

# Spin–Orbit interaction

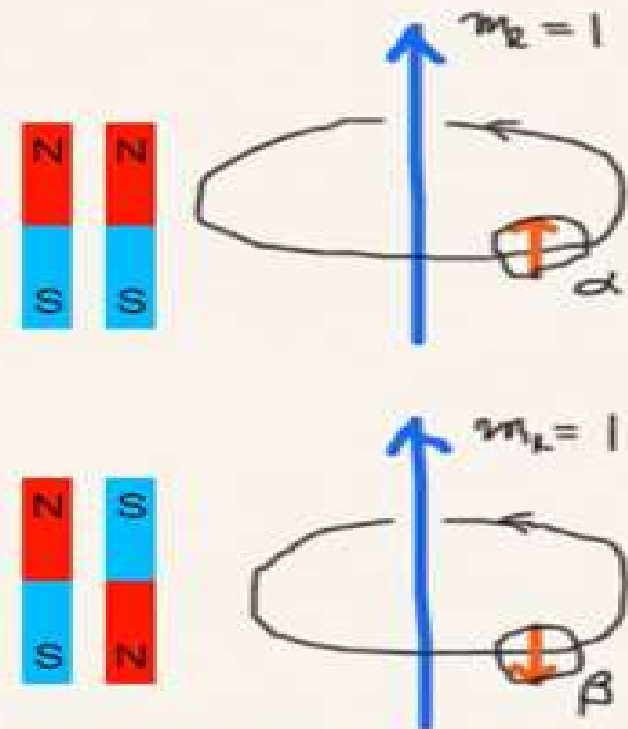
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# Spin-Orbit interaction

## 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.



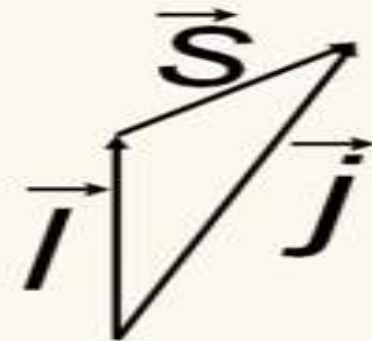
# Spin –Orbit interaction

## 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.

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

Total                  Orbital                  Spin



# Spin –Orbit interaction

## Sum of angular momenta

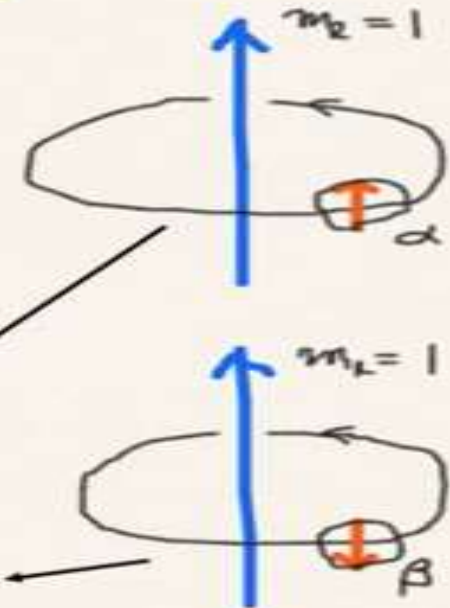
- $\vec{J}$  must be (space) quantized.
- So its total angular momentum quantum number  $j$  is either a full or half integer in the range:

$$j = j_{\min} (0 \text{ or greater}), j_{\min} + 1, \dots, j_{\max} - 1, j_{\max}$$

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

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

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

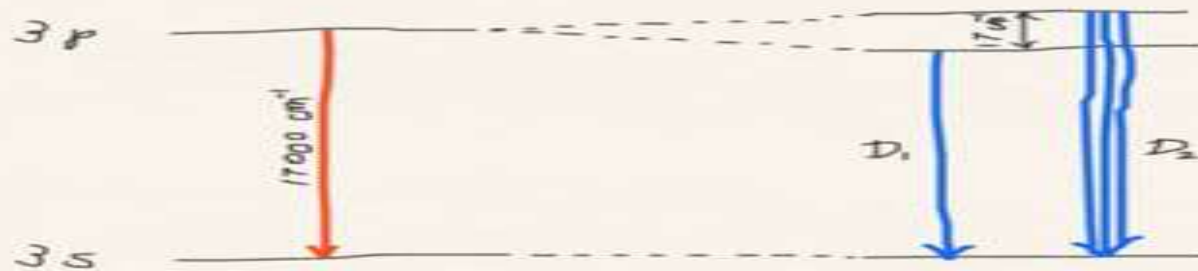


## Examples

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

### Examples

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



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

**The spin-orbit interaction**

In the absence of an external magnetic field, internal field generated by electron motion (proportional to orbital angular momentum) will interact with spin dipole moment

when  $\vec{L}$  is parallel to  $\vec{S}$

**Frame of nucleus**

**Frame of electron**

Nucleus circulates around electron  
 $\Rightarrow$  a  $B$ -field due to the nuclear motion

Orbital dipole moment is anti-parallel to spin dipole moment

$$U_{\uparrow} = -\vec{\mu}_s \cdot \vec{B} > 0$$
(spin up) *higher energy state*

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

when  $\vec{L}$  is anti-parallel to  $\vec{S}$

Frame of nucleus

Frame of electron

Nucleus circulates around electron  
 $\Rightarrow$  a  $B$ -field due to the nuclear motion

Orbital dipole moment is parallel to spin dipole moment

$$U_{\downarrow} = -\vec{\mu}_s \cdot \vec{B} < 0$$

(spin down)

lower energy state

The spin-orbit interaction causes fine structure doubling of atomic spectral lines

(3/3/2010)

# Total Angular Momentum (J)

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

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

$$\text{z-component: } J_z = m_j \hbar \quad m_j = -j, -j+1, \dots, j-1, j$$

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

Permissible values for the total angular momentum quantum number  $j$

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

(maximum value) (minimum value)

For an atomic electron  $s = 1/2$


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

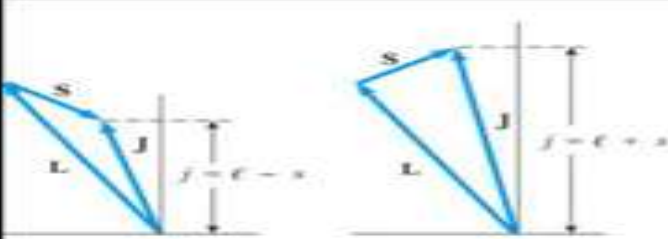
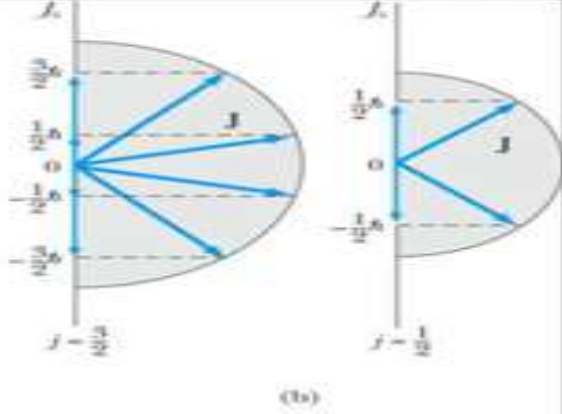
Example,

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)



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

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

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

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

**$m_j$  has an even number of values**

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

(b) The allowed orientations of the total angular momentum  $\mathbf{J}$  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  $\mathbf{L}$  alone

## Energy Shift Due to spin-orbit interaction

Energy shift due to spin-orbit interaction

$$U_{LS} = \mu_B \vec{L} \cdot \vec{B}_{\text{internal}}$$

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

Square of total angular momentum

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

Spin-orbit interaction energy (a relativistic effect):

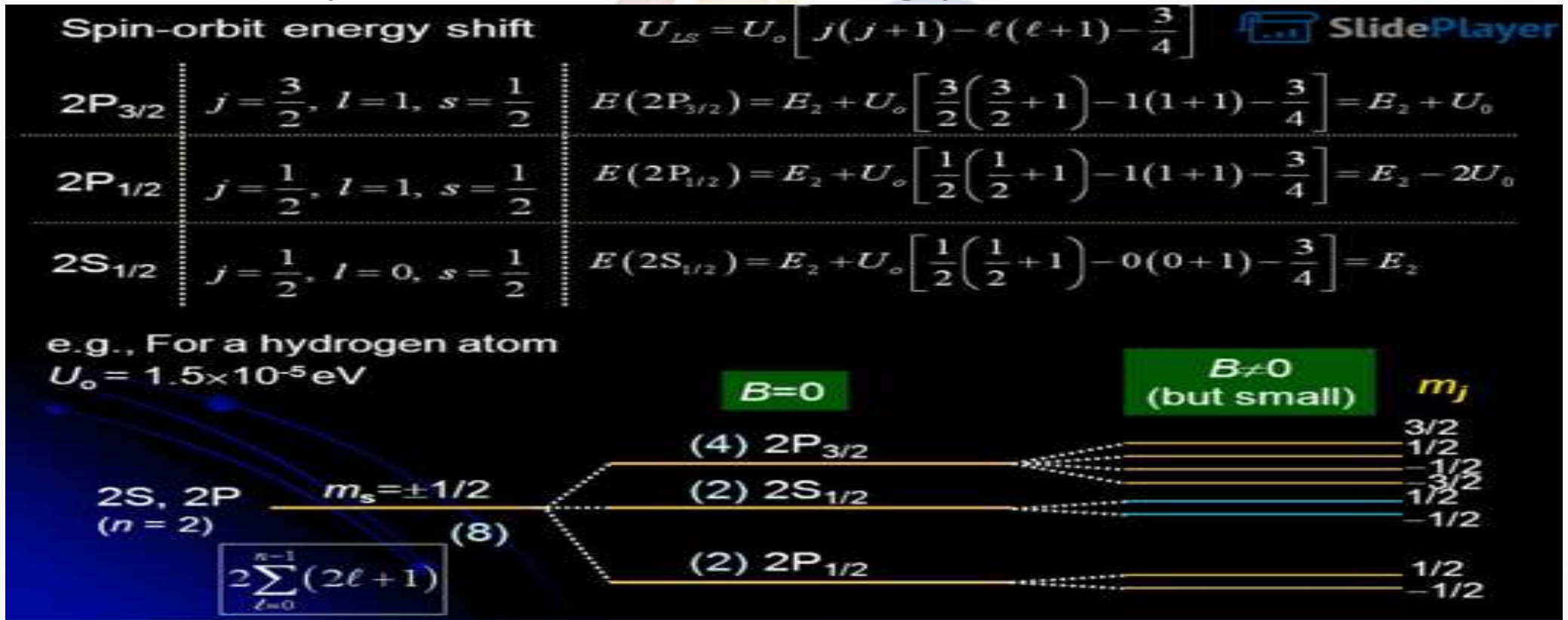
$$U_{LS} = \frac{Ze^2}{4\pi\epsilon_0} \frac{g_e}{2} \frac{1}{4m_e^2 c^2 r^3} (\vec{L} \cdot \vec{S})$$

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

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

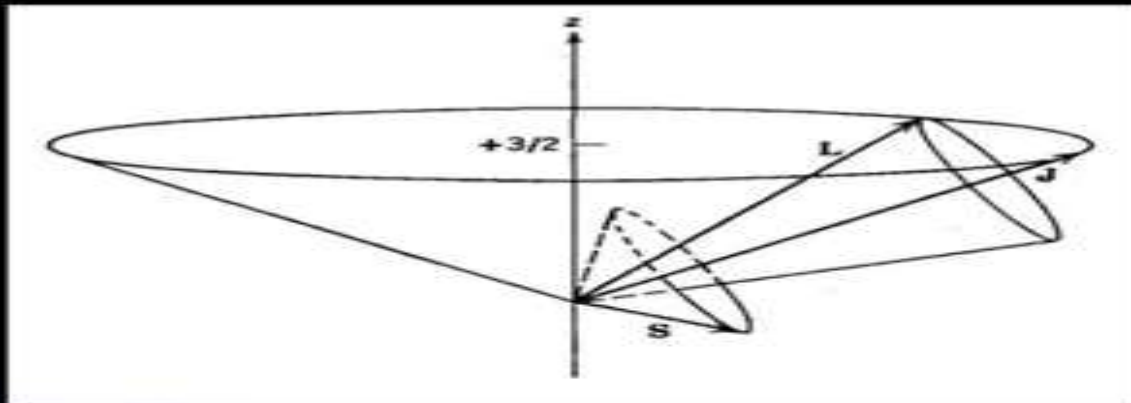
Write  $U_{LS} = U_o \left[ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right]$

# Spin-Orbit energy Shift



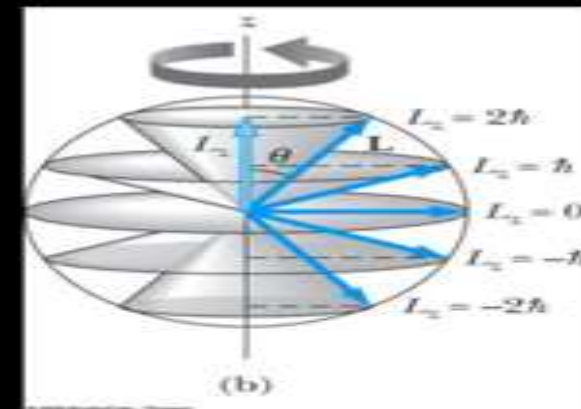
## Effect of Magnetic Fields ( Weak and Strong Field)

Weak  $B$  field



The angular momentum vectors  $L$ ,  $S$ , and  $J$  for a typical case of a state with  $l = 2$ ,  $j = 5/2$ ,  $m_j = 3/2$ . The vectors  $L$  and  $S$  precess uniformly about their sum  $J$ , as  $J$  precesses randomly about the  $z$  axis

Strong  $B$  field



In a strong  $B$  field, the orbital angular momentum  $L$  precesses about the  $z$  axis. (Similarly for the spin angular momentum  $S$ )

(3/8/2010)

# Remarks

SlidePlayer

## Remarks:

In a small external  $B$  field, the **spin-orbit interaction** is dominant and the total angular momentum  $\mathbf{J}$  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  $\mathbf{L}$  and the spin angular momentum  $\mathbf{S}$  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  $n = 2$

$(n, l, m_l, m_s)$

$$\begin{aligned} & \left(2, 0, 0, \frac{1}{2}\right), \left(2, 0, 0, -\frac{1}{2}\right) \\ & \left(2, 1, 0, \frac{1}{2}\right), \left(2, 1, 0, -\frac{1}{2}\right) \\ & \left(2, 1, 1, \frac{1}{2}\right), \left(2, 1, 1, -\frac{1}{2}\right) \\ & \left(2, 1, -1, \frac{1}{2}\right), \left(2, 1, -1, -\frac{1}{2}\right) \end{aligned}$$

(in the absence of spin-orbit interaction)

$(n, l, j, m_j)$

$$\begin{aligned} & \left(2, 0, \frac{1}{2}, \frac{1}{2}\right), \left(2, 0, \frac{1}{2}, -\frac{1}{2}\right) \\ & \left(2, 1, \frac{3}{2}, \frac{3}{2}\right), \left(2, 1, \frac{3}{2}, \frac{1}{2}\right) \\ & \left(2, 1, \frac{3}{2}, -\frac{1}{2}\right), \left(2, 1, \frac{3}{2}, -\frac{3}{2}\right) \\ & \left(2, 1, \frac{1}{2}, \frac{1}{2}\right), \left(2, 1, \frac{1}{2}, -\frac{1}{2}\right) \end{aligned}$$

(in the presence of spin-orbit interaction)

# School of Basic and Applied Science

Course Code :MSCP 6002

Course Name: ATOMIC AND MOLECULAR PHYSICS

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