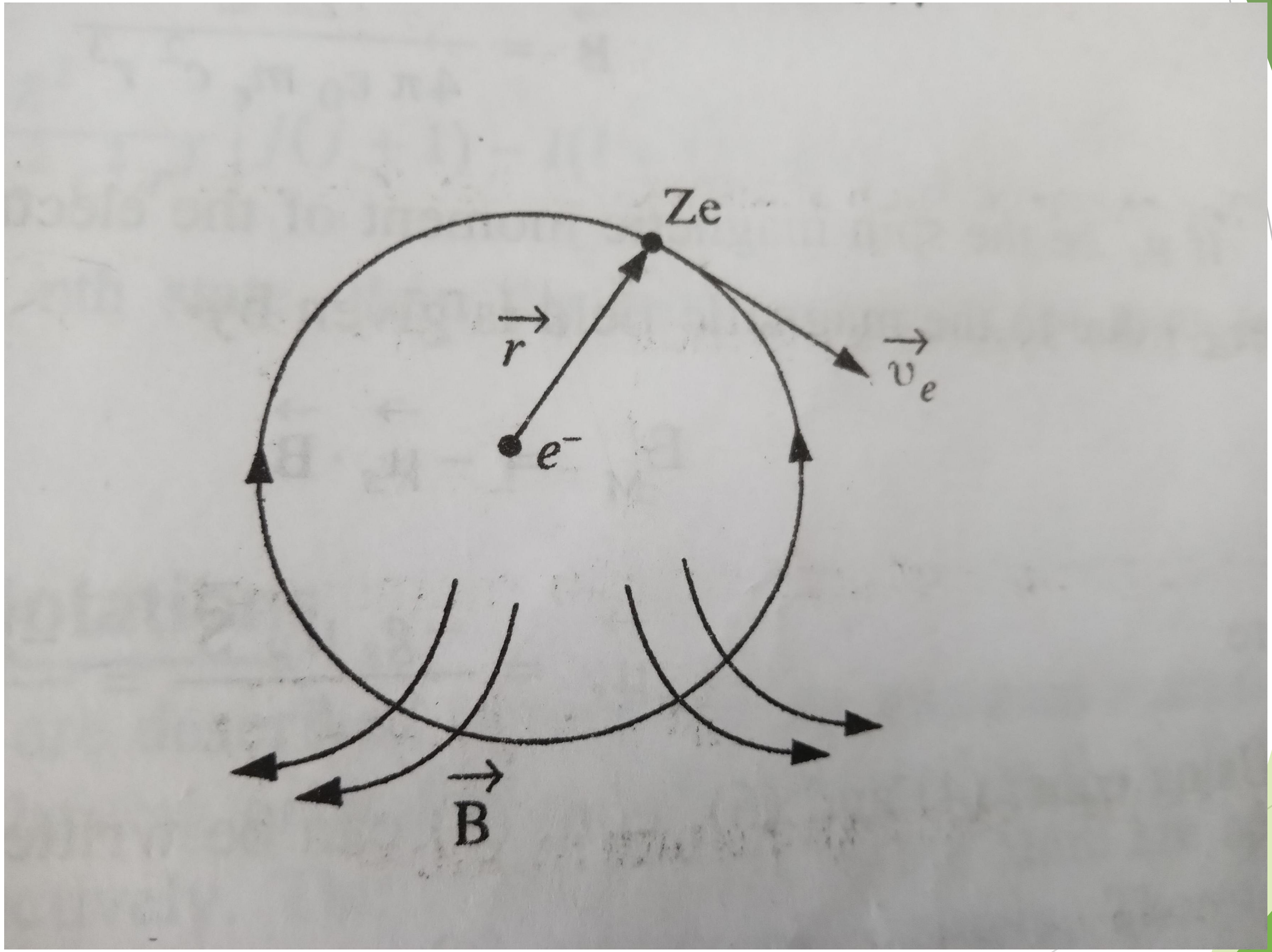
Spin orbit coupling

Definition

- The electron in an atom has angular momenta associated with it’s orbital motion and spin motion. The orbital motion of the electron give rise to an internal magnetic field.
- The spin magnetic moment of the electron interact with this internal magnetic field which leads to the modification of the energy level of atom.
- In fact this interaction is between the orbital magnetic moment and the spin magnetic moment and hence is called spin orbit coupling.

Derivation

- Suppose an electron is moving in a circular orbit of radius r around the nucleus with a speed 've. Since the motion is relative therefore we can consider that the nucleus is moving in a circular orbit of radius r around the fixed electron, but in a direction opposite to that of the electron with the same speed. The motion of nucleus in a circular orbit is equivalent to the flow of current in a circular loop of radius r.


Ze
$\vec{r}$
$\vec{v}_e$
e^-
$\vec{B}$

The magnetic field due to such a current loop at its centre is given by

$$B = \frac{\mu_0 I}{2r}$$

But

$$I = \frac{Ze}{T}$$

Where

$$T = \frac{\text{Circumference of the orbit}}{\text{Speed of the nucleus}} = \frac{2\pi r}{v_e}$$

∴

$$I = \frac{Ze v_e}{2\pi r}$$

Hence

$$B = \frac{\mu_0 Zev_e}{4\pi r^2}$$

Eqn. (2) can also be written as

$$B = \frac{\mu_0 Ze}{4\pi r^2}\frac{(\vec{r}\times\vec{v}_e)}{r^3} = \frac{\mu_0 Ze(\vec{r}\times m_e\vec{v}_e)}{4\pi m_e r^3}$$

Since $\vec{r}\times m_e\vec{v}_e = \vec{r}\times\vec{p} = \vec{L}$

∴

$$\vec{B} = \frac{\mu_0 Ze\vec{L}}{4\pi m_e r^3}$$

Now $\mu_0\varepsilon_0 = \frac{1}{c^2}$, where $c = 3\times10^8$ m s^{-1} is the speed of light in vacuu

or

$$\mu_0 = \frac{1}{\varepsilon_0 c^2}$$

∴

$$\vec{B} = \frac{Ze\vec{L}}{4\pi\varepsilon_0 m_e c^2 r^3}$$

If $\vec{\mu}_s$ be the spin magnetic moment of the electron, then the interaction energy (*i.e.*, poten energy) due to the magnetic field is given by

$$E'_M = -\vec{\mu}_s\cdot\vec{B}$$

where

$$\vec{\mu}_s = \frac{-g_s\mu_B\vec{S}}{\hbar} = \frac{-2\mu_B\vec{S}}{\hbar} \quad (\because g_s = 2)$$

Using eqns. (4) and (6), eqn. (5) can be written as

$$E'_M = \frac{2\mu_B}{\hbar}\times\frac{Ze}{4\pi\varepsilon_0 m_e c^2 r^3}\vec{S}\cdot\vec{L}$$

$|\vec{a}\times\vec{b}| = |\vec{a}||\vec{b}| \sin\theta$ sin 90°

$|r\times v_e|$ = r ve

$\therefore$

$$\vec{B} = \frac{Ze\,\vec{L}}{4\pi\,\varepsilon_0\, m_e\, c^2\, r^3} \qquad \ldots(4)$$

If $\vec{\mu}_s$ be the spin magnetic moment of the electron, then the interaction energy (*i.e.*, potential energy) due to the magnetic field is given by

$$E'_M = -\vec{\mu}_s \cdot \vec{B} \qquad \ldots(5)$$

where

$$\vec{\mu}_s = \frac{-g_s\, \mu_B\, \vec{S}}{\hbar} = \frac{-2\, \mu_B\, \vec{S}}{\hbar} \qquad (\because g_s = 2) \ \ldots(6)$$

Using eqns. (4) and (6), eqn. (5) can be written as

$$E'_M = \frac{2\,\mu_B}{\hbar} \times \frac{Ze}{4\pi\,\varepsilon_0\, m_e\, c^2\, r^3}\, \vec{S}\cdot\vec{L} \qquad \ldots(7)$$

Put $\mu_B = \frac{e\hbar}{2m_e}$ or $\frac{2\mu_B}{\hbar} = \frac{e}{m_e}$ in eqn. (7), we get

$$E'_M = \frac{Ze^2}{4\pi\varepsilon_0 m_e^2 c^2 r^3}\vec{S}\cdot\vec{L} \quad ...(8)$$

This is the energy in a frame of reference in which the electron is at rest. On relativistic transformation to the normal frame of reference, where nucleus is at rest, the energy is reduced by a factor 2. This is known as **Thomas precession.** Thus, spin-orbit interaction energy comes

$$E_M = \frac{1}{2}E'_M = \frac{Ze^2}{8\pi\varepsilon_0 m_e{}^2 c^3 r^3}\vec{S}\cdot\vec{L} \quad ...(9)$$

Now, we know $\vec{J} = \vec{L} + \vec{S}$

$\therefore$ $\vec{J}\cdot\vec{J} = (\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S}) = L^2 + \vec{L}\cdot\vec{S} + \vec{S}\cdot\vec{L} + S^2$

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

$$\therefore \quad \vec{S}\cdot\vec{L} = \frac{J^2 - L^2 - S^2}{2} \quad ...(10)$$

Since

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

$$L = \sqrt{l(l+1)}\,\hbar$$

$$S = \sqrt{s(s+1)}\,\hbar$$

$$\therefore \quad \vec{S}\cdot\vec{L} = \frac{[j(j+1) - l(l+1) - s(s+1)]\hbar^2}{2}$$

Hence, eqn. (9) becomes

$$E_M = \frac{Ze^2\hbar^2}{16\pi\varepsilon_0 m_e{}^2 c^2 r^3}[j(j+1) - l(l+1) - s(s+1)] \quad ...(11)$$

If E_n be the energy of the atom in the nth state, than the total energy of the atom in the presence of spin-orbit coupling is given by

$$E = E_n + E_M \quad ...(12)$$

Thank you