11.12 Hydrogen in Magnetic Field:

Zeeman effekt (weak B) $\longleftrightarrow$ Paschen-Back effect (strong B)

11.12.1 Minimal Coupling: see QFT lecture notes

Interaction of a charge $q = -e$ with a magnetic field $\vec{B}(\vec{x}) = \text{rot}\,\vec{A}(\vec{x})$ follows from minimal coupling:

$$\hat{\vec{p}} \to \hat{\vec{p}} - q\vec{A}(\vec{x}) = \frac{\hbar}{i}\vec{\nabla} + e\vec{A}(\vec{x})$$

Kinetic energy:

$$\hat{H}_{kin} = \frac{\hat{\vec{p}}^2}{2m} \Rightarrow \frac{1}{2m}\left[\frac{\hbar}{i}\vec{\nabla} + e\vec{A}(\vec{x})\right]^2$$

$$= -\frac{\hbar^2}{2m}\Delta + \frac{e}{2m}\Big[\underbrace{\frac{\hbar}{i}\vec{\nabla}\,\vec{A}(\vec{x})}_{\text{operator ordering}} + \vec{A}(\vec{x})\frac{\hbar}{i}\vec{\nabla}\Big] + \frac{e^2}{2m}\vec{A}(\vec{x})^2$$

wave function

$$= -\frac{\hbar^2}{2m}\Delta + \frac{e}{m}\left[\vec{A}\frac{\hbar}{i}\vec{\nabla} + \cancel{\frac{\hbar}{2i}\,\text{div}\,\vec{A}}\right] + \frac{e^2}{2m}\vec{A}(\vec{x})^2$$

Homogeneous magnetic field: $\vec{A}(\vec{x}) = \frac{1}{2}\underbrace{\vec{B}}_{\text{konst.}}\times\vec{x}$, $\text{rot}\,\vec{A}(\vec{x}) = \vec{B}$

Homogeneous magnetic field in z-direction:

$$\vec{B}(\vec{x}) = B\,\vec{e}_z \Rightarrow \vec{A}(\vec{x}) = \frac{B}{2}\begin{pmatrix}-y\\ x\\ 0\end{pmatrix}, \quad \underline{\text{div}\,\vec{A}(\vec{x}) = 0}$$

$$\hat{H}_{kin} = -\frac{\hbar^2}{2m}\Delta + \frac{e}{2m}B\underbrace{\left(x\frac{\hbar}{i}\frac{\partial}{\partial y} - y\frac{\hbar}{i}\frac{\partial}{\partial x}\right)}_{=\hat{L}_z} + \cancel{\frac{e^2}{2m}(x^2+y^2)B^2}$$

linear in B
(linear Zeeman effect)

quadratic in B
(quadratic Zeeman effect)

neglected in the following

linear energy shift due to orbital angular momentum:

$$\hat{H}_B = \frac{eB}{2m}\hat{L}_z = -\underbrace{\frac{-e\hbar}{2m}}_{=\ \mu_B}\underbrace{g_e}_{=1}\vec{B}\cdot\frac{\hat{\vec{L}}}{\hbar}$$

Bohr magneton   Landé factor

analogous shift due to spin:

$$\hat{H}_B = -\frac{-e\hbar}{2m}\underbrace{g_s}_{=2}\vec{B}\cdot\frac{\hat{\vec{S}}}{\hbar}$$

$= 2$ (due to Dirac equation)

Total energy shift:

$$\hat{H}_B = \frac{eB}{2m}(\hat{L}_z + \underbrace{2}_{=g_s}\hat{S}_z)$$

Outlook:

$\hat{H}_{SO} \gg \hat{H}_B$: B weak Zeeman

$\hat{H}_{SO} \ll \hat{H}_B$: B strong Paschen Back

Total Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_{KE} + \underbrace{\hat{H}_{SO}}_{=\frac{e^2}{8\pi\varepsilon_0 m^2c^2r^3}\hat{\vec{L}}\cdot\hat{\vec{S}}} + \hat{H}_D + \hat{H}_B$$

11.12.2 Linear Zeeman Effect: "$\hat{H}_{SO}$" $\gg$ "$\hat{H}_B$"

$\hat{H}_B$ – effect to be treated perturbated

unperturbed $\hat{H}_{SO}$ is diagonal with respect $|j, m\rangle$

$$E_B = \langle j,m|\hat{H}_B|j,m\rangle = \frac{eB}{2m}\langle j,m|\underbrace{\hat{L}_z + 2\hat{S}_z}_{=\hat{J}_z + \hat{S}_z}|j,m\rangle = \frac{e\hbar}{2m}B\left\{m + \langle j,m|\frac{\hat{S}_z}{\hbar}|j,m\rangle\right\}$$

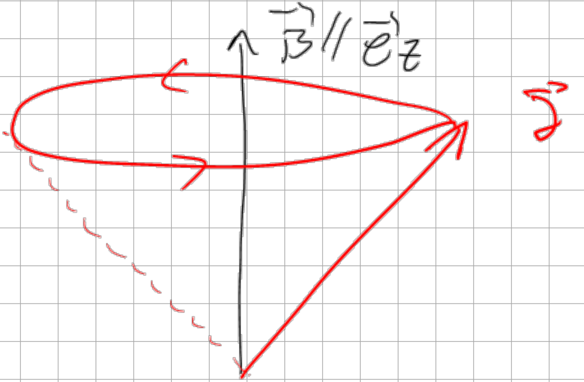
Recall spinorial spherical harmonics:

$$|j=l\pm\tfrac{1}{2}, m\rangle = \pm\sqrt{\frac{l\pm m+1/2}{2l+1}}\,|m_l=m-\tfrac{1}{2}, m_s=+\tfrac{1}{2}\rangle + \sqrt{\frac{l\mp m+1/2}{2l+1}}\,|m_l=m+\tfrac{1}{2}, m_s=-\tfrac{1}{2}\rangle$$

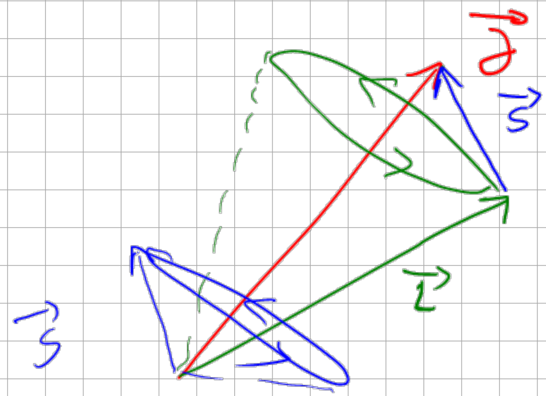
$$\langle j,m|\hat{S}_z|j,m\rangle = \frac{\hbar}{2}\left\{\frac{l\pm m+1/2}{2l+1} - \frac{l\mp m+1/2}{2l+1}\right\} = \pm\frac{m\hbar}{2l+1}$$

$$\Rightarrow E_B = \frac{e\hbar}{2m}\, m\left(1\pm\frac{1}{2l+1}\right) = -\frac{-e\hbar}{2m}\underbrace{g_j}_{\text{Landé factor}} B\, m \quad ; \quad \boxed{g_j = 1\pm\frac{1}{2l+1}}$$

This result also follows from semiclassical vector model (based on the Wigner-Eckart theorem)



slow precession due to weak magnetic field



fast precession due to strong LS coupling

Due to fast precession of $\vec{L}$ and $\vec{S}$ around $\vec{J}$ only their temporal average is physically relevant, which points along $\vec{J}$-direction

$$\langle\vec{S}\rangle = \frac{\vec{S}\cdot\vec{J}}{|\vec{J}|}\frac{\vec{J}}{|\vec{J}|} \qquad \langle\vec{L}\rangle = \frac{\vec{L}\cdot\vec{J}}{|\vec{J}|}\frac{\vec{J}}{|\vec{J}|}$$

$$E_B = \frac{e\vec{B}}{2M}\cdot\Big(\underbrace{g_e}_{=1}\langle\vec{L}\rangle + \underbrace{g_s}_{=2}\langle\vec{S}\rangle\Big) = \frac{e\vec{B}}{2M}\cdot\left(\vec{L}\cdot\vec{J} + 2\vec{S}\cdot\vec{J}\right)\frac{\vec{J}}{\vec{J}^2} = \frac{eB\hbar}{2M}\, m \quad g_j$$

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

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

$$g_j = \frac{j(j+1) + l(l+1) - s(s+1) + 2\left[j(j+1) + s(s+1) - l(l+1)\right]}{2j(j+1)}$$

$$= 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$$

(Please note: analogy for hyperfine spin structure and its Zeeman effect)

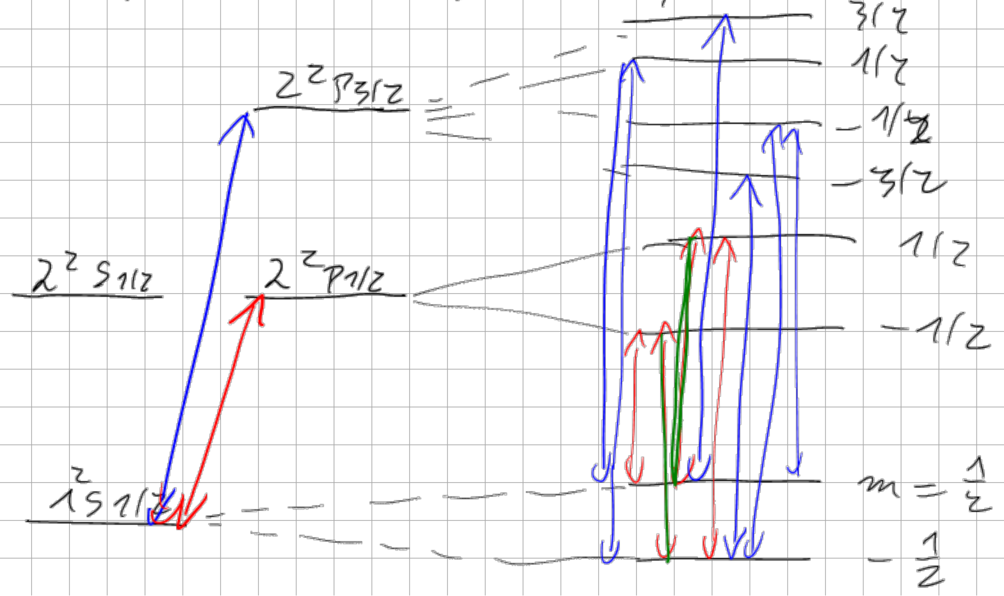
1. Case: $j = l + 1/2$, $s = 1/2$

$$g_{l+\frac{1}{2}} = \dots = 1 + \frac{1}{2l+1}$$

2. Case: $j = l - 1/2$, $s = 1/2$

$$g_{l-\frac{1}{2}} = 1 - \frac{1}{2l+1}$$

3. Case: $j = 1/2$, $s = 1/2$, $l = 0$ $\Rightarrow$ $g_{1/2} = 2$



$g_j = \frac{4}{3}$

$g_j = \frac{2}{3}$

$g_j = 2$

selection rule

$\Delta l = \pm 1$

$\Delta m = 0, \pm 1$

$B = 0$ $\quad$ $B > 0$

1 line $\quad$ 4 lines

1 line $\quad$ 6 lines

$n = 2, \ell = 1$ initial state $\quad$ $n = 1, \ell = 0$ final states $\quad$ $\Delta E / \mu_B B$

- $\left| \frac{1}{2}, \pm \frac{1}{2} \right\rangle \quad \left| \frac{1}{2}, \pm \frac{1}{2} \right\rangle \quad \left(\pm \frac{1}{2}\right) \cdot \frac{2}{3} - \left(\pm \frac{1}{2}\right) 2 = \mp \frac{2}{3}$

all changes calculated involve $m_{s, \text{init.}}$, $m_{s \text{ final}}$, $g_{J \text{ initial}}$, $g_{J \text{ final}}$

11.12.3 Paschen Back effect:

B strong $\Rightarrow \hat{H}_B$ is far more important than $\hat{H}_{SO}$

unperturbed system: $\hat{H}_0 + \hat{H}_{KE} + \underbrace{\hat{H}_B}_{} + \hat{H}_D$, perturbed system: $\hat{H}_{SO}$

$$= \frac{e\hbar}{2m} B(\hat{L}_z + 2\hat{S}_z)$$

unperturbed eigenstates: $|\ell, s = 1/2; m_\ell, m_s\rangle$

$$E_B = \langle \ell, s = \tfrac{1}{2}; m_\ell, m_s | \hat{H}_B | \ell, s = \tfrac{1}{2}; m_\ell, m_s \rangle = \frac{e\hbar}{2m} B \left(\underline{m_\ell + 2 m_s}\right)$$

$\hat{H}_0$: degeneracy with respect to $m_\ell, m_s \Rightarrow 2(2\ell+1)$ degeneracy

E_B states are degenerate with the same $m_\ell + 2 m_s$

Expectation value of $\hat{H}_{SO} = C \cdot \vec{L} \cdot \vec{S}$

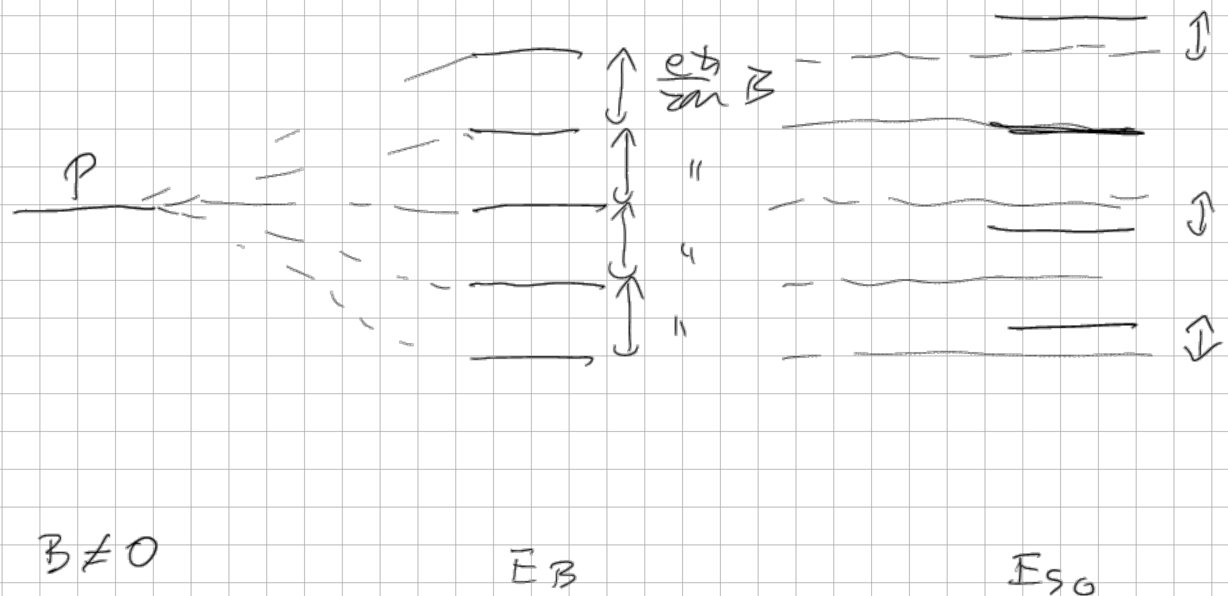
$$\langle \hat{\vec{L}} \cdot \hat{\vec{S}} \rangle_{m_\ell, m_s} = \left\langle \frac{1}{2}\left(\hat{L}_+ \hat{S}_- + \hat{L}_- \hat{S}_+\right) + \hat{L}_z \cdot \hat{S}_z \right\rangle_{m_\ell, m_s} = m_\ell \cdot m_s$$

$$\langle \hat{L}_\pm \rangle_{m_\ell, m_s} = 0 = \langle \hat{S}_\pm \rangle_{m_\ell, m_s}$$

$$\langle \hat{H}_{SO} \rangle_{m_\ell, m_s} = \frac{e^2 \hbar^2}{8\pi \varepsilon_0 m^2 c^2} \left\langle \frac{1}{r^3} \right\rangle \cdot m_\ell m_s$$

example $\ell = 1$: $P_{1/2}$, $P_{3/2}$

m_ℓ	m_s	$E_B \sim m_\ell + 2 m_s$	$m_\ell \cdot m_s$
1	1/2	2	1/2
1	−1/2	0	−1/2
0	1/2	1	0
0	−1/2	−1	0
−1	1/2	0	−1/2
−1	−1/2	−2	1/2



12 Klein-Gordon Equation:

Motivation:

- Unifying quantum mechanics and special relativity
- Schrödinger was the first to setup Klein-Gordon equation, application to Coulomb potential led to wrong energy level due to the lack of spin 1/2; therefore Schrödinger focused on nonrelativistic limit, i.e. Klein-Gordon equation
- Today Klein-Gordon equation correctly describes spin 0 particles as, i.e. $\pi^{\pm}$, π^0