Spin–Orbit interaction

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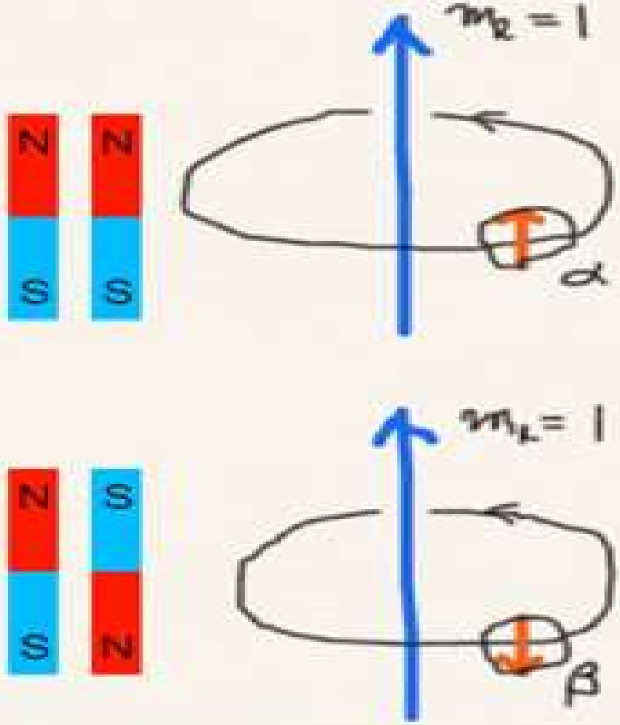
Spin-Orbit interaction

Spin-orbit coupling

- Spin of an electron makes it a magnet. Orbital motion of the electron also makes it a magnet. These two magnetic moments can interact or "couple" (**spin-orbit coupling**) and cause energy level splitting.

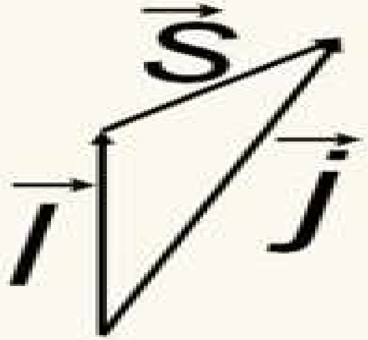


Spin –Orbit interaction

Sum of angular momenta

- Each electron has two angular momenta (a dual magnet): orbital angular momentum and spin angular momentum.
- The total momentum is the most naturally defined as their vector addition.

$$\underset{\text{Total}}{\vec{j}} = \underset{\text{Orbital}}{\vec{l}} + \underset{\text{Spin}}{\vec{s}}$$



Spin –Orbit interaction

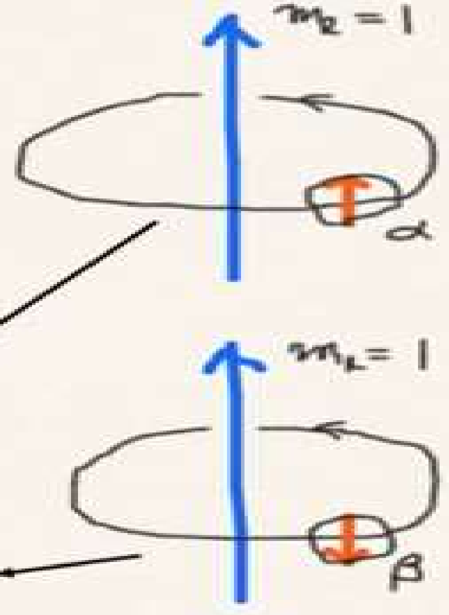
Sum of angular momenta

- $\vec{j}$ must be (space) quantized.
- So its total angular momentum quantum number j is either a full or half integer in the range: $j = j_{min}$ (0 or greater), $j_{min}+1, \ldots, j_{max}-1, j_{max}$

$$\vec{j} = \vec{l} + \vec{s}$$

$$j_{max} = l + s = l + \tfrac{1}{2}$$

$$j_{min} = |l - s| = |l - \tfrac{1}{2}|$$



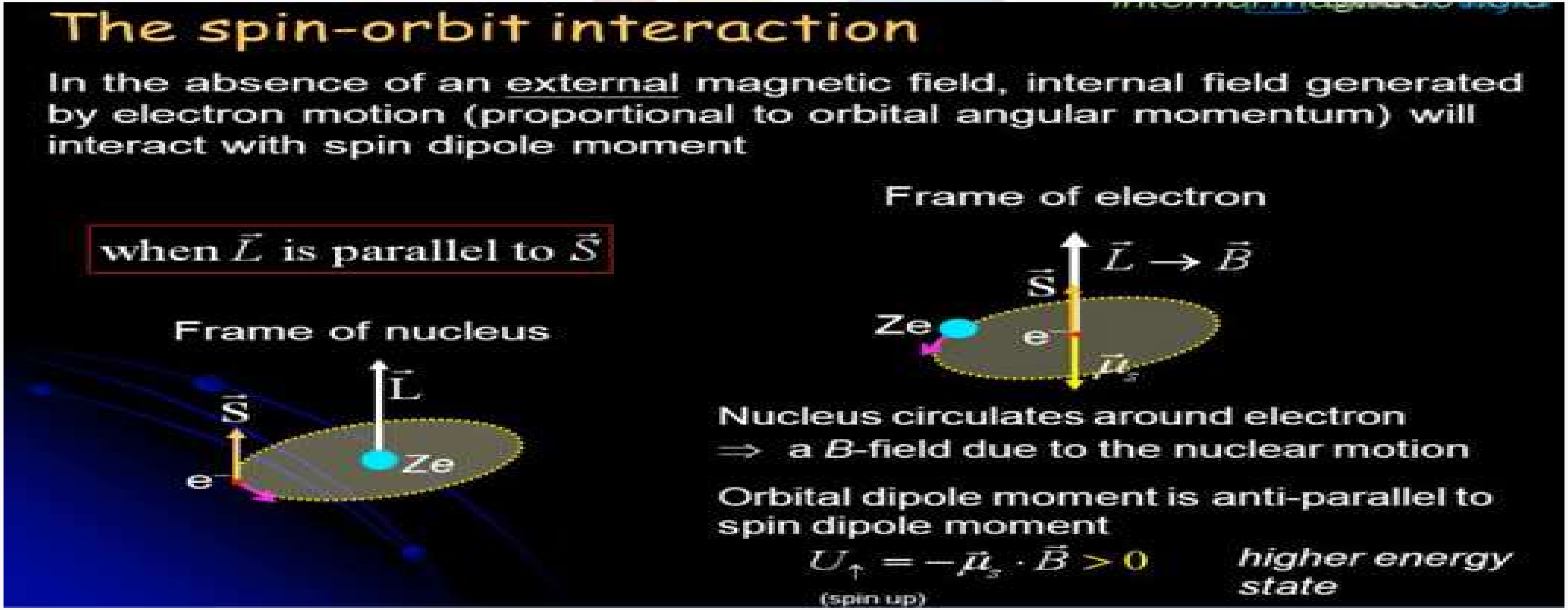
Examples

- Identify the levels that may arise from the configurations (a) $(3p)^1$, (b) $(3s)^1$.

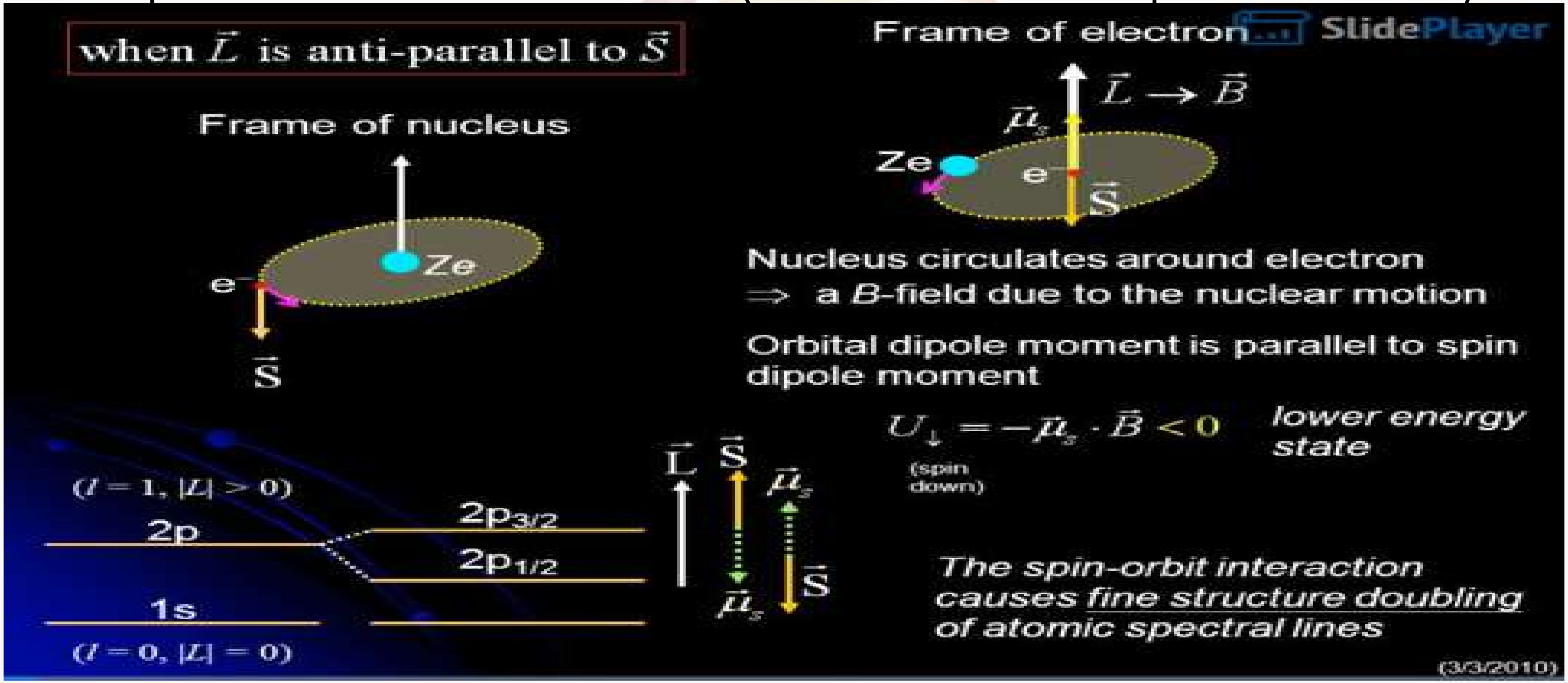
Examples

- (a) $3p$ orbital $\rightarrow l = 1$. $j = l \pm ½ = 3/2$ or $1/2$.
- (b) $3s$ orbital $\rightarrow l = 0$. $j = 0 + ½ = ½$ ($j = 0 - ½$ is not allowed because j is non negative).

Spin – Orbit interaction(When L is parallel to S)



Spin – Orbit interaction(When L is ani-parallel to S)



Total Angular Momentum (J)

Total angular momentum (as a result of spin-orbit interaction)

$\vec{J} = \vec{L} + \vec{S}$ magnitude: $|\vec{J}| = \sqrt{j(j+1)}\hbar$

z-component: $J_z = m_j\hbar \quad m_j = -j, -j+1, \cdots, j-1, j$

Neither $\vec{L}$ nor $\vec{S}$ is conserved separately!

Permissible values for the total angular momentum quantum number j

$$j = l+s, \quad l+s-1, \quad \cdots, \quad |l-s|$$

(maximum value) (minimum value)

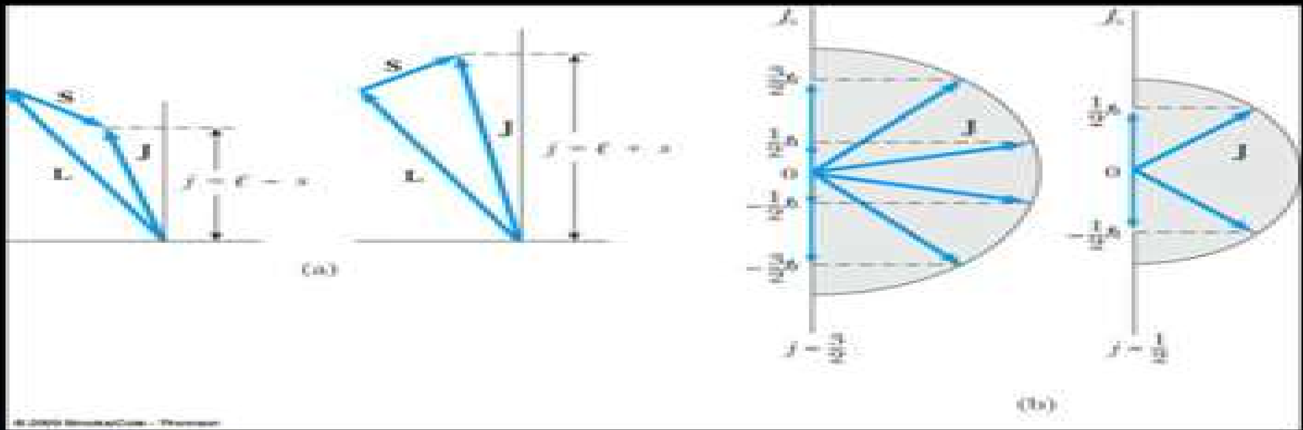
For an atomic electron $s = 1/2$

$$j = l + \frac{1}{2}, \quad l - \frac{1}{2}$$

Example,
for the 2p state $l = 1$, $j = 3/2$ or $1/2$
for the 3d state $l = 2$, $j = 5/2$ or $3/2$
for the s state $l = 0$, $j = 1/2$

Total Angular Momentum (J)

$l = 1$



$j = 1/2 \quad |J| = \frac{\sqrt{3}}{2}\hbar$

$m_j = -\frac{1}{2}, +\frac{1}{2}$

$j = 3/2 \quad |J| = \frac{\sqrt{15}}{2}\hbar$

$m_j = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

m_j has an even number of values

(a) A vector model for determining the total angular momentum $J = L + S$ of a single electron

(b) The allowed orientations of the total angular momentum J for the states $j = 3/2$ and $j = 1/2$. Notice that there are now an even number of orientations possible, not the odd number familiar from the space quantization of L alone

Energy Shift Due to spin-orbit interaction

Energy shift due to spin-orbit interaction

$$U_{LS} = -\vec{\mu}_s \cdot \vec{B}_{\text{internal}}$$

$$\vec{B}_{\text{internal}} = ?$$

Square of total angular momentum

$$\vec{J}^2 = (\vec{L}+\vec{S})^2 = (\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S})$$
$$= \vec{L}^2 + \vec{S}^2 + 2\vec{L}\cdot\vec{S} \quad \Rightarrow \quad \vec{L}\cdot\vec{S} = \frac{\vec{J}^2 - \vec{L}^2 - \vec{S}^2}{2}$$

Spin-orbit interaction energy (a relativistic effect):

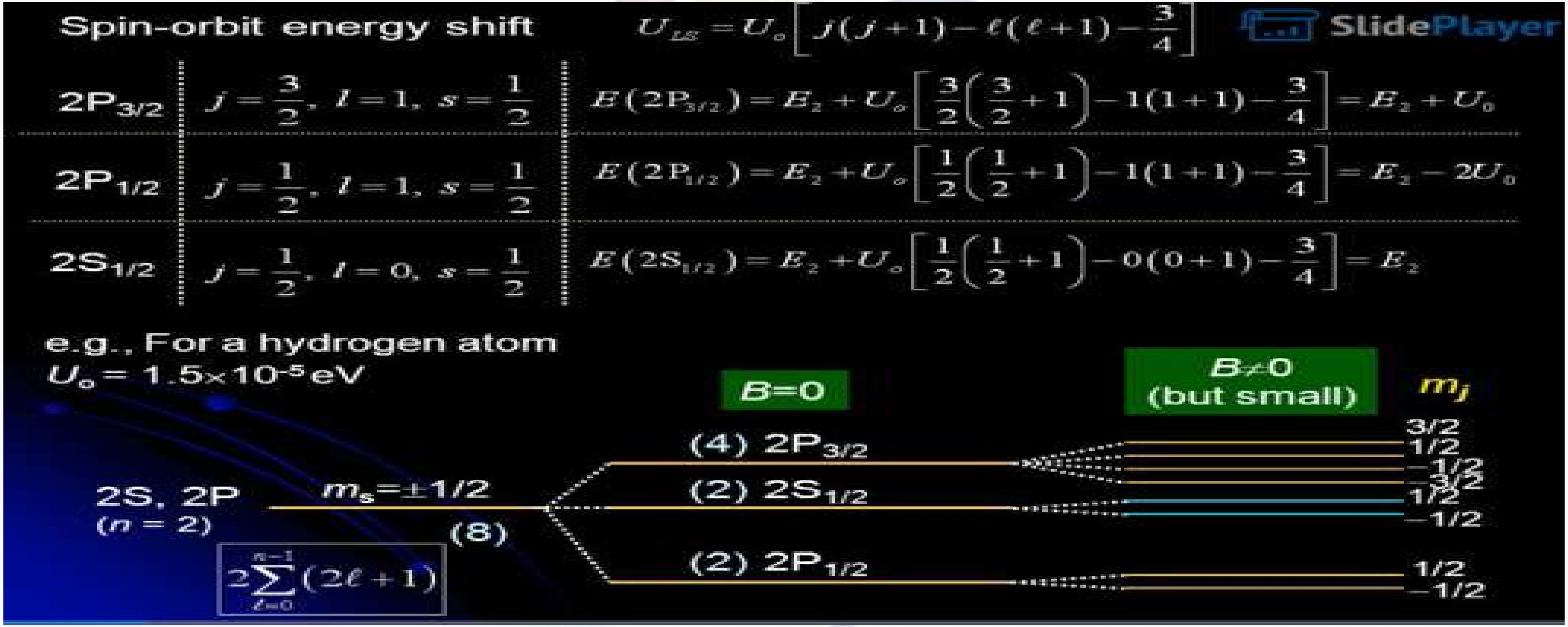
$$U_{LS} = \frac{Ze^2}{4\pi\varepsilon_o}\frac{g_e}{2}\frac{1}{4m_e^2c^2r^3}(\vec{L}\cdot\vec{S})$$

r: radius of the orbiting electron
c: speed of light

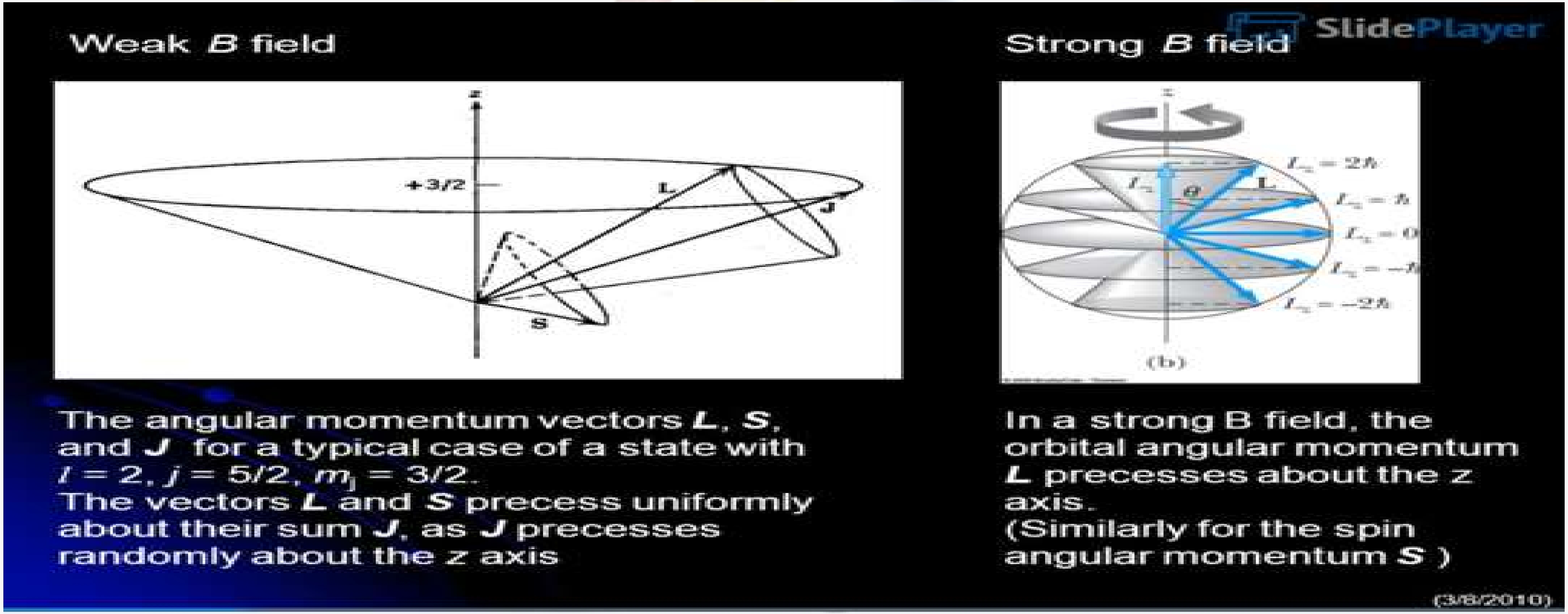
$$U_{LS} \propto \vec{L}\cdot\vec{S} = \frac{\hbar^2}{2}[j(j+1) - \ell(\ell+1) - s(s+1)]$$

Write $U_{LS} = U_o\left[j(j+1) - \ell(\ell+1) - \frac{3}{4}\right]$

Spin- Orbit energy Shift



Effect of Magnetic Fields (Weak and Strong Field)



Remarks

Remarks:

In a small external *B* field, the **spin-orbit interaction** is dominant and the total angular momentum ***J*** as a whole precesses around the *B* field. The no. of split lines = the no. of m_j values

In a large external *B* field, both the orbital angular momentum ***L*** and the spin angular momentum ***S*** precess **independently** around the *B* field. The no. of splitting lines = $2 \times (2l + 1)$

Quantum numbers – in the absence of spin-orbit effect, a state of an atomic electron is specified by (n, l, m_l, m_s). If the spin-orbit interaction is taken into account, the state may be specified by (n, l, j, m_j)

$2P_{3/2}$, $2P_{1/2}$, $2S_{1/2}$

Example

Example: electronic states associated with the principle quantum number $n = 2$

(n, l, m_l, m_s)

$\left(2,0,0,\frac{1}{2}\right), \left(2,0,0,-\frac{1}{2}\right)$

$\left(2,1,0,\frac{1}{2}\right), \left(2,1,0,-\frac{1}{2}\right)$

$\left(2,1,1,\frac{1}{2}\right), \left(2,1,1,-\frac{1}{2}\right)$

$\left(2,1,-1,\frac{1}{2}\right), \left(2,1,-1,-\frac{1}{2}\right)$

(in the absence of spin-orbit interaction)

(n, l, j, m_j)

$\left(2,0,\frac{1}{2},\frac{1}{2}\right), \left(2,0,\frac{1}{2},-\frac{1}{2}\right)$

$\left(2,1,\frac{3}{2},\frac{3}{2}\right), \left(2,1,\frac{3}{2},\frac{1}{2}\right)$

$\left(2,1,\frac{3}{2},-\frac{1}{2}\right), \left(2,1,\frac{3}{2},-\frac{3}{2}\right)$

$\left(2,1,\frac{1}{2},\frac{1}{2}\right), \left(2,1,\frac{1}{2},-\frac{1}{2}\right)$

(in the presence of spin-orbit interaction)

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