Hydrogen Atom in Magnetic Field

(strong) magnetic field: $\vec{B} = B_0 \hat{z}$

magnetic moment of electron

$$\vec{\mu} = -\frac{e}{2m_e}\left(\vec{L} + g_e \vec{S}\right)$$

$$g_e = 2.00232 \approx 2$$

magnetic energy:

$$H_{mag} = -\vec{\mu}\cdot\vec{B}$$

$$= -\mu_z B_0$$

$$= \frac{e}{2m_e} B_0 \left(L_z + 2S_z\right)$$

electron in hydrogen atom

$$H = \frac{1}{2m}\vec{P}^2 - \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{r} + H_{mag}$$

quantum state: $|n\, l\, m_l\, m_s\rangle$

energies: $E_{nlm_lm_s} = -\frac{Ry}{n^2} + \frac{e\hbar}{2m_e} B_0 \left(m_l + 2m_s\right)$

weak magnetic field:

magnetic energy << fine structure splitting

$$H = H_0 + H_1$$

$$H_0 = \frac{1}{2m_e}\vec{P}^2 - \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{r} + H_{spin\text{-}orbit} + H_{relativistic}$$

$$H_1 = \frac{e}{2m_e} B_0 (L_z + 2S_z)$$

eigenvalue problem for H_0:

eigenstates: $|n\, l\, j\, m_j\rangle$

$$\begin{aligned} n &= 1, 2, 3, \ldots \\ l &= 0, 1, \ldots, n-1 \\ j &= \tfrac{1}{2} \qquad\qquad\quad l = 0 \\ &= l - \tfrac{1}{2}, l + \tfrac{1}{2} \quad l = 1, 2, \ldots \\ m_j &= -j, -j+1, \ldots, +j \end{aligned}$$

energies depend only on n, j:

$$E_{n,j} = -\frac{Ry}{n^2} + \frac{\alpha^2 Ry}{n^3}\left(\frac{3}{4} - \frac{n}{j+\frac{1}{2}}\right)$$

1st order perturbation theory:

$$E^{(1)}_{n\ell j m_j} = \frac{e}{2m_e} B_0 \langle n \ell j m_j | L_z + 2S_z | n \ell j m_j \rangle$$

can evaluate by

- expressing $|\ell\ j\ m_j\rangle$ as linear combination of $|\ell\ m_\ell\ m_s\rangle$
- using $L_z |\ell\ m_\ell\ m_s\rangle = m_\ell \hbar\, |\ell\ m_\ell\ m_s\rangle$
  $S_z |\ell\ m_\ell\ m_s\rangle = m_s \hbar\, |\ell, m_\ell\ m_s\rangle$

Alternative: use Wigner-Eckardt Theorem

$$\langle L_z \rangle = \left\langle \frac{\vec{L}\cdot\vec{J}}{\vec{J}^2} J_z \right\rangle$$

$$\langle S_z \rangle = \left\langle \frac{\vec{S}\cdot\vec{J}}{\vec{J}^2} J_z \right\rangle$$

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

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

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

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

$$\langle L_z \rangle_{n,\ell,j,m_j} = \langle n \ell j m_j | \frac{\vec{L}\cdot\vec{J}}{\vec{J}^2} J_z | n \ell j m_j \rangle$$

$$= \langle n \ell j m_j | \frac{\vec{J}^2 + \vec{L}^2 - \vec{S}^2}{2\vec{J}^2} J_z | n \ell j m_j \rangle$$

$$= \frac{[j(j+1) + \ell(\ell+1) - s(s+1)]\hbar^2}{2j(j+1)\hbar^2} \langle n \ell j m_j | J_z | n \ell j m_j \rangle$$

$$= \frac{j(j+1) + \ell(\ell+1) - \frac{3}{4}}{2j(j+1)} m_j \hbar$$

$$\langle S_z \rangle_{n\ell j m_j} = \langle n \ell j m_j | \frac{\vec{S}\cdot\vec{J}}{\vec{J}^2} J_z | n \ell j m_j \rangle$$

$$= \langle n \ell j m_j | \frac{\vec{J}^2 + \vec{S}^2 - \vec{L}^2}{2\vec{J}^2} J_z | n \ell j m_j \rangle$$

$$= \frac{[j(j+1) + s(s+1) - \ell(\ell+1)]\hbar^2}{2j(j+1)\hbar^2} \langle n \ell j m_j | J_z | n \ell j m_j \rangle$$

$$= \frac{j(j+1) + \frac{3}{4} - \ell(\ell+1)}{2j(j+1)} m_j \hbar$$

$$E^{(1)}_{n\ell j m_j} = \frac{e}{2m_e} B_0 \left[\frac{j(j+1) + \ell(\ell+1) - \frac{3}{4}}{2j(j+1)} m_j \hbar + 2 \frac{j(j+1) + \frac{3}{4} - \ell(\ell+1)}{2j(j+1)} m_j \hbar \right]$$

$$= \frac{e}{2m_e} B_0 \frac{3j(j+1) - \ell(\ell+1) + \frac{3}{4}}{2j(j+1)} (m_j \hbar)$$

$$= g(j,\ell) \frac{e}{2m_e} B_0 (m_j \hbar)$$

Landé g-factor: $g(j,\ell) = \dfrac{3j(j+1) - \ell(\ell+1) + \frac{3}{4}}{2j(j+1)}$

$$= \frac{2j+1}{2\ell+1} \quad \text{for } j = \ell \pm \tfrac{1}{2}$$