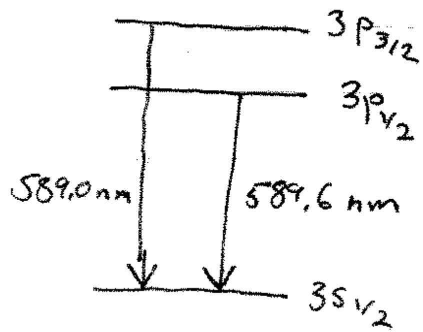
Phys 522 P.S. # 9 Solutions

Problem # 1

Alkali atoms look a lot like Hydrogen with its one valance electron. The difference is that different l-values are nondegenerate due to the overlap of the valence wavefunction with the core.

Like Hydrogen spin-orbit coupling gives rise to fine structure

Not to scale



These closely spaced spectral lines are knows a D1 and D2.

The nuclear spin gives rise to hyperfine structure. For the common isotope with atomic mass 23 amu: ^{23}Na the nuclear spin is $I = 3/2$

(a) The total angular momentum $\vec{F} = \vec{I} + \vec{J}$ has possible values according to the triangle inequality

$$|I - J| \leq F \leq I + J$$

Ground state $3S_{1/2}$: $J = 1/2$ $I = 3/2$ $\Rightarrow F = 2$ or 1

Excited states: $3P_{1/2}$: $J = 1/2$ $I = 3/2$ $\Rightarrow F = 2$ or 1

$3P_{3/2}$: $J = 3/2$ $I = 3/2$ $\Rightarrow F = 3\ 2\ 1\ 0$

radial wave function 3S understood

C-G expansion

$$|(nl_j)\ F M_F\rangle = \sum_{m_j\, m_I} \langle F M_F | j m_j\, I m_I\rangle\ |j m_j\rangle \otimes |I m_I\rangle$$

$$= \sum_{m_j} \langle F M_F | j m_j\, I\, M_F - m_j\rangle |j m_j\rangle \otimes |I\, M_F - m_j\rangle$$

<u>$3S_{1/2}$ state $F=2$</u>

$$\boxed{|3S_{1/2};\ F=2, M_F=2\rangle = |\tfrac{1}{2}\ \tfrac{1}{2}\rangle \otimes |\tfrac{3}{2}\ \tfrac{3}{2}\rangle}$$ (stretched state)

$$|3S_{1/2};\ F=2, M_F=1\rangle = \langle 2 1 | \tfrac{1}{2} \tfrac{1}{2}\ \tfrac{3}{2} \tfrac{1}{2}\rangle\ |\tfrac{1}{2}\ \tfrac{1}{2}\rangle |\tfrac{3}{2}\ \tfrac{1}{2}\rangle + \langle 2 1 | \tfrac{1}{2} -\tfrac{1}{2}\ \tfrac{3}{2} \tfrac{3}{2}\rangle\ |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle |\tfrac{3}{2}\ \tfrac{3}{2}\rangle$$

$$\boxed{|3S_{1/2};\ F=2, M_F=1\rangle = \frac{\sqrt{3}}{2} |\tfrac{1}{2} \tfrac{1}{2}\rangle |\tfrac{3}{2} \tfrac{1}{2}\rangle + \frac{1}{2} |\tfrac{1}{2} -\tfrac{1}{2}\rangle |\tfrac{3}{2}\ \tfrac{3}{2}\rangle}$$

$$|3S_{1/2};\ F=2, M_F=0\rangle = \langle 2 0 | \tfrac{1}{2} \tfrac{1}{2}\ \tfrac{3}{2} -\tfrac{1}{2}\rangle |\tfrac{1}{2} \tfrac{1}{2}\rangle |\tfrac{3}{2} -\tfrac{1}{2}\rangle + \langle 2 0 | \tfrac{1}{2} -\tfrac{1}{2}\ \tfrac{3}{2} \tfrac{1}{2}\rangle |\tfrac{1}{2} -\tfrac{1}{2}\rangle |\tfrac{3}{2} \tfrac{1}{2}\rangle$$

$$\boxed{|3S_{1/2};\ F=2, M_F=0\rangle = \frac{1}{\sqrt{2}} |\tfrac{1}{2} \tfrac{1}{2}\rangle |\tfrac{3}{2} -\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}} |\tfrac{1}{2} -\tfrac{1}{2}\rangle |\tfrac{3}{2} \tfrac{1}{2}\rangle}$$

Now use rule $\langle J\, -M | j_1\, -m_1\ j_2\, -m_2\rangle = (-1)^{j_1+j_2-j} \langle J M | j_1 m_1\ j_2 m_2\rangle$

$$\Rightarrow \boxed{|3S_{1/2};\ F=2;\ M_F=-1\rangle = \frac{\sqrt{3}}{2} |\tfrac{1}{2} -\tfrac{1}{2}\rangle |\tfrac{3}{2} -\tfrac{1}{2}\rangle + \frac{1}{2} |\tfrac{1}{2} +\tfrac{1}{2}\rangle |\tfrac{3}{2} -\tfrac{3}{2}\rangle}$$

$$\boxed{|3S_{1/2},\ F=2\ M_F=-2\rangle = |\tfrac{1}{2} -\tfrac{1}{2}\rangle |\tfrac{3}{2}\ -\tfrac{3}{2}\rangle}$$

(stretched state)

The $3s_{1/2}$ state, $F=1$

We can determine these (up to an overall phase) just by orthogonality and selection rules. ~~Here~~ I will just use C-G coeffs

$$\boxed{\begin{aligned}
|3s_{1/2};\ F=1\ M_F=1\rangle &= \tfrac{1}{2}\,|\tfrac{1}{2}\,\tfrac{1}{2}\rangle|\tfrac{3}{2}\,\tfrac{1}{2}\rangle - \tfrac{\sqrt{3}}{2}\,|\tfrac{1}{2}\,\tfrac{-1}{2}\rangle|\tfrac{3}{2}\,\tfrac{3}{2}\rangle \\
|3s_{1/2};\ F=1\ M_F=0\rangle &= \tfrac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\,\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle - |\tfrac{1}{2}\,\tfrac{-1}{2}\rangle|\tfrac{3}{2}\,{+\tfrac{1}{2}}\rangle\right) \\
|3s_{1/2};\ F=1\ M_F=-1\rangle &= -\tfrac{1}{2}\,|\tfrac{1}{2}\,\tfrac{-1}{2}\rangle|\tfrac{3}{2}\,\tfrac{-1}{2}\rangle + \tfrac{\sqrt{3}}{2}\,|\tfrac{1}{2}\,{+\tfrac{1}{2}}\rangle|\tfrac{3}{2}\,\tfrac{-3}{2}\rangle
\end{aligned}}$$

We clearly see that $\langle F'M_F'|FM_F\rangle = \delta_{FF'}\,\delta_{M_F' M_F}$ for all states in this manifold

The $3p_{1/2}$ state $F=2$ or 1

These states have the same addition of $\vec{J}+\vec{I}$ as the $3s_{1/2}$ state and thus have the same ~~decomps~~ decomposition in the uncoupled basis $|j\,M_j\rangle|I\,M_I\rangle$. These states differ from $3s_{1/2}$ in the radial wave funct.

$3P_{3/2}$ state $F=3$

Now $j=3/2$ $I=3/2$

Stretched state $\boxed{|3p_{3/2};\ F=3\ M_F=3\rangle = |\tfrac{3}{2}\,\tfrac{3}{2}\rangle \otimes |\tfrac{3}{2}\,\tfrac{3}{2}\rangle}$

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$$|3P_{3/2};\ F=3, M_F=2\rangle = \langle 32|\tfrac{3}{2}\tfrac{3}{2}\ \tfrac{3}{2}\tfrac{1}{2}\rangle\ |\tfrac{3}{2}\tfrac{3}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{1}{2}\rangle + \langle 32|\tfrac{3}{2}\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{3}{2}\rangle\ |\tfrac{3}{2}\tfrac{1}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{3}{2}\rangle$$

$$\boxed{|F=3, M_F=2\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle\right)}$$

$$|3P_{3/2};\ F=3, M_F=1\rangle = \langle 31|\tfrac{3}{2}\tfrac{3}{2}\ \tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle\ |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \langle 31|\tfrac{3}{2}\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\rangle\ |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \langle 31|\tfrac{3}{2}\,{-\tfrac{1}{2}}\ \tfrac{3}{2}\tfrac{3}{2}\rangle\ |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$

$$= \frac{1}{\sqrt{5}}|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \sqrt{\tfrac{3}{5}}\,|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \frac{1}{\sqrt{5}}|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$

$$|3P_{3/2};\ F=3, M_F=0\rangle = \langle 30|\tfrac{3}{2}\tfrac{3}{2}\ \tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle\ |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle + \langle 30|\tfrac{3}{2}\tfrac{1}{2}\ \tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle\ |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \langle 30|\tfrac{3}{2}\,{-\tfrac{1}{2}}\ \tfrac{3}{2}\tfrac{1}{2}\rangle\ |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \langle 30|\tfrac{3}{2}\,{-\tfrac{3}{2}}\ \tfrac{3}{2}\tfrac{3}{2}\rangle\ |\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$

$$= \frac{1}{2\sqrt{5}}|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle + \frac{3}{2\sqrt{5}}|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \frac{3}{2\sqrt{5}}|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \frac{1}{2\sqrt{5}}|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$

Again using the $M \to -M$ C-G rule

$$|3P_{3/2};\ F=3\ M_F=-1\rangle = \frac{1}{\sqrt{5}}|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \sqrt{\tfrac{3}{5}}\,|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \frac{1}{\sqrt{5}}|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle$$

$$|3P_{3/2};\ F=3\ M_F=-2\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle\right)$$

$$|3P_{3/2};\ F=3\ M_F=-3\rangle = |\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle$$

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$3P_{3/2}$ F = 2 state

Again, up to a phase we can find these through selection rules and orthogonality to $3P_{1/2}$ F = 2 states. Here I will use C-G coefficients.

$$|3P_{3/2}\ F=2, M_F=2\rangle = \langle 2\,2|\tfrac{3}{2}\tfrac{3}{2}\ \tfrac{3}{2}\tfrac{1}{2}\rangle |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \langle 2\,2|\tfrac{3}{2}\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\rangle |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$
$$= \frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle - |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle\right)$$

$$|3P_{3/2}\ F=2\ M_F=1\rangle = \langle 2\,1|\tfrac{3}{2}\tfrac{3}{2}\ \tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \langle 2\,1|\tfrac{3}{2}\tfrac{1}{2}\ \tfrac{3}{2}\tfrac{1}{2}\rangle |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \langle 2\,1|\tfrac{3}{2}\,{-\tfrac{1}{2}}\ \tfrac{3}{2}\tfrac{3}{2}\rangle |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$
$$= \frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle - |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle\right)$$

$$|3P_{3/2}, F=2\ M_F=0\rangle = \langle 2\,0|\tfrac{3}{2}\tfrac{3}{2}\ \tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle + \langle 2\,0|\tfrac{3}{2}\tfrac{1}{2}\ \tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle + \langle 2\,0|\tfrac{3}{2}\,{-\tfrac{1}{2}}\ \tfrac{3}{2}\tfrac{1}{2}\rangle |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle + \langle 2\,0|\tfrac{3}{2}\,{-\tfrac{3}{2}}\ \tfrac{3}{2}\tfrac{3}{2}\rangle |\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle$$
$$= +\frac{1}{2}\left(|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle + |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle - |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle - |\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle\right)$$

~~Again~~

$$3P_{3/2}\quad |F=2\ M_F=-1\rangle = -\frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle - |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle\right)$$
$$|F=2\ M_F=-2\rangle = -\frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle - |\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle\right)$$

$3p_{3/2}$ F=1 state

$$\boxed{\begin{aligned}|3p_{3/2};\ F=1\ M_F=1\rangle = &\sqrt{\tfrac{3}{10}}\left(|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{-1}{2}\rangle\right) - \sqrt{\tfrac{2}{5}}\,|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle \\ &+\sqrt{\tfrac{3}{10}}\,|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle|\tfrac{3}{2}\ \tfrac{3}{2}\rangle\end{aligned}}$$

$$\boxed{\begin{aligned}|3p_{3/2};\ F=1\ M_F=0\rangle = \tfrac{1}{\sqrt{5}}\Big(&\tfrac{3}{2}|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\text{-}\tfrac{3}{2}\rangle - \tfrac{1}{2}|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\text{-}\tfrac{1}{2}\rangle - \tfrac{1}{2}|\tfrac{3}{2}\text{-}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle \\ &+ \tfrac{3}{2}|\tfrac{3}{2}\text{-}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle\end{aligned}}$$

$$\boxed{\begin{aligned}|3p_{3/2};\ F=1\ M_F=-1\rangle = &\sqrt{\tfrac{3}{10}}\ |\tfrac{3}{2}\text{-}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle - \sqrt{\tfrac{2}{5}}\,|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle \\ &+\sqrt{\tfrac{3}{10}}\,|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\ -\tfrac{3}{2}\rangle\end{aligned}}$$

Finally!

$$\boxed{\begin{aligned}|3p_{3/2};\ F=0\ M=0\rangle = \tfrac{1}{2}\Big(&|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\text{-}\tfrac{3}{2}\rangle - |\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\text{-}\tfrac{1}{2}\rangle + |\tfrac{3}{2}\text{-}\tfrac{1}{2}\rangle|\tfrac{3}{2}\ \tfrac{1}{2}\rangle \\ &- |\tfrac{3}{2}\text{-}\tfrac{3}{2}\rangle|\tfrac{3}{2}\ \tfrac{3}{2}\rangle\Big)\end{aligned}}$$

This will always be an equally weighted ~~supperpo~~ superposition, i.e. for $j+j \rightarrow J=0$

$|0\ 0\rangle$ = equally weighted superposition of anti correllated state $|j\,m\rangle|j\,-m\rangle$

The simplest example is the spin-singlet

$$|0\,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

(b) Check using recursion relations

Start with streched state

$$|F=3\ M_F=3\rangle = |\tfrac{3}{2}\ \tfrac{3}{2}\rangle \otimes |\tfrac{3}{2}\ \tfrac{3}{2}\rangle$$

$$\hat{F}_- = \hat{J}_- + \hat{I}_- \Rightarrow \hat{F}_-|F=3, M_F=3\rangle = \hat{J}_-|\tfrac{3}{2}\tfrac{3}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{3}{2}\rangle + |\tfrac{3}{2}\tfrac{3}{2}\rangle \otimes \hat{I}_-|\tfrac{3}{2}\ \tfrac{3}{2}\rangle$$

$$\Rightarrow \sqrt{3(3+1) - 3(3-1)}\,|F=3, M_F=2\rangle = \sqrt{\tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{3}{2}(\tfrac{3}{2}-1)}\left(|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle + |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle\right)$$

$$\Rightarrow \boxed{|F=3, M_F=2\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle + |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\ \tfrac{1}{2}\rangle\right)} \checkmark$$

$$\hat{F}_-|F=3, M_F=2\rangle = \frac{1}{\sqrt{2}}\hat{J}_-|\tfrac{3}{2}\tfrac{1}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{3}{2}\rangle + \frac{1}{\sqrt{2}}|\tfrac{3}{2}\tfrac{1}{2}\rangle \otimes I_-|\tfrac{3}{2}\ \tfrac{3}{2}\rangle + \frac{1}{\sqrt{2}}\hat{J}_-|\tfrac{3}{2}\tfrac{3}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}}|\tfrac{3}{2}\tfrac{3}{2}\rangle \otimes I_-|\tfrac{3}{2}\ \tfrac{1}{2}\rangle$$

$$\sqrt{3(3+1) - 2(2-1)}\,|F=3, M_F=1\rangle = \frac{1}{\sqrt{2}}\sqrt{\tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}-1)}\left(|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{3}{2}\rangle + |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle\right) + \frac{2}{\sqrt{2}}\sqrt{\tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{3}{2}(\tfrac{3}{2}-1)}\left(|\tfrac{3}{2}\tfrac{1}{2}\rangle \otimes |\tfrac{3}{2}\tfrac{1}{2}\rangle\right)$$

$$\Rightarrow \boxed{|F=3, M_F=1\rangle = \frac{1}{\sqrt{5}}\left(|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle \otimes |\tfrac{3}{2}\ \tfrac{3}{2}\rangle + |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle\right) + \sqrt{\frac{3}{5}}\left(|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle\right)} \checkmark$$

$$\sqrt{3(3+1) - 0}\,|F=3, M_F=0\rangle = \frac{1}{\sqrt{5}}\sqrt{\tfrac{3}{2}(\tfrac{3}{2}+1) + \tfrac{1}{2}(-\tfrac{1}{2}-1)}\left(|\tfrac{3}{2} -\tfrac{3}{2}\rangle|\tfrac{3}{2}\ \tfrac{3}{2}\rangle + |\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2} -\tfrac{3}{2}\rangle\right) + \frac{1}{\sqrt{5}}\sqrt{\tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{3}{2}(\tfrac{3}{2}-1)}\left(|\tfrac{3}{2}\ \tfrac{1}{2}\rangle|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle + |\tfrac{3}{2} -\tfrac{1}{2}\rangle|\tfrac{3}{2}\ \tfrac{1}{2}\rangle\right) + \sqrt{\frac{3}{5}}\sqrt{\tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}-1)}\left(|\tfrac{3}{2}\ \tfrac{1}{2}\rangle|\tfrac{3}{2}\ -\tfrac{1}{2}\rangle + |\tfrac{3}{2} -\tfrac{1}{2}\rangle|\tfrac{3}{2}\ \tfrac{1}{2}\rangle\right)$$

$$\Rightarrow |F=3, M_F=0\rangle = \frac{1}{2\sqrt{5}}\left(|\tfrac{3}{2}\tfrac{3}{2}\rangle|\tfrac{3}{2} -\tfrac{3}{2}\rangle + |\tfrac{3}{2} -\tfrac{3}{2}\rangle|\tfrac{3}{2}\tfrac{3}{2}\rangle\right) + \frac{3}{2\sqrt{5}}\left(|\tfrac{3}{2}\tfrac{1}{2}\rangle|\tfrac{3}{2} -\tfrac{1}{2}\rangle + |\tfrac{3}{2} -\tfrac{1}{2}\rangle|\tfrac{3}{2}\tfrac{1}{2}\rangle\right)$$

(6) Dipole matrix elements $\langle 3p_{1/2}\ F' M_F' \,|\, \hat{d}_z \,|\, 3s_{1/2}\ F M_F \rangle$

In problem set 1 we found

$\langle P_{1/2}\ m_j' \,|\, \hat{d}_z \,|\, S_{1/2}\ m_j \rangle$ <u>vanished</u> unless $m_j = m_j'$

Example: $\langle 3P_{1/2}\ F=1\ M_F' \,|\, \hat{d}_z \,|\, 3S_{1/2}\ F=1\ 0 \rangle$

$M_F' = 1$:
$$\left(\tfrac{1}{2}\langle \tfrac{1}{2}\,\tfrac{1}{2}|\langle \tfrac{3}{2}\,\tfrac{1}{2}| - \tfrac{\sqrt{3}}{2}\langle \tfrac{1}{2}\,-\tfrac{1}{2}|\langle \tfrac{3}{2}\,\tfrac{3}{2}|\right)\hat{d}_z \left(\tfrac{1}{\sqrt{2}}|\tfrac{1}{2}\,\tfrac{1}{2}\rangle|\tfrac{3}{2}\,-\tfrac{1}{2}\rangle - \tfrac{1}{\sqrt{2}}|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle|\tfrac{3}{2}\,\tfrac{1}{2}\rangle\right)$$

$$= \frac{1}{2\sqrt{2}}\langle \underset{j}{\tfrac{1}{2}}\,\underset{m_j}{\tfrac{1}{2}}|\, d_z \,|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle$$ using orthogonality of $|I\ m_I\rangle$ states

$= 0$ from above

$M_F' = 0$
$$\left(\tfrac{1}{\sqrt{2}}\langle \tfrac{1}{2}\,\tfrac{1}{2}|\langle \tfrac{3}{2}\,-\tfrac{1}{2}| - \tfrac{1}{\sqrt{2}}\langle \tfrac{1}{2}\,-\tfrac{1}{2}|\langle \tfrac{3}{2}\,\tfrac{1}{2}|\right) \hat{d}_z \left(\tfrac{1}{\sqrt{2}}|\tfrac{1}{2}\,\tfrac{1}{2}\rangle|\tfrac{3}{2}\,-\tfrac{1}{2}\rangle - \tfrac{1}{\sqrt{2}}|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle|\tfrac{3}{2}\,\tfrac{1}{2}\rangle\right)$$

$$= \frac{1}{2}\langle P_{1/2}\,\tfrac{1}{2}|\,\hat{d}_z\,|S_{1/2}\,\tfrac{1}{2}\rangle + \frac{1}{2}\langle P_{1/2}\,-\tfrac{1}{2}|\,\hat{d}_z\,|S_{1/2}\,-\tfrac{1}{2}\rangle$$

$M_F' = -1$
$$\left(-\tfrac{1}{2}\langle \tfrac{1}{2}\,-\tfrac{1}{2}|\langle \tfrac{3}{2}\,-\tfrac{1}{2}| + \tfrac{\sqrt{3}}{2}\langle \tfrac{1}{2}\,\tfrac{1}{2}|\langle \tfrac{3}{2}\,-\tfrac{3}{2}|\right)\hat{d}_z \left(\tfrac{1}{\sqrt{2}}|\tfrac{1}{2}\,\tfrac{1}{2}\rangle|\tfrac{3}{2}\,-\tfrac{1}{2}\rangle - \tfrac{1}{\sqrt{2}}|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle|\tfrac{3}{2}\,\tfrac{1}{2}\rangle\right)$$

$$= -\frac{1}{2}\langle \tfrac{1}{2}\,-\tfrac{1}{2}|\,\hat{d}_z\,|\tfrac{1}{2}\,\tfrac{1}{2}\rangle = 0$$

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Thus we see the selection rule

$$\langle 3p_{1/2}\ F' M_F' \mid \hat{d}_z \mid 3s_{1/2}\ F M_F \rangle$$

vanishes unless $M_F = M_F'$

This is another example of the Wigner-Eckart theorem. We will find a <u>MUCH</u> simpler and less tedious way of instantly determining this rule

Problem 2: Zeeman effect in ground state of hydrogen

$$\hat{H} = \underbrace{A\,\hat{\vec{\imath}}\cdot\hat{\vec{s}}}_{\substack{\text{hyperfine}\\ \text{coupling}}} + \underbrace{g_e \mu_B \vec{B}\cdot\hat{\vec{s}} - g_p \mu_N \vec{B}\cdot\hat{\vec{\imath}}}_{\text{coupling to external } \vec{B}\text{-field}}$$

$$\equiv \hat{H}_{HF} + \hat{H}_B$$

(a) Weak field: $\mu_B B \ll A$.

$\frac{A}{h} \cong 1.42\,\text{GHz}$ for 1s of hydrogen

$\frac{\mu_B}{h} \cong 1.4\ \text{MHz/Gauss}$ (Bohr Magneton)

$$\Rightarrow \boxed{\text{Weak } B \lesssim\!< 1\,\text{kG} \quad (1{,}000 \text{ Gauss})}$$

In the weak-field limit $\hat{H}_B$ is a perturbation to $\hat{H}_{HF}$. The "good quantum numbers" are those that ~~eigen~~ define the eigenvector of $\hat{H}_{HF}$. These are the coupled angular momentum.

$$\boxed{|F\, M_F,\, i, s\rangle \quad (\text{also principle quantum number } n\text{, and orbital } l)}$$

The shifts, to lowest nonvanish order are first order

$$\delta E^{(1)}_{FM_F} = \langle F M_F, i, s|\, \hat{H}_B\, |F M_F, i s\rangle$$

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From Lecture, we have the eigenstates in coupled representation

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

F=0
$$\left\{ |F=0, M_F=0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right) \right.$$

Where $|\pm, \pm\rangle$ — electron spin up/down, proton spin up/down

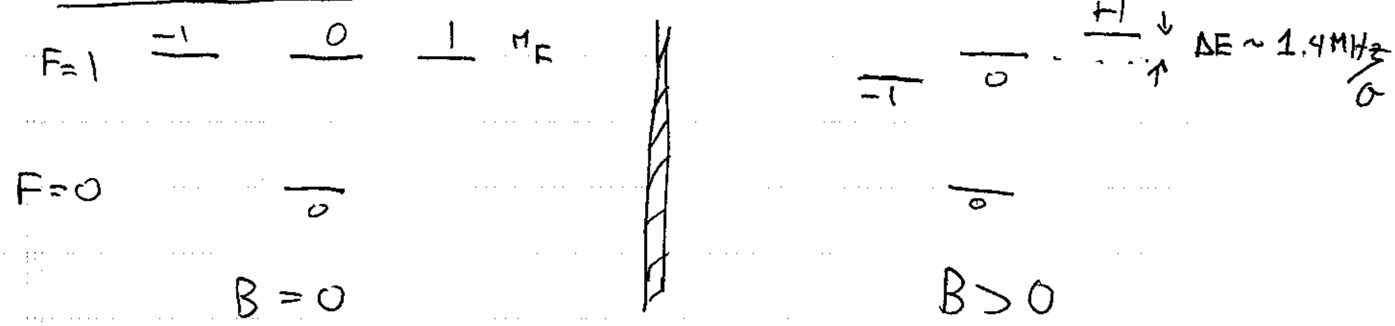
Aside: In the uncoupled basis

$$\langle m_s', m_i' | \hat{H}_B | m_s, m_i \rangle = g_e \mu_B B\, m_s\, \delta_{m_s m_s'} \cancel{- g_p \mu_N B\, m_i\, \delta_{m_i m_i'}}$$ neglect

In the weak field regime $\mu_N B$ is negligible

$$\Rightarrow \boxed{\begin{aligned} \delta E^{(1)}_{F=1, M_F=1} &= g_e \frac{\mu_B B}{2} \cong (1.4\ \text{MHz/Gauss})\, B \\ \delta E^{(1)}_{F=1, M_F=0} &= 0 \\ \delta E^{(1)}_{F=1, M_F=-1} &= -g_e \frac{\mu_B B}{2} \cong (-1.4\ \text{MHz/Gauss})\, B \\ \delta E^{(1)}_{F=0, M_F=0} &= 0 \end{aligned}}$$

Zeeman Shifts in Weak-field limit



Zeeman shift linear w/ B

(b) In the very strong field limit (Pashen-Back regime) $\hat{H}_B$ is dominant; $\hat{H}_{HF}$ is a perturbation

$\hat{H}_B$ commutes with $\hat{S}_z$ and $\hat{i}_z$ (taking $\vec{B}$ in the z-direction) $\Rightarrow$ Good quantum numbers are the "uncoupled representation"

$$|s\, m_s\rangle |i\, m_i\rangle$$

- To zeroth order, the energy levels are the eigenstates of $\hat{H}_B$

$$\boxed{E^{(0)}_{m_s,m_i} = g_e \mu_B B m_s - g_p \mu_N B m_i \quad \text{Typically negligible}}$$

Again linear in B, but near degenerate in m_i

- The first-order correction (due to hyperfine coupling)

$$\delta E^{(1)}_{m_s m_i} = \langle m_s m_i | A \hat{\vec{I}} \cdot \hat{\vec{S}} | m_s m_i \rangle = A \langle m_s m_i | \left(\frac{\hat{I}_+ \hat{S}_- + \hat{I}_- \hat{S}_+}{2} + \hat{I}_z \hat{S}_z \right) | m_s m_i \rangle$$

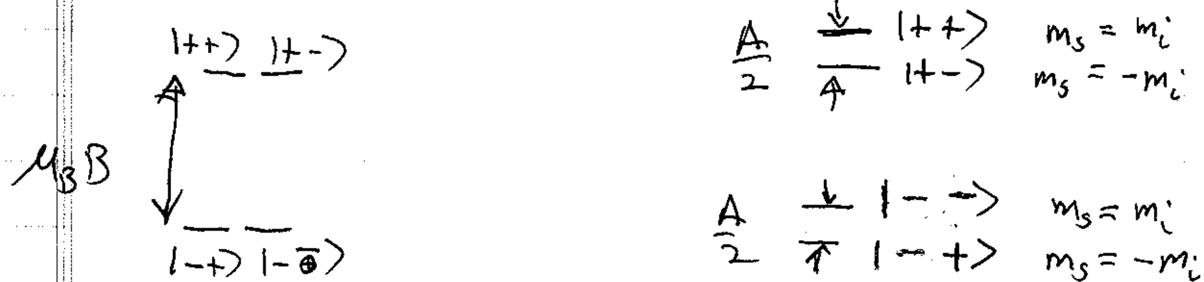
$$\Rightarrow \boxed{\delta E^{(1)}_{m_s m_i} = A\, m_s m_i}$$

(b) Continued

$$\Rightarrow \quad \delta E^{(1)}_{m_s m_i} = \frac{A}{4} \qquad m_s = m_i = \pm\frac{1}{2}$$

$$\delta E^{(1)}_{m_s m_i} = -\frac{A}{4} \qquad -m_s = m_i = \pm\frac{1}{2}$$

<u>Zeeman shift in Pashen-Back regime</u>



No Hyperfine
(neglecting nuclear)

Note: For very very large fields such that $\mu_N B >> A$ the nuclear spin cannot be neglected and nuclear spin-up is shifted down in energy relative to nuclear spin-down.

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(c) Exact diagonalization in 1s subspace

$$\hat{H} = \underbrace{A\hat{\vec{I}}\cdot\hat{\vec{S}}}_{\hat{H}_{HF}} + \underbrace{g_e \mu_B B \hat{S}_z - g_p \mu_N B \hat{I}_z}_{\hat{H}_B}$$

Consider: $\hat{F}_z = \hat{S}_z + \hat{I}_z$

Since $[\hat{S}_z, \hat{F}_z] = 0$ and $[\hat{I}_z, \hat{F}_z] = 0$

$$\Rightarrow [\hat{H}_B, \hat{F}_z] = 0$$

Also, since $\vec{I}\cdot\vec{S} = \dfrac{F^2 - I^2 - S^2}{2}$

and $[\hat{F}^2, \hat{F}_z] = 0$, $[\hat{I}^2, \hat{F}_z] = 0$, $[\hat{S}^2, \hat{F}_z] = 0$

$$\Rightarrow [\hat{H}_{HF}, \hat{F}_z] = 0$$

$$\Rightarrow \boxed{[\hat{H}, \hat{F}_z] = 0}$$

$\Rightarrow$ $\hat{H}$ is block-diagonal in subspaces with a given value of $\hat{F}_z$

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We will write a matrix representation of $\hat{H}$ is the coupled basis. The three possible values of M_F determine three subspaces

$\underline{M_F = 1}$: Only one state: $|F=1, M_F=1\rangle$

$\underline{M_F=-1}$: Only one state: $|F=1, M_F-1\rangle$

$\underline{M_F=0}$: 2D subspace $\underbrace{|F=0, M_F=0\rangle \text{ and } |F=1, M_F=0\rangle}$

$\hat{H}_{HF}$ is diagonal in this basis. $\hat{H}_B$ has off-diagonal elements in the $M_F=0$ subspace.

Ordering the basis $\{|\underset{F}{1},\underset{M_F}{1}\rangle, |1\,{-1}\rangle, |1\,0\rangle, |0,0\rangle\}$

$$\hat{H} = \underbrace{\begin{bmatrix} \frac{A}{4} & 0 & 0 & 0 \\ 0 & \frac{A}{4} & 0 & 0 \\ 0 & 0 & \frac{A}{4} & 0 \\ 0 & 0 & 0 & -3\frac{A}{4} \end{bmatrix}}_{\hat{H}_{HF}} + \underbrace{\begin{bmatrix} (g_e \mu_B - g_p \mu_N)\frac{B}{2} & 0 & 0 & 0 \\ 0 & -(g_e\mu_B - g_p\mu_N)B & 0 & 0 \\ 0 & 0 & 0 & \langle 10|\hat{H}_B|00\rangle \\ 0 & 0 & \langle 00|\hat{H}_B|10\rangle & 0 \end{bmatrix}}_{\hat{H}_B}$$

Aside: $\langle 10|\hat{H}_B|00\rangle = \left(\frac{\langle +-| + \langle -+|}{\sqrt{2}}\right)\left(g_e\mu_B B\hat{S}_z - g_p\mu_N \hat{I}_z\right)\left(\frac{|+-\rangle - |-+\rangle}{\sqrt{2}}\right)$

$$= \frac{g_e\mu_B B}{2} + \frac{g_p \mu_N B}{2}$$

In the $M_F = \pm 1$ subspaces $|1,1\rangle$ and $|1,-1\rangle$ are eigenvectors of the total Hamiltonian, with eigenvalue

$$\boxed{E(M_F = \pm 1) = \frac{A}{4} \pm (g_e \mu_B - g_p \mu_N)\frac{B}{2}}$$

In the $M_F = 0$ subspace, we must diagonalize the 2X2 block

$$\hat{H}_{M_F=0} = \begin{bmatrix} \frac{A}{4} & (g_e \mu_B + g_p \mu_N)\frac{B}{2} \\ (g_e \mu_B + g_p \mu_N)\frac{B}{2} & -\frac{3A}{4} \end{bmatrix}$$

$$= A \begin{bmatrix} \frac{1}{4} & \frac{x}{2} \\ \frac{x}{2} & -\frac{3}{4} \end{bmatrix}$$

where

$$\boxed{x \equiv (g_e \mu_B + g_p \mu_N)\frac{B}{A}}$$

Eigenvalues: $A\left(-\frac{1}{4} \pm \frac{1}{2}\sqrt{1+x^2}\right)$

$$\Rightarrow \boxed{E_{\pm}(M_F=0) = -\frac{A}{4} \pm \frac{A}{2}\sqrt{1+x^2}}$$

Check w/ Breit-Rabi formula

$$E_{\pm}(M_F) = -g_p \mu_N B m_F - \frac{A}{4} \pm \frac{A}{2}\sqrt{1 + 2m_F x + x^2}$$

$M_F = \pm 1$ $\quad E_{\pm}(\pm 1) = \mp g_p \mu_N B - \frac{A}{4} \pm \frac{A}{2}(x \pm 1)$

Here 10, so only one root (+ root for $M_F = +1$
− root for $M_F = -1$)

$$\Rightarrow E(M_F=\pm 1) = \frac{A}{4} \pm \frac{A}{2}\chi \mp g_p \mu_N B$$

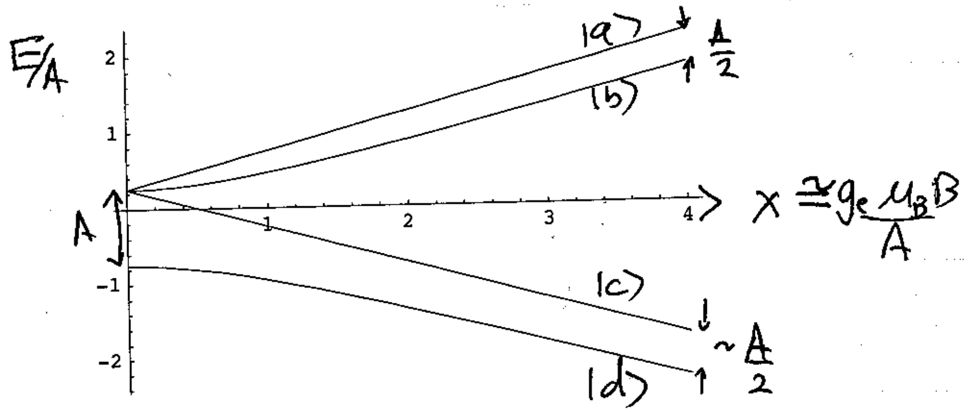
$$= \frac{A}{4} \pm (g_e \mu_B + g_p \mu_N)\frac{B}{2} \mp g_p \mu_N B$$

$$\Rightarrow \boxed{E(M_F \pm 1) = \frac{A}{4} \pm (g_e \mu_B - g_p \mu_N)\frac{B}{2}}$$

For $M_F = 0$, we have two roots

$$\boxed{E(M_F=0) = -\frac{A}{4} \pm \frac{A}{2}\sqrt{1+\chi^2}}$$

(d)



Breit - Rabi diagram (neglecting nuclear magneton)

- For $x \ll 1$ (weak field) we see shifts within the hyperfine manifold $|F M_F\rangle$
- For $x \gg 1$ (strong field) the spins decouple and separately shift.

$$|a\rangle = |F=1, M_F=1\rangle = |++\rangle$$
$$|c\rangle = |F=1, M_F-1\rangle = |--\rangle$$

$|b\rangle \longrightarrow |F=1, M_F=0\rangle$ (weak) $\quad |+-\rangle$ (strong)

$|d\rangle \rightarrow |F=0, M=0\rangle$ (weak) $\quad |-+\rangle$ (strong)

(e) ~~Assump~~ Asymptotic expansions

- For $M_F = \pm 1$, the eigenvalue has the same form, independent of B (stretched state)

$$E(M_F = \pm 1) = \frac{A}{4} \pm g_e \mu_B B \quad (\text{neglecting } \mu_N)$$

- For $M_F = 0$ we must expand $-\frac{A}{4} \pm \frac{A}{2}\sqrt{1+x^2}$

Weak Field $\quad x = \frac{\mu_B B}{A} \ll 1$

$$\delta E^{(1)}(M_F = \pm 1) = \pm g_e \mu_B B$$

$$\delta E^{(1)}(M_F = 0) = 0 \quad (\text{no shift in first order})$$

Strong Field $\quad x \gg 1$

$$\delta E^{(1)}(M_F = \pm 1) = \frac{A}{4} = (\pm\tfrac{1}{2})(\pm\tfrac{1}{2})A \checkmark$$

$$\delta E^{(1)}(M_F = 0) = -\frac{A}{4} = (\pm\tfrac{1}{2})(\mp\tfrac{1}{2})A \checkmark$$

These agree with perturbation theory