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Tutorial V

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Reminder

EXERCISE I : Zeeman effect and spin-orbit coupling on the $2p$ state of the hydrogen atom

Including spin-orbit (LS) coupling, the Hamiltonian of the hydrogen atom can be written

$$H = H_0 + \xi(\vec{l} \cdot \vec{s})$$

whereξ is the spin-orbit coupling strength and H_0 is given by

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{r}$$

In this problem we concentrate on the $2p$ state.

1. Decompose the states $|J, M_J\rangle$ in terms of $\left|l, \frac{1}{2}, m_l, m_s\right\rangle$, where $\vec{J} = \vec{l} + \vec{s}$ is the total angular momentum operator and M_J are the projections of the total angular momentum (eigenvalues of J_z). For this you can make use of the following Clebsch-Gordon coefficients :

$$\left|J = \frac{3}{2}, m_J\right\rangle = A\,|l, m_l = m_J + 1/2, s, m_s = -1/2\rangle + B\,|l, m_l = m_J - 1/2, s, m_s = 1/2\rangle$$
$$\left|J = \frac{1}{2}, m_J\right\rangle = C\,|l, m_l = m_J + 1/2, s, m_s = -1/2\rangle + D\,|l, m_l = m_J - 1/2, s, m_s = 1/2\rangle$$

$$A = \sqrt{\frac{l - m_J + 1/2}{2l + 1}}, \qquad B = \sqrt{\frac{l + m_J + 1/2}{2l + 1}}$$
$$C = \sqrt{\frac{l + m_J + 1/2}{2l + 1}}, \qquad D = -\sqrt{\frac{l - m_J + 1/2}{2l + 1}}$$

2. Write expressions for all of the fine structure states of the $2p$ state and make a sketch labeling the relevant energy scales and the degrees of degeneracy, noting that $\vec{l} \cdot \vec{s} = \frac{1}{2}[J^2 - l^2 - s^2]$ is diagonal in the $|J, M_J\rangle$ basis.

$$\begin{cases}
\left|\frac{3}{2}, +\frac{3}{2}\right\rangle = \left|1, 1, \frac{1}{2}, \frac{1}{2}\right\rangle \\
\left|\frac{3}{2}, +\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1, 1, \frac{1}{2}, -\frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|1, 0, \frac{1}{2}, \frac{1}{2}\right\rangle \\
\left|\frac{3}{2}, -\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1, 0, \frac{1}{2}, -\frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|1, -1, \frac{1}{2}, \frac{1}{2}\right\rangle \\
\left|\frac{3}{2}, -\frac{3}{2}\right\rangle = \left|1, -1, \frac{1}{2}, -\frac{1}{2}\right\rangle \\
\left|\frac{1}{2}, +\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1, 1, 1, -\frac{1}{2}\right\rangle - \sqrt{\frac{1}{3}}\left|1, 0, \frac{1}{2}, \frac{1}{2}\right\rangle \\
\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1, 0, \frac{1}{2}, -\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1, -1, \frac{1}{2}, \frac{1}{2}\right\rangle
\end{cases}$$

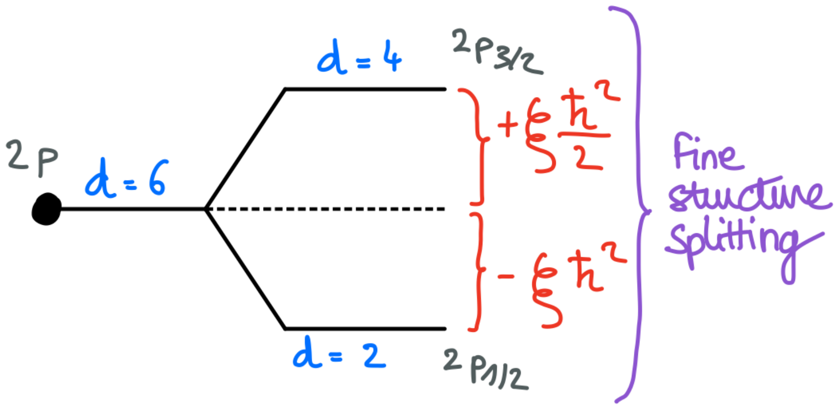
We can also write,

$$J^2 = L^2 + S^2 + 2(L \cdot S) \longrightarrow L \cdot S = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$$

Meaning,

$$\begin{aligned} \delta E &= \xi \langle J, m_J | \vec{L} \cdot \vec{S} \, | J, m_J \rangle \\ &= \frac{\xi \hbar^2}{2} \left(J(J+1) - L(L+1) - S(S+1) \right) \end{aligned}$$

$\lvert J, m_J \rangle$	$J,\ L,\ s$	δE
$\left\lvert \frac{3}{2}, +\frac{3}{2} \right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$\frac{\hbar^2}{2}\xi$
$\left\lvert \frac{3}{2}, +\frac{1}{2} \right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$\frac{\hbar^2}{2}\xi$
$\left\lvert \frac{3}{2}, -\frac{1}{2} \right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$\frac{\hbar^2}{2}\xi$
$\left\lvert \frac{3}{2}, -\frac{3}{2} \right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$\frac{\hbar^2}{2}\xi$
$\left\lvert \frac{1}{2}, +\frac{1}{2} \right\rangle$	$\frac{1}{2},\ 1,\ \frac{1}{2}$	$-\hbar^2\xi$
$\left\lvert \frac{1}{2}, -\frac{1}{2} \right\rangle$	$\frac{1}{2},\ 1,\ \frac{1}{2}$	$-\hbar^2\xi$



3. Show that the interaction Hamiltonian with an external magnetic field $\vec{B}$ applied parallel to $\vec{z}$ can be written.

$$H_B = \omega_0(l_z + 2s_z) \quad \text{where} \quad \omega_0 = -\frac{eB}{2m} \quad \text{and} \quad B = ||\vec{B}||$$

We know that,

$$\vec{\mu}_L = \frac{g_L \mu_B}{\hbar} \vec{L}, \qquad \vec{\mu}_S = \frac{g_S \mu_B}{\hbar} \vec{S}$$

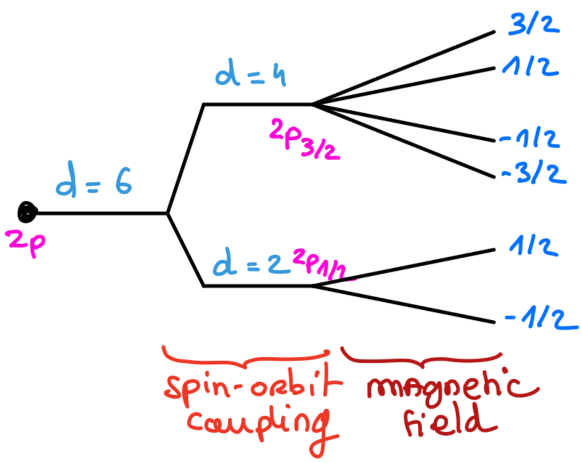
With $g_L = 1$ and $g_S = 2$.

$$\begin{aligned} H_B &= -\vec{\mu} \cdot \vec{B} \\ &= -(\vec{\mu}_L + \vec{\mu}_S) \cdot \vec{B} \\ &= -\frac{\mu_B}{\hbar}(\vec{L} + 2\vec{S}) \cdot \vec{B} \\ &= -\frac{e}{2m_e}\left(\vec{L} + 2\vec{S}\right) \cdot \vec{B} \\ &= \omega_0(l_z + 2s_z) \end{aligned}$$

4. We assume that the influence of the magnetic field is weak compared to the spin-orbit coupling. Write an expression for the modification of the energy levels as a function of B using first order perturbation theory.

$$\begin{aligned} \delta E &= \langle J, m_J| \, H_B \, |J, m_J\rangle \\ &= \omega_0 \hbar \left[m_l + 2m_s\right] \end{aligned}$$

$\|J, m_J\rangle$	$J,\ L,\ s$	δE
$\left\|\frac{3}{2}, +\frac{3}{2}\right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$2\hbar\omega_0$
$\left\|\frac{3}{2}, +\frac{1}{2}\right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$\frac{2}{3}\hbar\omega_0$
$\left\|\frac{3}{2}, -\frac{1}{2}\right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$-\frac{2}{3}\hbar\omega_0$
$\left\|\frac{3}{2}, -\frac{3}{2}\right\rangle$	$\frac{3}{2},\ 1,\ \frac{1}{2}$	$-2\hbar\omega_0$
$\left\|\frac{1}{2}, +\frac{1}{2}\right\rangle$	$\frac{1}{2},\ 1,\ \frac{1}{2}$	$\frac{1}{3}\hbar\omega_0$
$\left\|\frac{1}{2}, -\frac{1}{2}\right\rangle$	$\frac{1}{2},\ 1,\ \frac{1}{2}$	$-\frac{1}{3}\hbar\omega_0$



As long as the magnetic field B is weak in comparison to the spin-orbit coupling, the application of this field does lift the degeneracy.

5. Now we assume that the magnetic field is strong enough to dominate over the spin-orbit coupling. Write an expression for the modification of the levels as a function of B in first order perturbation theory.

$\lvert l, m_l, s, m_s\rangle$	$E^{(0)}$
$\lvert 1, 1, \frac{1}{2}, +\frac{1}{2}\rangle$	$E_0 + 2\hbar\omega_0$
$\lvert 1, 1, \frac{1}{2}, -\frac{1}{2}\rangle$	E_0
$\lvert 1, 0, \frac{1}{2}, +\frac{1}{2}\rangle$	$E_0 + \hbar\omega_0$
$\lvert 1, 0, \frac{1}{2}, -\frac{1}{2}\rangle$	$E_0 - \hbar\omega_0$
$\lvert 1, -1, \frac{1}{2}, +\frac{1}{2}\rangle$	E_0
$\lvert 1, -1, \frac{1}{2}, -\frac{1}{2}\rangle$	$E_0 - 2\hbar\omega_0$

First order perturbation for non-degenerate states,

$$\begin{aligned} E^{(1)} &= \langle l, m_l, s, m_s\rvert H_{\text{spin-orbit}} \lvert l, m_l, s, m_s\rangle \\ &= \xi \langle l, m_l, s, m_s\rvert \vec{l}\cdot\vec{s} \lvert l, m_l, s, m_s\rangle \end{aligned}$$

$$\vec{l}\cdot\vec{s} = l_z s_z + \frac{1}{2}(l_+ s_- + l_- s_+)$$

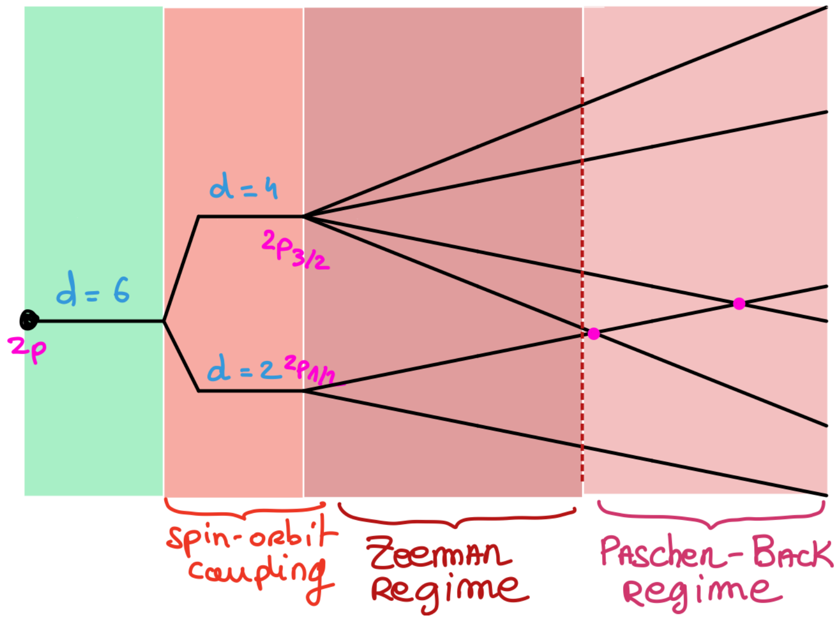
$\lvert l, m_l, s, m_s\rangle$	$E^{(1)}$
$\lvert 1, 1, \frac{1}{2}, +\frac{1}{2}\rangle$	$+\xi\frac{\hbar^2}{2}$
$\lvert 1, 0, \frac{1}{2}, +\frac{1}{2}\rangle$	0
$\lvert 1, 0, \frac{1}{2}, -\frac{1}{2}\rangle$	0
$\lvert 1, -1, \frac{1}{2}, -\frac{1}{2}\rangle$	$+\xi\frac{\hbar^2}{2}$

$$(\xi\vec{l}\cdot\vec{s}) = \xi\frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

First order perturbation for degenerate states,

$\lvert l, m_l, s, m_s\rangle$	$E^{(1)}$
$\lvert 1, 1, \frac{1}{2}, -\frac{1}{2}\rangle$	$-\xi\frac{\hbar^2}{2}$
$\lvert 1, -1, \frac{1}{2}, +\frac{1}{2}\rangle$	$-\xi\frac{\hbar^2}{2}$

$$(\xi\vec{l}\cdot\vec{s}) = -\xi\frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$


d = 6
2p
d = 4
$^2p_{3/2}$
d = 2
$^2p_{1/2}$
spin-orbit coupling
Zeeman Regime
Paschen-Back regime