Hamiltonian: Hydrogen in Magnetic Field

$$\hat H = \underbrace{\hat H_0}_{\text{Schrödinger}} + \underbrace{\hat H_{KE} + \underbrace{\hat H_{SO}}_{\sim \hat{\vec L}\cdot\hat{\vec S}} + \hat H_D}_{\text{special relativistic corrections}} + \underbrace{\hat H_B}_{= \frac{eB}{2m}\left(\hat L_z + 2\hat S_z\right)}$$

diagonal with respect to option B

diagonal with respect to option A

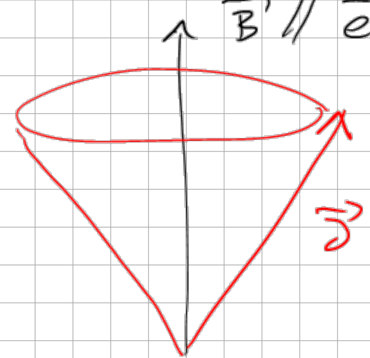
Zeeman Effect: "$\hat H_{SO} \gg \hat H_B$" $\hat{=}$ weak magnetic field

see last time: $\Delta E_B = \langle j, m_j | \hat H_B | j, m_j \rangle = \ldots = \frac{e\hbar}{2m} B\, m_j\, g_j$

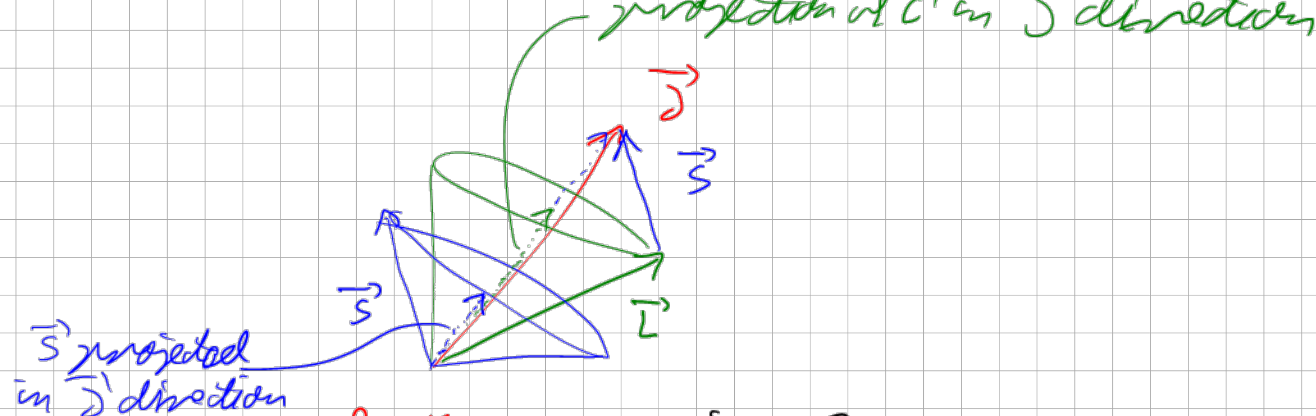
spinorial spherical harmonics

Landé factor: $g_j = 1 \pm \frac{1}{2\ell+1}$, $j = \ell \pm 1/2$

semiclassical vector model:



slow precession of $\vec J$ around $\vec B$



fast precession of $\vec L, \vec S$ around $\vec J$

$\Rightarrow$ temporal average is relevant

$$\langle \vec{S}\rangle = \left(\frac{\vec{S}\cdot\vec{J}}{|\vec{J}|}\right)\frac{\vec{J}}{|\vec{J}|}\,, \qquad \langle \vec{L}\rangle = \left(\frac{\vec{L}\cdot\vec{J}}{|\vec{J}|}\right)\frac{\vec{J}}{|\vec{J}|}$$

$$\Delta E_B = \frac{e\vec{B}}{2m}\left(\underbrace{g_\ell}_{=1}\langle \vec{L}\rangle + \underbrace{g_s}_{=2}\langle \vec{S}\rangle\right) \qquad \vec{B} = B\vec{e}_z$$

$$= \frac{e\vec{B}}{2m}\overbrace{\left(\vec{L}\cdot\vec{J} + 2\,\underbrace{\vec{S}\cdot\vec{J}}\right)\cdot\frac{\vec{J}}{|\vec{J}|^2}}^{\parallel\, g_j} = \frac{eB\hbar}{2m}\, m_j \underbrace{g_j}_{=?}$$

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

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

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

$$= \ldots = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)} \quad (*)$$

Note: by analogy similar formulas occur for the ~~Zee~~ Zeeman effect of hyperfine structure

fine structure	ℓ	s	$\longrightarrow$	j	$\Rightarrow$ Landé factor g_j
hyperfine structure	j	i	$\longrightarrow$	f	$\Rightarrow$ Landé factor g_f

^{87}Rb: $L = 0,\ S = 1/2 \Rightarrow J = 1/2$

$I = 3/2 \Rightarrow F = 1,\ 2$

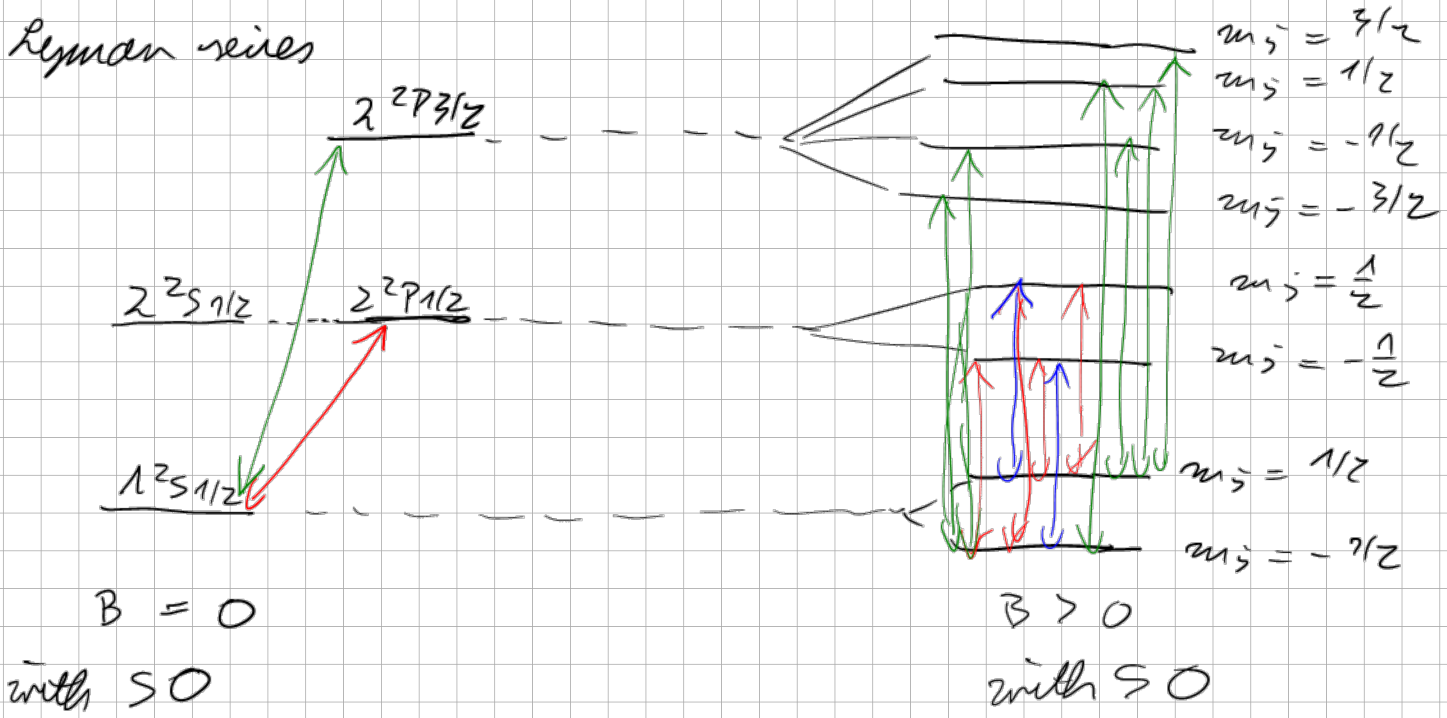
Comparison with previous Landé factor

1. Case: $j = l + 1/2,\ s = 1/2$ 2. Case: $j = l - 1/2,\ s = 1/2$ $(l \neq 0)$

$g_j \overset{(*)}{=} \dots = 1 + \frac{1}{2l+1}$ $g_j = \underline{(*)} = 1 - \frac{1}{2l+1}$ ✓

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

Lyman series



$g_j = \frac{4}{3}$ $(l = 1,\ s = \frac{1}{2},\ j = \frac{3}{2})$

$\underline{g_j = \frac{2}{3}}$ $(l = 1,\ s = 1/2,\ j = \frac{1}{2})$

$g_{\frac{1}{2}} = 2$ $(l = 0,\ s = 1/2,\ j = \frac{1}{2})$

selection rules

$\Delta l = \pm 1$

$\Delta m_j = 0, \pm 1$

ΔE_B is in units $\mu_B \cdot B$: $(m_j\, g_j)_{\text{final}} - (m_j\, g_j)_{\text{initial}}$

$$\Big|\underbrace{\tfrac{1}{2}}_{=j},\ \underbrace{\pm\tfrac{1}{2}}_{=m_j}\Big\rangle \longrightarrow \Big|\tfrac{1}{2},\ \pm\tfrac{1}{2}\Big\rangle : \left(\pm\tfrac{1}{2}\right)\cdot\tfrac{2}{3} - \left(\pm\tfrac{1}{2}\right)\cdot 2 = \mp\tfrac{2}{3}$$

Paschen – Back – Effect:

$\vec{B}$ is strong: $\underbrace{\hat{H}_B}_{\sim \hat{L}_z + 2\hat{S}_z}$ as unperturbed, $\underbrace{\hat{H}_{SO}}_{= C \cdot \hat{\vec{L}} \cdot \hat{\vec{S}}}$ as perturbation

$$|l, s = \tfrac{1}{2}; m_l, m_s\rangle$$

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

$\hat{H}_0$ degeneracy with respect to m_l, m_s: $2 \cdot (2l+1)$

E_B states are degenerate with respect to $m_l + 2m_s$

$$\langle \hat{H}_{SO}\rangle_{m_l, m_s} = C \langle \hat{\vec{L}} \cdot \hat{\vec{S}}\rangle_{m_l, m_s} = C \langle \tfrac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z \cdot \hat{S}_z\rangle_{m_l, m_s} = \underline{C\, m_l \cdot m_s}$$

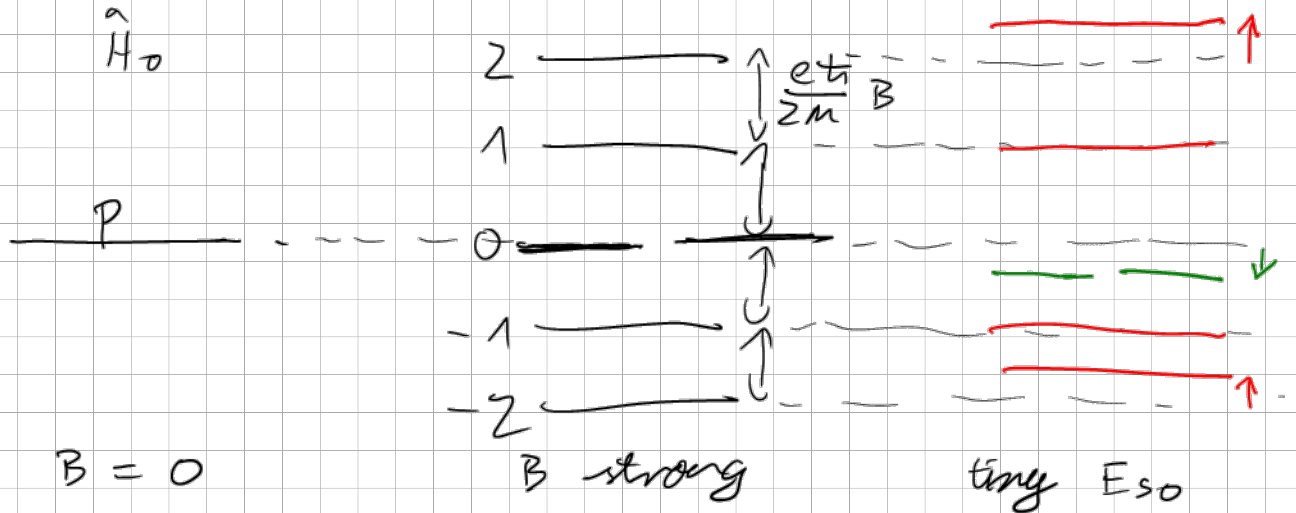
$$\langle m_l | \hat{L}_\pm | m_l\rangle = 0, \quad \langle m_s | \hat{S}_\pm | m_s\rangle = 0$$

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

example: $l = 1 \Rightarrow p_{1/2}$ and $p_{3/2}$

m_l	m_s	$E_B \sim (m_l + 2m_s)$	$m_l \cdot m_s$
1	1/2	2	1/2
1	−1/2	0	$\underline{-1/2}$
0	1/2	1	0
0	−1/2	−1	0
−1	1/2	0	$\underline{-1/2}$

$$\underbrace{-1 \qquad -1/2}_{2\cdot(2\cdot 1+1) = 6} \qquad -2 \qquad 1/2$$



12 Klein-Gordon Equation

Motivation:

- Unify quantum mechanics with special relativity
- Schrödinger was the first to set up Klein-Gordon equation, but application to Coulomb potential lead to wrong spectra due to missing spin ½
  → Schrödinger in non-relativistic limit his equation
- Today Klein-Gordon equation correctly describe spin 0 particles i.e. pions $\pi^\pm$, π^0

12.1 Schrödinger Equation:

nonrelativistic dispersion: $E = \frac{\vec{p}^2}{2m}$ $\Big\}$ $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi \quad |\cdot\psi^*$

Jordan rule: $\vec{p} \to \hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}$, $E \to \hat{E} = i\hbar\frac{\partial}{\partial t}$ $\Big\}$ $\underline{-i\hbar\frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi^*}$ $|\cdot\psi$

$$i\hbar\underbrace{\left\{\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\right\}}_{\frac{\partial}{\partial t}\underbrace{\psi^*\psi}_{=\rho}} + \frac{\hbar^2}{2m}\underbrace{\left\{\psi^*\Delta\psi - \psi\Delta\psi^*\right\}}_{\vec{\nabla}\left\{\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right\}} = 0$$

Continuity equation: $\frac{\partial}{\partial t}\rho + \operatorname{div}\underbrace{\vec{j}}_{\text{current density}} = 0$ (local conservation law)

$$\vec{j} = \frac{\hbar}{2mi}\left\{\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right\}$$

global conservation law:

$$\frac{\partial}{\partial t}\int d^3x\,(\rho) = -\int d^3x\,\operatorname{div}\vec{j} \overset{\text{Gauß}}{=} -\oint_\infty \vec{j}\cdot d\vec{\sigma} \equiv 0$$

$$\Rightarrow \underline{\int d^3x\,\rho = \text{const.}} \underset{\text{w.l.g.}}{\Rightarrow} \int d^3x\,\psi^*\psi = 1$$

Schrödinger for charged particle moving in electromagnetic field

→ minimal coupling

$$\vec{p} \to \vec{p} - q\vec{A} \xrightarrow{\text{Jordan}} \hat{\vec{p}} \to \frac{\hbar}{i}\vec{\nabla} - q\vec{A}$$

$$E \to E - q\varphi \xrightarrow{\text{Jordan}} \hat{E} \to i\hbar\frac{\partial}{\partial t} - q\varphi$$

local gauge transformation:

$$\psi(\vec{x},t) = \psi'(\vec{x},t)\,e^{\frac{i}{\hbar}q\overbrace{\Lambda(\vec{x},t)}^{\text{gauge function}}}$$

$$\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)\psi(\vec{x},t) = e^{\frac{i}{\hbar}q\Lambda(\vec{x},t)}\left\{\frac{\hbar}{i}\vec{\nabla}\underbrace{+q\vec{\nabla}\Lambda(\vec{x},t) - q\vec{A}}_{=-q\vec{A}'}\right\}\psi'(\vec{x},t)$$

$$\vec{A}'(\vec{x},t) = \vec{A}(\vec{x},t) - \vec{\nabla}\Lambda(\vec{x},t) \longleftarrow$$

$$\left(i\hbar\frac{\partial}{\partial t} - q\varphi\right)\psi(\vec{x},t) = e^{\frac{i}{\hbar}q\Lambda(\vec{x},t)}\left\{i\hbar\frac{\partial}{\partial t}\underbrace{-q\frac{\partial\Lambda(\vec{x},t)}{\partial t} - q\varphi}_{=-q\varphi'}\right\}\psi'(\vec{x},t)$$

$$\varphi'(\vec{x},t) = \varphi(\vec{x},t) + \frac{\partial}{\partial t}\Lambda(\vec{x},t) \longleftarrow$$

These gauge transformation of $\vec{A}$, φ

$$\vec{B} = \mathrm{rot}\,\vec{A} \Rightarrow \vec{B} = \mathrm{rot}\,\vec{A}', \quad \vec{E} = -\vec{\nabla}\varphi - \frac{\partial\vec{A}}{\partial t} \rightarrow \vec{E}' = -\vec{\nabla}\varphi' - \frac{\partial\vec{A}'}{\partial t}$$

$$\frac{\partial}{\partial t}\vec{\nabla}\Lambda - \vec{\nabla}\frac{\partial}{\partial t}\Lambda = 0$$

Schwarz theorem

Schrödinger equation in presence of electromagnetic field:

$$i\hbar\frac{\partial\psi}{\partial t} = \left\{-\frac{\hbar^2}{2m}\Delta + i\frac{q\hbar}{m}\vec{A}\cdot\vec{\nabla} + \frac{iq\hbar}{2m}\,\mathrm{div}\,\vec{A} + \frac{q^2\vec{A}^2}{2m} + q\varphi\right\}\psi$$

~~1) non-rel. dispersion~~ $\rightarrow$ relativistic dispersion

2) Jordan rule

3) minimal

$\longrightarrow$ Schrödinger $\qquad\qquad \rightarrow$ Klein-Gordon