11.10 LS-Coupling:

Important example: adding orbital angular momentum and spin 1/2

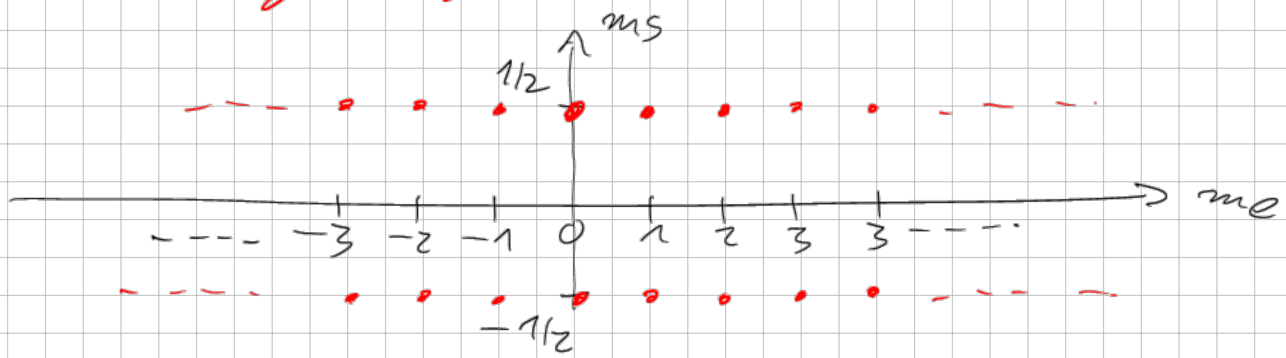
$j_1 = l$ (integer), $m_1 = m_l$
$j_2 = s = \frac{1}{2}$, $m_2 = m_s = \pm\frac{1}{2}$

} allowed values of j
1) $l = 0$: $j = 1/2$
2) $l > 0$: $j = l \pm 1/2$

example: p state $\hat{=}$ $l = 1$

$\Rightarrow$ $j = 1/2$, $j = 3/2$ $\Rightarrow$ $P_{1/2}$, $P_{3/2}$ (subscript to j; P: $l = 1$)

m_l, m_s - plane is particularly simple: two rows corresponding to $m_s = \pm 1/2$



Concentrate on $j = l + \frac{1}{2}$ $(l > 0)$:

$$\underbrace{\hat{J}_-}_{=(\hat{L}_- + \hat{S}_-)} \underbrace{|\underbrace{l+\tfrac{1}{2}}_{=j}, \underbrace{m+1}_{=m_j}\rangle}_{=\sum_{m_l', m_s'} |m_l', m_s'\rangle\langle m_l', m_s'| l+\frac{1}{2}, m+1\rangle} = \hbar\sqrt{(\underbrace{l+\tfrac{1}{2}}_{=j} + \underbrace{m+1}_{=m_j})(\underbrace{l+\tfrac{1}{2}}_{j} \underbrace{- m - 1}_{=-m_j} + 1)}\ |\underbrace{l+\tfrac{1}{2}}_{=j}, m\rangle$$

$$= \sum_{\substack{m_l', m_s' \\ m_j = m+1 = m_l' + m_s'}} (\hat{L}_- + \hat{S}_-)\, |m_l', m_s'\rangle \langle m_l', m_s' | l + \tfrac{1}{2}, m+1\rangle$$

$$= \sum_{m_l', m_s'} \hbar \Big\{ \sqrt{(l + m_l')(l - m_l' + 1)}\ |m_l' - 1, m_s'\rangle \langle m_l', m_s' | l + \tfrac{1}{2}, m+1\rangle$$

$m+1 = m_\ell' + m_s'$

$$+\sqrt{\left(\tfrac{1}{2}+m_s'\right)\left(\tfrac{1}{2}-m_s'+1\right)}\ |m_\ell', m_s'-1\rangle\langle m_\ell' m_s' | \ell+\tfrac{1}{2}, m+1\rangle \Big\} \quad (2)$$

Apply $\langle m_\ell, m_s|$ to this equation:

(1) $m_\ell = m_\ell' - 1,\ m_s = m_s' \Rightarrow m_\ell' = m_\ell + 1,\ m_s' = m_s.$ $\quad m + 1 = m_\ell' + m_s' = m_\ell + 1 + m_s$

(2) $m_\ell = m_\ell',\ m_s = m_s' - 1 \Rightarrow m_\ell' = m_\ell,\ m_s' = m_s + 1;$ $\quad m+1 = m_\ell' + m_s' = m_\ell + 1 + m_s$

$\Rightarrow m = m_\ell + m_s$

choice: $m_\ell = m - \tfrac{1}{2},\ m_s = \tfrac{1}{2} \Rightarrow m = m_\ell + m_s$ ✓

(1) $m_\ell' = m_\ell + 1 = m + \tfrac{1}{2},\ m_s' = m_s = \tfrac{1}{2}$

(2) $m_\ell' = m_\ell = m - \tfrac{1}{2},\ m_s' = m_s + 1 = \tfrac{3}{2}$

$$\sqrt{\left(\ell+m+\tfrac{3}{2}\right)\left(\ell-m+\tfrac{1}{2}\right)}\ \langle m-\tfrac{1}{2}, \tfrac{1}{2} | \ell+\tfrac{1}{2}, m\rangle$$

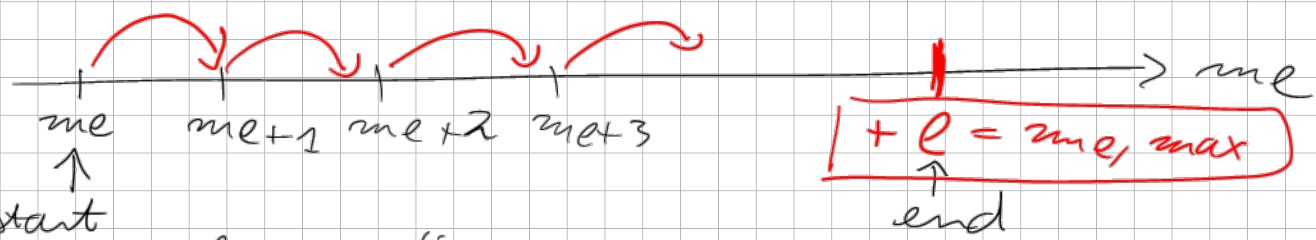
$$= \sqrt{\left(\ell+m+\tfrac{1}{2}\right)\left(\ell-m-\tfrac{1}{2}+1\right)}\ \underbrace{\langle m-\tfrac{1}{2}, \tfrac{1}{2} | m-\tfrac{1}{2}, \tfrac{1}{2}\rangle}_{=1}\langle m+\tfrac{1}{2}, \tfrac{1}{2} | \ell+\tfrac{1}{2}, m+1\rangle \quad (1)$$

$$+\sqrt{\left(\tfrac{1}{2}+\tfrac{3}{2}\right)\underbrace{\left(\tfrac{1}{2}-\tfrac{3}{2}+1\right)}_{=0}}\ \underbrace{\langle m-\tfrac{1}{2}, \tfrac{1}{2} | m-\tfrac{1}{2}, \tfrac{3}{2}-1\rangle}_{=1}\langle m-\tfrac{1}{2}, \underbrace{\tfrac{3}{2}}_{=m_s} | \ell+\tfrac{1}{2}, m+1\rangle \quad (2)$$

$$\langle \underbrace{m-\tfrac{1}{2}}_{=m_\ell}, \underbrace{\tfrac{1}{2}}_{=m_s} | \ell+\tfrac{1}{2}, m\rangle = \sqrt{\frac{\ell+m+1/2}{\ell+m+3/2}}\ \langle \underbrace{m+\tfrac{1}{2}}_{m_\ell+1}, \tfrac{1}{2} | \ell+\tfrac{1}{2}, m+1\rangle \quad (*)$$

$\hat{=}\ m = m_\ell + \tfrac{1}{2}$

$m_s = \frac{1}{2}$:



$\ell - m_\ell$ times

$\hat{=}\ \ell - m_\ell = \ell + \frac{1}{2} - \underbrace{(m_\ell + \frac{1}{2})}_{=m} = \ell + \frac{1}{2} - m$ iterations

$$(*) = \sqrt{\frac{\ell+m+\frac{1}{2}}{\ell+m+\frac{3}{2}}} \cdot \sqrt{\frac{\ell+m+\frac{3}{2}}{\ell+m+\frac{5}{2}}} \quad \langle m+\tfrac{3}{2}, \tfrac{1}{2} | \ell+\tfrac{1}{2}, m+2 \rangle$$

$$\overset{\ell+\frac{1}{2}-m \text{ times}}{=} - - - \dots = \sqrt{\frac{\ell+m+\frac{1}{2}}{\ell+m+\frac{1}{2}+\ell+\frac{1}{2}-m}} \quad \langle m-\tfrac{1}{2}+\ell+\tfrac{1}{2}-m, \tfrac{1}{2} | \ell+\tfrac{1}{2}, m+\ell+\tfrac{1}{2}-m \rangle$$

$$= \sqrt{\frac{\ell+m+\frac{1}{2}}{2\ell+1}} \quad \langle \underbrace{\ell}_{m_{\ell,max}}, \underbrace{\tfrac{1}{2}}_{m_{s,max}} | \underbrace{\ell+\tfrac{1}{2}}_{=j}, \underbrace{\ell+\tfrac{1}{2}}_{=m_{j,max}} \rangle$$

$$|\underbrace{\ell}_{m_{\ell,max}}, \underbrace{\tfrac{1}{2}}_{m_{s,max}}\rangle \equiv |\underbrace{\ell+\tfrac{1}{2}}_{j}, \underbrace{\ell+\tfrac{1}{2}}_{=m_{j,max}}\rangle \Rightarrow \langle \ell, \tfrac{1}{2} | \ell+\tfrac{1}{2}, \ell+\tfrac{1}{2} \rangle \equiv 1$$

$$\langle m-\tfrac{1}{2}, \tfrac{1}{2} | \ell+\tfrac{1}{2}, m \rangle = \sqrt{\frac{\ell+m+1/2}{2\ell+1}}$$

This result is 1/4 of the whole story:

$$|j = \ell+\tfrac{1}{2}, m\rangle = \sqrt{\frac{\ell+m+1/2}{2\ell+1}}\, |m_\ell = m-\tfrac{1}{2}, m_s = \tfrac{1}{2}\rangle + (*)\, |m_\ell = m+\tfrac{1}{2}, m_s = -\tfrac{1}{2}\rangle$$

$$|j = l - \tfrac{1}{2}, m\rangle = (*)\ |m_l = m - \tfrac{1}{2}, m_s = \tfrac{1}{2}\rangle + (*)\ |m_l = m + \tfrac{1}{2}, m_s = -\tfrac{1}{2}\rangle$$

$$\underbrace{\begin{pmatrix} |l + \tfrac{1}{2}, m\rangle \\ |l - \tfrac{1}{2}, m\rangle \end{pmatrix}}_{j, m\text{ - basis states}} = \underbrace{\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}}_{\text{orthonormal transformation}} \underbrace{\begin{pmatrix} |m - \tfrac{1}{2}, \tfrac{1}{2}\rangle \\ |m + \tfrac{1}{2}, -\tfrac{1}{2}\rangle \end{pmatrix}}_{m_l, m_s\text{ - basis states}}$$

$$\cos\alpha = \sqrt{\frac{l + m + 1/2}{2l + 1}} \Rightarrow \sin\alpha = \pm\sqrt{1 - \cos^2\alpha} = \pm\sqrt{\frac{l - m + 1/2}{2l + 1}}$$

$$\Rightarrow \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{l + m + 1/2}{2l + 1}} & \sqrt{\frac{l - m - \frac{1}{2}}{2l + 1}} \\ -\sqrt{\frac{l - m + 1/2}{2l + 1}} & \sqrt{\frac{l + m + 1/2}{2l + 1}} \end{pmatrix}$$

Spinorical spherical harmonics:

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

$$|m_l, \tfrac{1}{2}\rangle \mathrel{\hat{=}} Y_l^m(\vartheta, \varphi) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |m_l, -1/2\rangle = Y_l^m(\vartheta, \varphi) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$Y_{l, \frac{1}{2}}^{j = l \pm \frac{1}{2}, m}(\vartheta, \varphi) = \pm\sqrt{\frac{l \pm m + 1/2}{2l + 1}}\ Y_l^{m - \frac{1}{2}}(\vartheta, \varphi) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l \mp m + 1/2}{2l + 1}}\ Y_l^{m + 1/2}(\vartheta, \varphi) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Later application:

1) fine structure
2) Zeemann effect, Landé factor

} important for understanding

3) solving Dirac equation for hydrogen atom | atomic physics

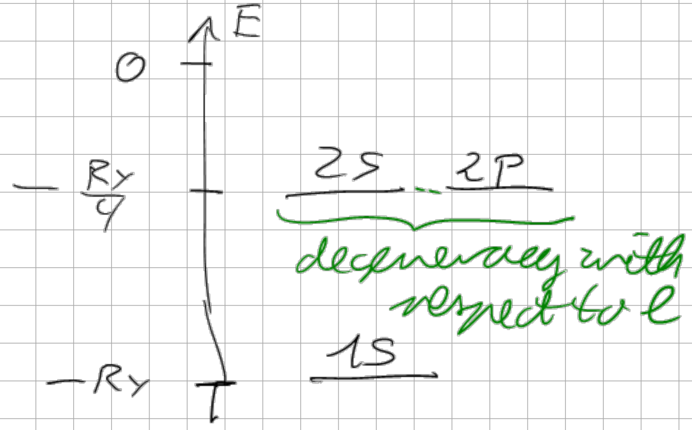
11.11 Fine structure of Hydrogen Structure:

Lecture QM I deals with non-relativistic hydrogen atom

$$\hat{H}_0 = \frac{\vec{p}^{\,2}}{2m} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$E_n^{(0)} = -R_y \frac{1}{n^2}, \quad R_y = \frac{1}{2} \underbrace{mc^2}_{0.5\,MeV} \alpha^2 = 13.6\,eV$$

$$\alpha \approx \frac{1}{137}$$



Now: special relativistic corrections

There are now 3 different special relativistic corrections which sum up to the fine structure correction, determined by Dirac theory

11.11.1 Correction of Kinetic Energy:

$$T = \sqrt{\vec{p}^{\,2}c^2 + m^2c^4} = mc^2\left\{1 + \frac{\vec{p}^{\,2}}{m^2c^2}\right\}^{1/2} \xrightarrow{|\vec{p}| \ll mc} mc^2\left\{1 + \frac{1}{2}\frac{\vec{p}^{\,2}}{m^2c^2} + \frac{1}{2}\,\frac{1}{2}\left(\frac{1}{2}-1\right)\frac{\vec{p}^{\,4}}{m^4c^4} + \dots\right\}$$

$$= \underbrace{mc^2}_{\text{rest energy}} + \underbrace{\frac{\vec{p}^{\,2}}{2m}}_{\text{non-relativistic limit}} \underbrace{- \frac{\vec{p}^{\,4}}{8m^3c^2}}_{\text{relativistic correction}} + \dots$$

The consequences of this relativistic correction of kinetic energy was calculated on Problem Set 2 due to perturbation theory based on Feynman – Hellmann theory:

$$E_{kE} = E_n^{(0)} \alpha^2 \left\{ \frac{1}{n(\ell + \frac{1}{2})} - \frac{3}{4n^2} \right\}$$

↑ lifts degeneracy of $E_n^{(0)}$ with respect to ℓ

⇒ But spin of electron yields another special relativistic correction

11.11.2 Spin-Orbit Coupling:

According to Dirac theory the electron spin leads to a magnetic moment

$$\vec{\mu} = -\mu_B g_S \frac{\vec{S}}{\hbar}$$

Bohr magneton: $\mu_B = \frac{e\hbar}{2m}$

Landé factor: $g_S = 2$

$$\Rightarrow \vec{\mu} = -\frac{e}{m}\vec{S}$$

- Electron at rest: $\vec{E} = -\vec{\nabla}\varphi, \quad \varphi = -\frac{e}{4\pi\varepsilon_0 r}$
- Electron moving with velocity $\vec{v} = \frac{\vec{p}}{m}$ sees in addition a magnetic field

$$\vec{B} = \frac{\vec{v}}{c^2} \times \vec{E} \qquad \left(\frac{|\vec{v}|}{c} \ll 1\right)$$

Energy correction:

$$-\vec{\mu}\cdot\vec{B} = \frac{e}{m}\vec{S}\cdot\vec{B} = \frac{e}{mc^2}\vec{S}\cdot(\vec{v}\times\vec{E}) = \frac{e}{m^2c^2}\vec{S}(\vec{p}\times\underbrace{\vec{E}}_{=-\vec{\nabla}\varphi})$$

$$= -\frac{e}{m^2c^2}\vec{S}(\vec{p}\times\vec{\nabla}\varphi) \quad \text{with} \quad \vec{\nabla} = \vec{e}_r\frac{\partial}{\partial r} = \frac{\vec{x}}{r}\frac{\partial}{\partial r}$$

$$= \frac{e}{m^2c^2}\frac{1}{r}\frac{\partial\varphi}{\partial r}(\vec{x}\times\vec{p})\cdot\vec{S} = \frac{e}{m^2c^2}\frac{1}{r}\frac{\partial\varphi}{\partial r}\vec{L}\cdot\vec{S}$$

A factor 2 is wrong here due to Thomas precession

$$\hat{H}_{SO} = \frac{e}{2m^2c^2} \frac{1}{r} \underbrace{\frac{\partial \varphi}{\partial r}}_{\frac{e}{4\pi\varepsilon_0 r^2}} \hat{\vec{L}} \cdot \hat{\vec{S}} = \frac{e^2}{8\pi\varepsilon_0 r^3 m^2 c^2} \boxed{\hat{\vec{L}} \cdot \hat{\vec{S}}}$$