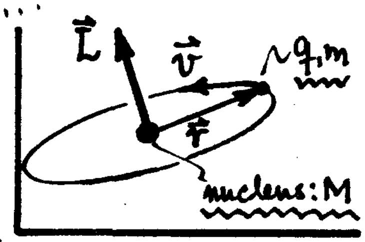
Magnetic Interactions in Atoms: Some Simple Facts

$\int$ no specific reference in Davydov or Sakurai

1) Classically, a circulating charge (or current loop) generates a magnetic field, conveniently described in terms of a "magnetic moment" μ, as...

$$\mu = (\text{current}) \times (\text{loop area}) = \left(\frac{q}{c} \Big/ \frac{2\pi r}{v}\right) \cdot \pi r^2 = \frac{q}{2mc}(mvr),$$



$$\xrightarrow{\text{or}} \vec{\mu} = \gamma \vec{L} \begin{cases} \gamma = q/2mc, \text{ called "gyromagnetic ratio"}, \\ \vec{L} = \vec{r} \times m\vec{v} = \text{orbital } \measuredangle \text{ momentum}. \end{cases} \quad (1)$$

For atomic systems, the charge $q = (-)e$, and $\vec{L}$ is measured in units of $\hbar$. For an electron $(-e, m_e)$ orbiting a nucleus of mass $M \gg m_e$...

$$L = r \cdot mv, \text{ w/ } m \rightarrow \mu = \frac{m_e M}{m_e + M} \simeq \left(1 - \frac{m_e}{M}\right) m_e \leftarrow \text{reduced mass correction}$$

Soy $L \rightarrow \left(1 - \frac{m_e}{M}\right) L$, and the electron orbital magnetic moment is:

$$\rightarrow \underline{\underline{\vec{\mu}_L}} = (-)\frac{e\hbar}{2m_e c}\left(1 - \frac{m_e}{M}\right)\frac{\vec{L}}{\hbar} = \underline{\underline{(-) g_L \mu_0 \vec{L}/\hbar}}, \quad (2)$$

where: $\mu_0 = e\hbar/2m_e c$, is the Bohr magneton $\int \mu_0 = 9.27 \times 10^{-21} \frac{\text{erg}}{\text{Gs}}$, $\mu_0/h = 1.40$ MHz/Gs;

and: $g_L = 1 - \frac{m_e}{M}$, is the orbital g-value.

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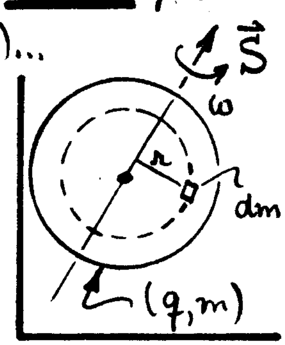
2) A spinning charge also generates a magnetic moment, and a relation similar to Eq. (2) exists between the spin $\measuredangle$ momentum $\vec{S}$ and the spin magnetic moment $\vec{\mu}_S$. This relation appears to be independent of charge structure (if any)...

$$\left.\begin{array}{l} \text{Spin } \measuredangle \text{ momentum: } S = \omega \int r^2 dm; \\ \text{Spin mag. moment: } \mu_S = \int \pi r^2 di, \quad di = \text{current element}. \end{array}\right\} \quad (3)$$



But: $di = \frac{dq}{c} \Big/ \frac{2\pi}{\omega}$, and: $dq = q\frac{dm}{m}$ (seems reasonable), so...

$$\mu_S = \int \pi r^2 \left(\frac{1}{c} q \frac{dm}{m} \Big/ \frac{2\pi}{\omega}\right) = \frac{q}{2mc}\omega \int r^2 dm = \gamma S \quad \int \text{same } \gamma \text{ as in Eq. (1)}. \quad (4)$$

$\vec{\mu}$: Simple Facts

For an electron, by analogy with the orbital moment $\vec{\mu}_L$ in Eq. (2), we write...

$$\underline{\vec{\mu}_S = -g_s \mu_0 \vec{S}/\hbar} \text{ ; spin magnetic moment ; } \mu_0 = \text{above Bohr magneton.} \tag{5}$$

$S/\hbar = \frac{1}{2}$ for electrons. g_s can be measured exptly... and provides a surprise...

$$\rightarrow g_s = \underset{\uparrow \text{ 2x orbital g-value!}}{\underline{2}} \cdot \left(1 + \frac{\alpha}{2\pi} + O(\alpha^2) + \ldots\right) \tag{6}$$

the factor 2 can be explained by Dirac theory. The $\alpha/2\pi \simeq 1/10^3$ and higher corrections require QED (quantized fields) for their explanation.

For a proton, the "natural" magneton (scale moment) is a nuclear magneton...

$$\mu_0 = e\hbar/2m_e c \longrightarrow \mu_N = e\hbar/2m_p c = \left(\frac{m_e}{m_p}\right)\mu_0 \tag{7}$$

m_e = electron mass, m_p = proton mass.

μ_N is 1/1836.11 as large as μ_0. But we still write--in analogy w/ Eqs. (2) & (5):

$$\underline{\vec{\mu}_p = -g_p \mu_0 \vec{I}/\hbar} \text{ ; proton spin mag. moment ; } \mu_0 = \text{above Bohr magneton ;} \tag{8}$$

w/ $\vec{I}$ = proton spin ($I/\hbar = \frac{1}{2}$),

&/ $g_p = (-)\, 2 \times 2.79 \times \dfrac{m_e}{m_p} = -3.04 \times 10^{-3}$, proton g-value.

↑ nobody knows how to calculate this anomalous factor!

Note the (−) sign in g_p... the proton charge is $+|e|$, so $\vec{\mu}_p$ & $\vec{I}$ are ∥ (not anti-∥).

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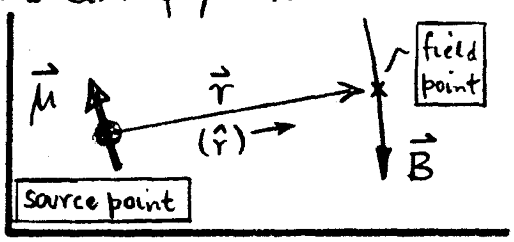
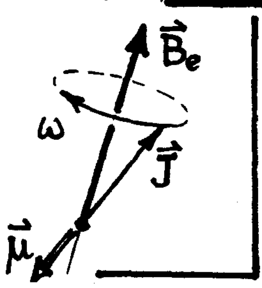
3) Three simple facts carry over from classical EM to the QM of $\vec{\mu}$'s...

A. $\vec{\mu}$ generates a magnetic dipole field:

$$\vec{B} = \frac{1}{r^3}\left[3(\vec{\mu}\cdot\hat{r})\hat{r} - \vec{\mu}\right], \quad \hat{r} = \frac{\vec{r}}{r}. \tag{9}$$



B. $\vec{\mu}$ precesses in an external magnetic field $\vec{B}_e$...



Let: $\vec{\mu} = \gamma \vec{J}$, $\gamma = -g(\mu_0/\hbar)$ for atoms. Then...

TORQUE on $\vec{\mu}$ due to ext'l $\vec{B}_e$ $\Big\}$
$$\frac{d\vec{J}}{dt} = \vec{\mu} \times \vec{B}_e = \gamma \vec{J} \times \vec{B}_e. \tag{10}$$

$\vec{\mu}$: Simple Facts

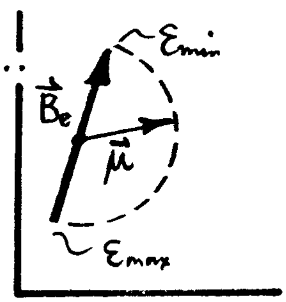
Let $\vec{B}_e$ be along the z-axis. Then the eqtn-of-motion for $\vec{J}$, Eq. (10), is...

$$\rightarrow \begin{pmatrix} \dot{J}_x \\ \dot{J}_y \end{pmatrix} = \gamma B_e \begin{pmatrix} J_y \\ -J_x \end{pmatrix} \Rightarrow \text{can be written: } \dot{J}_x + i\dot{J}_y = \gamma B_e (J_y - iJ_x),$$

or// $\dot{J}_+ = -i\gamma B_e J_+$, w/ $J_+ = J_x + iJ_y$; So// $\underline{\underline{J_+(t) = J_+(0)\, e^{-i\omega t}}}$, (11)

Where $\boxed{\omega = \gamma B_e = -g(\mu_0/\hbar)B_e}$ is the "Larmor precession frequency." The motion of $\vec{J}$, and hence $\vec{\mu}$, is a rapid rotation about the direction of $\vec{B}_e$.

C. $\vec{\mu}$ has an orientation-dependent energy in an external $\vec{B}_e$...



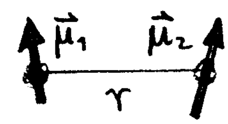
$$\underline{\underline{\mathcal{E} = -\vec{\mu}\cdot\vec{B}_e}} \quad \begin{cases} \text{min. for } \vec{\mu} \parallel \vec{B}_e, \\ \text{max. for anti-}\parallel. \end{cases} \tag{12}$$

This energy characterizes dipole-dipole coupling in an atom. If you have two magnetic dipole moments...

$$\rightarrow \vec{\mu}_1 = -g_1 \mu_0 \vec{J}_1, \quad \vec{\mu}_2 = -g_2 \mu_0 \vec{J}_2 \quad (\vec{J}_1 \,\&\, \vec{J}_2 \text{ are in units of } \hbar);$$

then// $\mathcal{E} = -\vec{\mu}_1 \cdot \vec{B}_2$, with: $\vec{B}_2 = \frac{1}{r^3}\left[3(\vec{\mu}_2\cdot\hat{r})\hat{r} - \vec{\mu}_2\right]$,

So// $$\boxed{\mathcal{E} = g_1 g_2 \frac{\mu_0^2}{r^3}\left[\vec{J}_1\cdot\vec{J}_2 - 3(\vec{J}_1\cdot\hat{r})(\vec{J}_2\cdot\hat{r})\right]}. \tag{13}$$

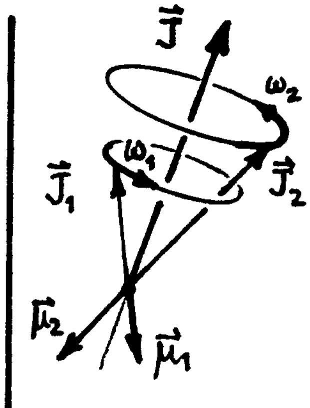


this term averages to zero, by mutual precession.

$\boxed{\text{NOTE}}$ Dipole-dipole coupling provides a mechanism by which two ∡ momenta $\vec{J}_1$ & $\vec{J}_2$ precess about their resultant $\vec{J} = \vec{J}_1 + \vec{J}_2$, as claimed in Vector Model.

$$\left.\begin{matrix}\text{precession} \\ \text{∡ freq.}\end{matrix}\right\} \quad \omega_1 = \gamma_1 B_2 \sim (g_1\mu_0/\hbar)\frac{g_2\mu_0}{a_0^3},$$

$$\omega_2 = \gamma_2 B_1 = \omega_1 \; ; \quad \text{i.e.// } \underline{\underline{\omega_1 = \omega_2 = \omega}}. \tag{14}$$



VECTOR MODEL

$\vec{J}_1$ & $\vec{J}_2$ remain in a plane which rotates uniformly about $\vec{J} = \vec{J}_1 + \vec{J}_2$ at a rapid rate (microwave to far infrared freqs):

$$\rightarrow f = \frac{\omega}{2\pi} \sim g_1 g_2 \frac{\mu_0^2}{a_0^3}/h = g_1 g_2 \alpha^4 \frac{mc^2}{h} = 300\, g_1 g_2 \text{ GHz}. \tag{15}$$

4) Magnetic dipole-dipole interaction energies within an atom are typically much smaller than the electronic (Coulomb) energies which characterize the overall structure and binding. Nevertheless, the magnetic interactions are important because they generate readily <u>observable</u> corrections to the Bohr energies... those corrections are known as atomic fs (fine structure) and hfs (hyperfine structure). For an order-of-magnitude survey...

<u>A.</u> <u>ELECTRONIC STRUCTURE</u> (Coulomb interaction between e & p):

$\rightarrow \mathcal{E}_{es} \sim e^2/a_0$, $a_0 = \hbar^2/m_e e^2 = 0.529 \times 10^{-8}$ cm (Bohr radius),

so// $\underline{\underline{\mathcal{E}_{es} \sim \alpha^2 m_e c^2 \sim 10\,\mathrm{eV}}}$* ; $\alpha = e^2/\hbar c \simeq 1/137$, finestructure const; $mc^2 = 0.511$ MeV, electron rest energy. (16)

<u>B.</u> <u>FINE STRUCTURE</u> (e-spin $\vec{\mu}_s$ coupled to e-orbital $\vec{\mu}_L$):

$\rightarrow \mathcal{E}_{fs} \sim g_L g_S \mu_0^2/a_0^3 \sim (e\hbar/m_e c)^2/(\hbar/m_e e^2) = \alpha^4 m_e c^2$,

so// $\underline{\underline{\mathcal{E}_{fs} \sim \alpha^2 \mathcal{E}_{es} \sim 10^{-4} \mathcal{E}_{es}}}$. (17)

<u>C.</u> <u>HYPERFINE STRUCTURE</u> (total e $\vec{\mu}_J$, $\vec{J} = \vec{L} + \vec{S}$, coupled to nuclear $\vec{\mu}_I$):

$\rightarrow \underline{\underline{\mathcal{E}_{hfs} \sim g_p g_J \mu_0^2/a_0^3 \sim \frac{m_e}{M} \mathcal{E}_{fs} \sim 10^{-3} \mathcal{E}_{fs}}}$. (18)

This is the hierarchy of major energy couplings <u>within</u> an atom. If the nucleus has a quadrupole moment Q (in units of $10^{-24}\,\mathrm{cm}^2$), then $\mathcal{E}_Q \sim N Q \alpha \mathcal{E}_{hfs}$, where N is a numerical factor ~ 10; usually $\mathcal{E}_Q < \mathcal{E}_{hfs}$. <u>Between</u> atoms, magnetic interactions (spin-spin couplings) of size $\sim \mathcal{E}_{fs}$ in Eq. (17) occur, and also there are Van der Waals interactions, with energies $\mathcal{E}_{vdW} \sim \left(\frac{a_0}{R}\right)^6 \mathcal{E}_{es}$, for atomic separations $R \gg a_0$. In <u>molecules</u>, one encounters also vibrational energies $\mathcal{E}_{vib} \sim \sqrt{m_e/M}\, \mathcal{E}_{es}$ and rotational energies $\mathcal{E}_{rot} \sim (m/M)\, \mathcal{E}_{es}$, w/ M = nuclear mass.

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* Of course we are just doing orders-of-magnitude. Actually $\alpha^2 m_e c^2 = 27.2$ eV.