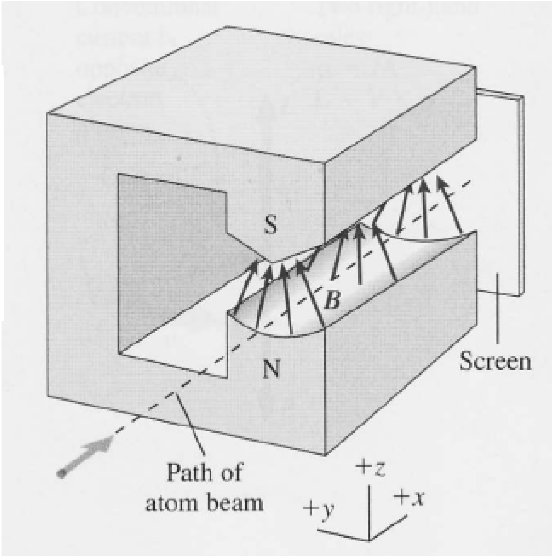
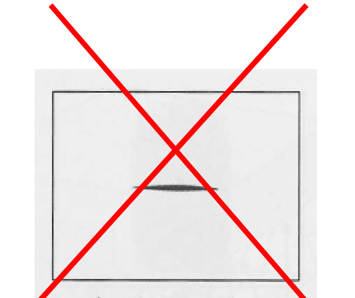
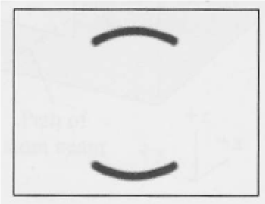
Since $\vec{\mu} = -\left(\frac{e}{2m}\right)\vec{L}$

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





$\ell = 0$ expectation



$\ell = 0$ observation

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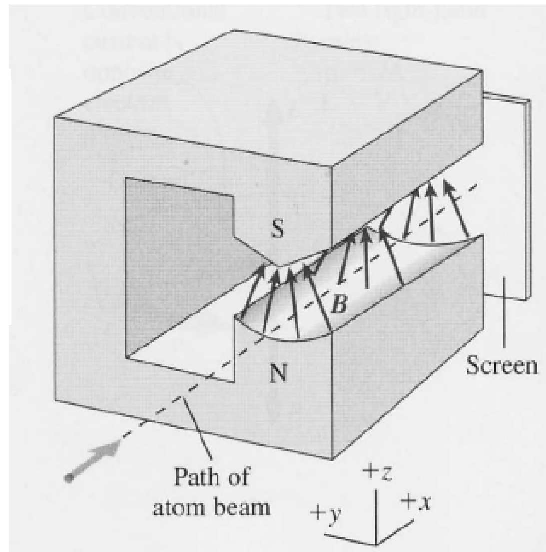

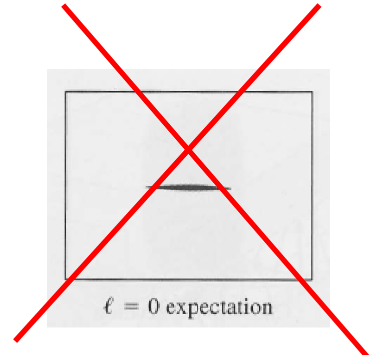

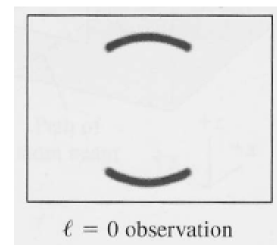

$$F = -\nabla\left(-\vec{\mu} \cdot \vec{B}\right) = -\left(\frac{e}{2m}\right) S_z \frac{\partial B_z}{\partial z}\hat{z} = -\left(\frac{e}{m}\right)(m_s \hbar)\frac{\partial B_z}{\partial z}\hat{z}$$

$$m_s = \pm\frac{1}{2}$$

Two lines! For *l* = 0

Four quantum numbers

- Principal quantum number: *n*

$$E_n = -13.6\ eV\left(\frac{1}{n^2}\right)$$

$$|\vec{L}| = \sqrt{l(l+1)}\hbar$$
$$L_z = m_l\hbar$$

$$|\vec{S}| = \sqrt{s(s+1)}\hbar$$
$$S_z = m_s\hbar$$

- Orbital quantum number: $l = 0, 1, 2, \ldots (n\text{-}1)$
- Magnetic quantum number: $m_l = 0, \pm 1, \pm 2, \ldots \pm l$
- Spin quantum number: $m_s = -s, -s+1, \ldots s-1, s$

Wave functions

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

$$\psi_{n,l,m_l,+\frac{1}{2}} = \psi_{n,l,m_l}(r,\theta,\phi)\uparrow$$

$$\psi_{n,l,m_l,-\frac{1}{2}} = \psi_{n,l,m_l}(r,\theta,\phi)\downarrow$$

- Spin should increase the degeneracy when no magnetic field is present n^2 to $2n^2$
- With the magnetic field, degeneracy can be
- broken due to LS coupling.

Spin-Orbit Interaction

- In a weak external magnetic field, we observe the combined angular momentum

Total Angular Momentum ($\vec{J}$) $\qquad \vec{J} = \vec{L} + \vec{S}$

$$\overrightarrow{|J|} = \sqrt{j(j+1)}\hbar$$
$$J_z = m_j\hbar$$
$$J_z = L_z \pm S_z$$
$$m_j\hbar = m_l\hbar + m_s\hbar$$

$where\ j = |l-s|, |l-s|+1, \ldots |l+s|-1, |l+s|$

where $m_j = -j, -j+1, \ldots, j-1, j$

$$|\vec{J}| = \sqrt{j(j+1)}\hbar \qquad where\ j = |l-s|, |l-s|+1, \ldots |l+s|-1, |l+s|$$

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$$J_z = L_z \pm S_z$$

$$m_j\hbar = m_l\hbar + m_s\hbar$$

$$|\vec{L}| = \sqrt{l(l+1)}\hbar \qquad where\ l = 0, 1, 2, \ldots n-1$$

$$L_z = m_l\hbar \qquad where\ m_l = -l, -l+1, \ldots l-1, l$$

$$|\vec{S}| = \sqrt{s(s+1)}\hbar \qquad where\ s\ is\ a\ number\ intrinsic\ to\ a\ given\ particle$$

$$S_z = m_s\hbar \qquad where\ m_s = -s, -s+1, \ldots s-1, s$$

Exercise *l*=2, *s*=1/2

- In a weak external magnetic field
  - Possible j values
  - Total angular momentum magnitude for each j
  - The number of possible states for each j

$$|\vec{J}| = \sqrt{j(j+1)}\hbar \qquad where\ j = |l-s|, |l-s|+1, \ldots |l+s|-1, |l+s|$$

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Exercise *l*=2, *s*=1/2

- In a weak external magnetic field
  - Possible j values
  - Total angular momentum magnitude for each j
  - The number of possible states for each j

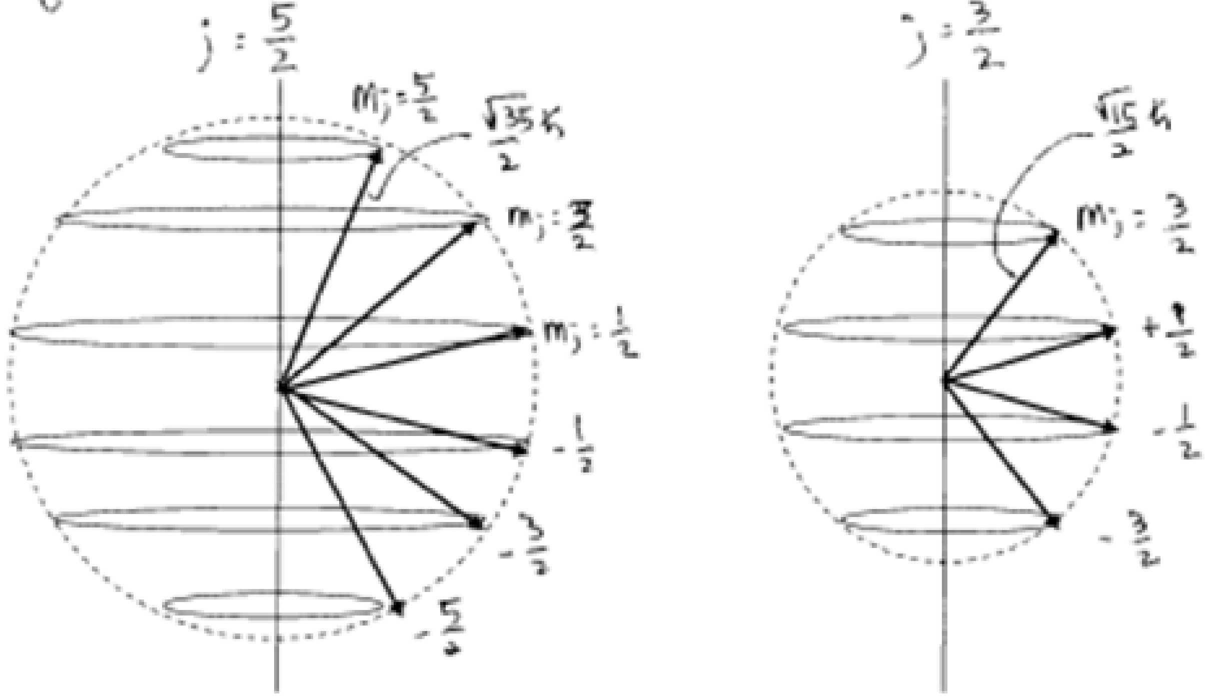
$$\text{for } j = \frac{5}{2} \rightarrow m_j = -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2}, +\frac{5}{2} \quad |\vec{J}| = \sqrt{j(j+1)}\hbar = \sqrt{\frac{5}{2}\frac{7}{2}}\hbar = \frac{\sqrt{35}}{2}\hbar$$

6 possible states (2*j*+1)

$$\text{for } j = \frac{3}{2} \rightarrow m_j = -\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2} \quad |\vec{J}| = \sqrt{j(j+1)}\hbar = \sqrt{\frac{3}{2}\frac{5}{2}}\hbar = \frac{\sqrt{15}}{2}\hbar \rightarrow$$

4 possible states

--L-S coupling --

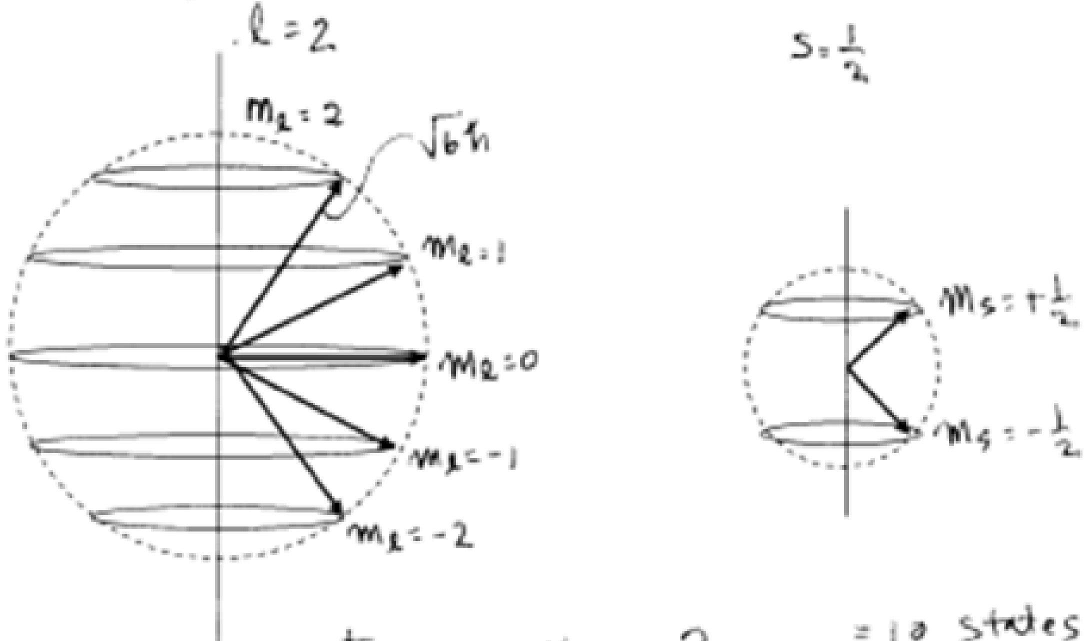


6 + 4 = 10 states

Exercise l=2, s=1/2

- In a strong external magnetic field
  - LS coupling breaks (LS coupling effect is very small)
  - L and S are independently quantized.

- separate -



5 × 2 = 10 states