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a) $H = H_0 + H_{so} + H_z$ where $H_{so} = \frac{\hbar}{4m^2c^2} (\nabla V \times p) \cdot \sigma$

note $H_0 |\psi\rangle = 0$ by definition

and $H_z = \frac{e\hbar}{mc} \vec{B} \cdot \sigma$

We assume $H_{so} \gg H_z$ and treat H_z as a perturbation on H_{so}
 first we find the eigenstates of H_{so}

Let us write

$$H_{so} = \frac{\hbar}{4m^2c^2} \frac{\partial V}{\partial x_j} P_k \epsilon_{jkm} \sigma_m$$

where $x_j \in \{x, y, z\}$ and $\sigma_m \in \{\sigma_x, \sigma_y, \sigma_z\}$
 $P_k \in \{P_x, P_y, P_z\}$ the Pauli matrices.

We need to consider terms like

$$\langle \uparrow | \langle X | H_{so} | Y \rangle | \uparrow \rangle = \frac{\hbar}{4m^2c^2} \langle X | \frac{\partial V}{\partial x} P_y | Y \rangle \langle \uparrow | \sigma_z | \uparrow \rangle$$

We can consider them at once by assigning indices

$$\langle X_p | \langle X_i | H_{so} | X_\ell \rangle | X_n \rangle = \frac{\hbar}{4m^2c^2} \langle X_i | \frac{\partial V}{\partial x_j} P_k | X_\ell \rangle \langle X_p | \sigma_m | X_n \rangle \epsilon_{jkm}$$

↳ this term is nothing more than the p^{th} row n^{th} column of the Pauli matrix

Now V is Even in each of the 3 dimensions of symmetry in the crystal, so $\frac{\partial V}{\partial x_j}$ is odd in x_j . Since $|X_\ell\rangle$ is odd in x_ℓ , $P_k |X_\ell\rangle$ is odd in x_k and x_ℓ (or even in all if $k=\ell$). Therefore j must equal k and $i=k$ or $i=j$ if $k=\ell$. Note j may not equal k because of the Levi-Civita symbol ϵ_{jkm} .

Note also that since both V and $|X_i\rangle$ are symmetric upon interchange $x \rightarrow y \rightarrow z \rightarrow x$ (not to mention the same symmetry of p) There are only two independent values of this matrix element:

$$\langle p | H_{30} | l n \rangle = \frac{\hbar}{4m^2 c^2} (A \delta_{kl} \delta_{ij} + B \delta_{ki} \delta_{jl}) \sigma_{pn}^{(m)} \epsilon_{jkm}$$

where $A = \langle X | \frac{\partial V}{\partial x} \frac{\partial}{\partial y} | Y \rangle \frac{\hbar}{i}$ and $B = \langle X | \frac{\partial V}{\partial y} \frac{\partial}{\partial x} | Y \rangle \frac{\hbar}{i}$

(note A & B are pure imaginary for real $|X_i\rangle$ and V)

simplifying, we have

$$\begin{aligned} \langle p | H_{30} | l n \rangle &= \frac{\hbar}{4m^2 c^2} (A \delta_{kl} \delta_{ij} \epsilon_{jkm} + B \delta_{ki} \delta_{jl} \epsilon_{jkm}) \sigma_{pn}^{(m)} \\ &= \frac{\hbar}{4m^2 c^2} (A \epsilon_{ilm} + B \epsilon_{lim}) \sigma_{pn}^{(m)} = \frac{\hbar}{4m^2 c^2} (A+B) \epsilon_{ilm} \sigma_{pn}^{(m)} \\ &= iC \epsilon_{ilm} \sigma_{pn}^{(m)} \quad \text{by letting } C = \frac{1}{i} \frac{\hbar}{4m^2 c^2} (A+B) \end{aligned}$$

in matrix form:

		i		2		3	
l	n	P	1	2	1	2	1
1		2					i
2		2					$-i$
3		2					$-i$

$$\cdot iC = iC \begin{bmatrix} 0 & -\sigma_z & \sigma_y \\ \sigma_z & 0 & \sigma_x \\ \sigma_y & \sigma_x & 0 \end{bmatrix}$$

Allowing Mathematica to find the eigensystem gives us eigenvectors

$$-|X\rangle\uparrow - i|Y\rangle\uparrow + |Z\rangle\downarrow$$

$$\& \quad |X\rangle\downarrow - i|Y\rangle\downarrow + |Z\rangle\uparrow \quad \text{with value } -2C$$

$$\text{(ie } \begin{bmatrix} -1 \\ 0 \\ -i \\ 0 \\ 0 \\ 1 \end{bmatrix} \& \begin{bmatrix} 0 \\ 1 \\ 0 \\ i \\ +1 \\ 0 \end{bmatrix} \text{)}$$

$$\text{and } |X\rangle\uparrow + |Z\rangle\downarrow \sim \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}$$

$$-|X\rangle\downarrow + |Z\rangle\uparrow \sim \begin{bmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$i|X\rangle\downarrow + |Y\rangle\downarrow \sim \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

with value +C

$$\& \quad -i|X\rangle\uparrow + |Y\rangle\uparrow \sim \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -C \\ 0 \end{bmatrix}$$

of course any linear combo within each subset is also an eigenvector

Let us adopt the ^{combinations} basis given in class, since it is designed to diagonalize H_z , and label them $|j m_j\rangle$

$|\frac{3}{2} m_j\rangle$ correspond to the 4-fold degeneracy and $|\frac{1}{2} m_j\rangle$ correspond to the two-fold (i.e. the HH and LH states and the SO states respectively)

Degenerate perturbation theory requires diagonalizing each degenerate set individually. Supposing $B = B_0 \hat{z}$, $H_2 = \frac{e\hbar B_0}{mc} \sigma_z = E_B \sigma_z$

$$\begin{vmatrix} \langle \frac{1}{2} +\frac{1}{2} | H_2 | \frac{1}{2} +\frac{1}{2} \rangle & \langle \frac{1}{2} +\frac{1}{2} | H_2 | \frac{1}{2} -\frac{1}{2} \rangle \\ \langle \frac{1}{2} -\frac{1}{2} | H_2 | \frac{1}{2} +\frac{1}{2} \rangle & \langle \frac{1}{2} -\frac{1}{2} | H_2 | \frac{1}{2} -\frac{1}{2} \rangle \end{vmatrix} = \begin{bmatrix} \langle \frac{1}{2} +\frac{1}{2} | \\ \langle \frac{1}{2} -\frac{1}{2} | \end{bmatrix} H_2 \begin{bmatrix} | \frac{1}{2} +\frac{1}{2} \rangle \\ | \frac{1}{2} -\frac{1}{2} \rangle \end{bmatrix}$$

$$= \frac{1}{3} \begin{bmatrix} 0 & -1 & 0 & i & 1 & 0 \\ 1 & 0 & i & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & & & \\ & -1 & & & & \\ & & 1 & & & \\ & & & -1 & & \\ & & & & 1 & \\ & & & & & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \\ 0 & -i \\ -i & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \frac{1}{3} E_B$$

↳ this is since $\langle X_i | X_j \rangle \langle X_i | \frac{1}{2} X_m \rangle E_B = E_B \sum_j \sigma_z^{jm}$
 $= E_B \begin{bmatrix} \sigma_z & & \\ & \sigma_z & \\ & & \sigma_z \end{bmatrix}$

this gives $\frac{1}{3} \begin{bmatrix} 0 & -1 & 0 & i & 1 & 0 \\ 1 & 0 & i & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & -i \\ i & 0 \\ 1 & 0 \\ 0 & -1 \end{bmatrix} E_B = \frac{1}{3} \begin{bmatrix} -1 & -1 & 1 & & & 0 \\ & 0 & & & & \\ & & 0 & & & \\ & & & 0 & & \\ & & & & 1 & \\ & & & & & -1 \end{bmatrix} E_B = \frac{1}{3} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} E_B$

This is already diagonal! (Why? because these states were chosen to diagonalize σ_z)

The energy shifts are $\pm \frac{E_B}{3}$ for $|\frac{1}{2} \pm \frac{1}{2}\rangle$

likewise we construct

$$\begin{pmatrix} \langle \frac{3}{2}, \frac{3}{2} | \\ \langle \frac{3}{2}, \frac{1}{2} | \\ \langle \frac{3}{2}, -\frac{1}{2} | \\ \langle \frac{3}{2}, -\frac{3}{2} | \end{pmatrix} \begin{bmatrix} \sqrt{3} & 0 & -\sqrt{3} & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & i\sqrt{3} & 0 & 0 \\ 0 & 1 & 0 & i & 2 & 0 \\ -1 & 0 & i & 0 & 0 & 2 \end{bmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = 6 \langle \frac{3}{2}, m_j | \sigma_z | \frac{3}{2}, m_j \rangle$$

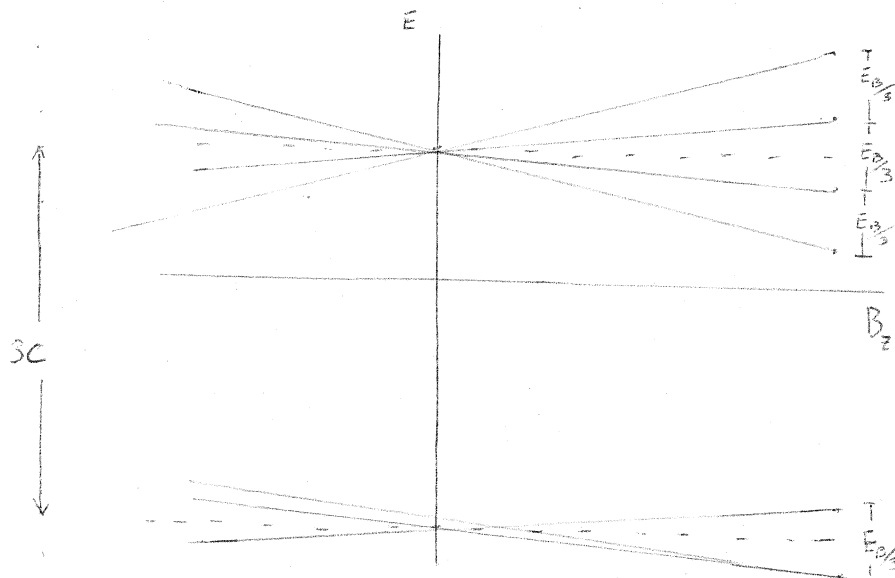
$$= \begin{bmatrix} 3+3 & 0 & 0 & -\sqrt{3}+\sqrt{3} \\ 0 & -3-3 & \sqrt{3}-\sqrt{3} & 0 \\ 0 & \sqrt{3}-\sqrt{3} & 1+i-i & 0 \\ \sqrt{3}+\sqrt{3} & 0 & 0 & -1+i+i \end{bmatrix} = \begin{bmatrix} 6 & & & \\ & -6 & & \\ & & 2 & \\ & & & -2 \end{bmatrix}$$

Again the $|\frac{3}{2}, m_j\rangle$ diagonalize. No coincidence.

so the energy shifts are $\pm 6 \frac{E_B}{6} = \pm E_B$ for $|\frac{3}{2}, \pm \frac{3}{2}\rangle$

and $\pm \frac{E_B}{3}$ for $|\frac{3}{2}, \pm \frac{1}{2}\rangle$

This is reasonable since the greater splitting is for the greater z component of spin, and the splitting is the same for both pairs w/ $m_j = \pm \frac{1}{2}$



b) Optical selection rules for conduction band

We need to evaluate matrix elements like

$$\langle j m_j | \mu \cdot \vec{E} | 1 \rangle | \chi \rangle \propto \langle j m_j | x_i E_i | 1 \rangle | \chi_k \rangle$$

but $|1\rangle$ is even in all dimensions, and $x_i |1\rangle \propto |X_i\rangle$

in matrix form we have

$$\langle j m_j | X_i | \chi_k \rangle = \sum_i E_i \langle j m_j | X_i | \chi_k \rangle = \langle j m_j | \left(E_x \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} + E_y \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + E_z \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

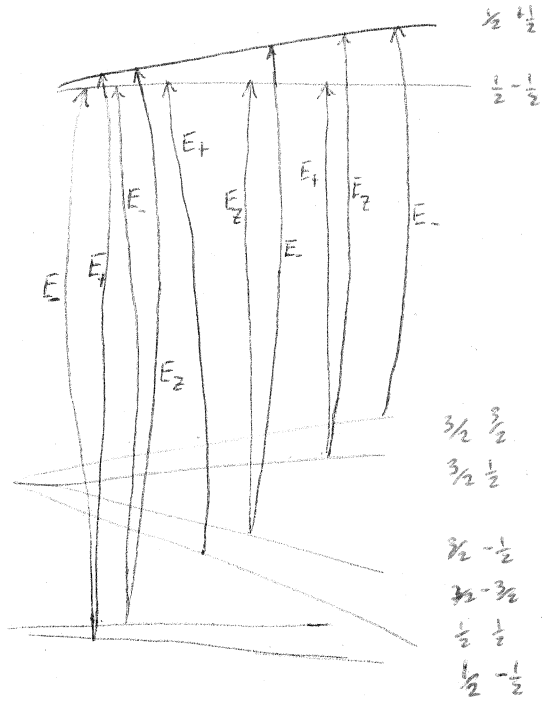
$$= \begin{bmatrix} \langle \frac{3}{2} \frac{3}{2} | X_i | \frac{1}{2} \frac{1}{2} \rangle \\ \langle \frac{3}{2} \frac{1}{2} | X_i | \frac{1}{2} \frac{1}{2} \rangle \\ \langle \frac{3}{2} \frac{1}{2} | X_i | \frac{1}{2} \frac{3}{2} \rangle \\ \langle \frac{3}{2} \frac{3}{2} | X_i | \frac{1}{2} \frac{3}{2} \rangle \\ \langle \frac{1}{2} \frac{1}{2} | X_i | \frac{1}{2} \frac{1}{2} \rangle \\ \langle \frac{1}{2} \frac{3}{2} | X_i | \frac{1}{2} \frac{3}{2} \rangle \end{bmatrix} \left(E_x \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + E_y \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + E_z \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$= \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & 0 \\ -\frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{6}} \\ 0 & -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \left(E_x \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + E_y \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + E_z \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$= E_x \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} & 0 \\ 0 & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} & 0 \end{bmatrix} + i E_y \begin{bmatrix} -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} & 0 \end{bmatrix} + E_z \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \frac{2}{\sqrt{6}} & 0 \\ 0 & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2}(E_x - iE_y) & 0 \\ 0 & \frac{1}{2}(E_x + iE_y) \\ \frac{2}{\sqrt{6}} E_z & \frac{1}{\sqrt{6}}(E_x + iE_y) \\ -\frac{1}{\sqrt{6}}(E_x - iE_y) & \frac{2}{\sqrt{6}} E_z \\ \frac{1}{\sqrt{3}} E_z & -\frac{1}{\sqrt{3}}(E_x - iE_y) \\ \frac{1}{\sqrt{3}}(E_x + iE_y) & \frac{1}{2} E_z \end{bmatrix}$$

or if we use circular polarizations $E_{\pm} = E_x \pm iE_y$

$$\frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3}E_+ & 0 & 3/2 & 3/2 \\ 0 & \sqrt{3}E_+ & 3/2 & -3/2 \\ 2E_2 & E_+ & 3/2 & 1/2 \\ -E_- & 2E_2 & 3/2 & -1/2 \\ \sqrt{2}E_2 & -\sqrt{2}E_- & 1/2 & 1/2 \\ \sqrt{2}E_+ & \sqrt{2}E_- & 1/2 & -1/2 \end{pmatrix} \begin{matrix} \uparrow\uparrow \\ \uparrow\downarrow \end{matrix}$$



c) Because the matrix elements that are non zero in $\langle X_i | \frac{\partial V}{\partial x_j} P_k | X_l \rangle \langle X_p | \sigma_m | X_n \rangle \epsilon_{ijkm}$ are the same as those of

$$\langle 2lm | x_j P_k | 2l'm' \rangle \langle X_p | \sigma_m | X_q \rangle \epsilon_{jkm}, \text{ we can identify}$$

$\nabla V \times p$ with L and σ with S and write $J = L + S$

This occurs because ∇V shares ^{some} the same symmetries as \bar{X}

The math may then be reproduced exactly to find the same solutions in atomic systems. If only we knew more group theory to identify the representation before beginning.

d) Because of these symmetries viz. $|x\rangle \rightarrow |y\rangle \rightarrow |z\rangle \rightarrow |x\rangle; x \rightarrow -x$

and so forth, a different set of Bloch states would not change the result apart from a possible change in the constant C representing the integration of the specific state. The relationships would hold.

including SO coupling

5. The unperturbed eigenstates are

$$J = \frac{3}{2} \begin{cases} \frac{1}{\sqrt{2}} (|x+iY\rangle \uparrow) & = | \frac{3}{2}, \frac{3}{2} \rangle \\ \frac{1}{\sqrt{6}} (2|z\rangle \uparrow + |x+iY\rangle \downarrow) & = | \frac{3}{2}, \frac{1}{2} \rangle \\ \frac{1}{\sqrt{6}} (2|z\rangle \downarrow - |x-iY\rangle \uparrow) & = | \frac{3}{2}, -\frac{1}{2} \rangle \\ \frac{1}{\sqrt{2}} (|x-iY\rangle \downarrow) & = | \frac{3}{2}, -\frac{3}{2} \rangle \end{cases} \quad \text{From notes}$$

$$J = \frac{1}{2} \begin{cases} \frac{1}{\sqrt{3}} (|z\rangle \uparrow - |x+iY\rangle \downarrow) & = | \frac{1}{2}, \frac{1}{2} \rangle \\ \frac{1}{\sqrt{3}} (|z\rangle \downarrow + |x-iY\rangle \uparrow) & = | \frac{1}{2}, -\frac{1}{2} \rangle \end{cases}$$

$$H = H_0 + H_{\text{strain}}$$

$$H_{\text{strain}} = -A_V (2S_{12} F + S_{11} \tilde{F}) - 3B_V [(L_x^2 + L_y^2 - \frac{2}{3}L^2) S_{12} F + (L_z^2 - \frac{L^2}{3}) S_{11} \tilde{F}]$$

$$L_x^2 + L_y^2 = L^2 - L_z^2, \text{ so}$$

$$H_{\text{strain}} = -A_V (2S_{12} + S_{11}) \tilde{F} - 3B_V \tilde{F} [(\frac{1}{3}L^2 - L_z^2) S_{12} + (L_z^2 - \frac{1}{3}L^2) S_{11}]$$

$$= -A_V \tilde{F} (2S_{12} + S_{11}) - 3B_V \tilde{F} (\frac{1}{3}L^2 - L_z^2) (S_{12} - S_{11})$$

Declare $-A_V \tilde{F} (2S_{12} + S_{11}) = \alpha$, $-3B_V \tilde{F} (S_{12} - S_{11}) = \beta$, constants

$$H_{\text{strain}} = \alpha + \beta (\frac{1}{3}L^2 - L_z^2)$$

Taking L^2 on any of the above states give $\ell(\ell+1)$, another constant, so

$$H_{\text{strain}} = \alpha + \frac{1}{3}\beta \ell(\ell+1) - \beta L_z^2$$

$$\text{Define } \gamma = \alpha + \frac{1}{3}\beta \ell(\ell+1)$$

$$H_{\text{strain}} = \gamma - \beta L_z^2$$

Looking at $| \frac{3}{2}, \frac{3}{2} \rangle$, $| \frac{3}{2}, \frac{1}{2} \rangle$ and $| \frac{1}{2}, \frac{1}{2} \rangle$, we find

$$\langle \frac{3}{2}, \frac{3}{2} | \gamma - \beta L_z^2 | \frac{3}{2}, \frac{3}{2} \rangle = \gamma - \beta$$

$$\langle \frac{3}{2}, \frac{1}{2} | \gamma - \beta L_z^2 | \frac{3}{2}, \frac{1}{2} \rangle = \langle \frac{3}{2}, \frac{1}{2} | \gamma - \beta L_z^2 | \frac{3}{2}, \frac{1}{2} \rangle = \langle \frac{1}{2}, \frac{1}{2} | \gamma - \beta L_z^2 | \frac{3}{2}, \frac{3}{2} \rangle = 0$$

$$\langle \frac{1}{2}, \frac{1}{2} | \gamma - \beta L_z^2 | \frac{1}{2}, \frac{1}{2} \rangle = \gamma - (\frac{1}{3} (2|\uparrow\rangle + \langle x+iY | \downarrow) (\frac{1}{3} |\uparrow\rangle + |x+iY\rangle \downarrow) \beta$$

$$= \gamma - \frac{1}{3}\beta$$

$$\langle \frac{3}{2}, \frac{1}{2} | \gamma - \beta L_z^2 | \frac{3}{2}, \frac{1}{2} \rangle = \gamma - \frac{\beta}{6} (2\langle z | \uparrow - \langle x+iY | \downarrow) (2|z\rangle \uparrow - |x+iY\rangle \downarrow)$$

$$= \gamma - \frac{2}{3}\beta$$

$$\langle \frac{3}{2}, \frac{1}{2} | \gamma - \beta L_z^2 | \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{3} (2|\uparrow\rangle - \langle x+iY | \downarrow) (\frac{1}{3} |z\rangle \uparrow + |x+iY\rangle \downarrow) \beta$$

$$= \frac{\sqrt{2}}{3}\beta = \frac{\sqrt{2}}{3}\beta$$

h's gives

$ \frac{3}{2}, \frac{3}{2} \rangle$	$\gamma - \beta$	0	0	0	0	0
$ \frac{1}{2}, \frac{1}{2} \rangle$	0	$\gamma - \frac{1}{3}\beta$	$\frac{\sqrt{2}}{3}\beta$	0	0	0
$ \frac{3}{2}, \frac{1}{2} \rangle$	0	$\frac{\sqrt{2}}{3}\beta$	$\gamma - \frac{2}{3}\beta$	0	0	0
$ \frac{3}{2}, -\frac{1}{2} \rangle$	0	0	0	$\gamma - \beta$	0	0
$ \frac{3}{2}, -\frac{3}{2} \rangle$	0	0	0	0	$\gamma - \frac{1}{3}\beta$	$\frac{\sqrt{2}}{3}\beta$
$ \frac{1}{2}, -\frac{1}{2} \rangle$	0	0	0	0	$\frac{\sqrt{2}}{3}\beta$	$\gamma - \frac{2}{3}\beta$
$ \frac{3}{2}, \frac{3}{2} \rangle$	$ \frac{1}{2}, \frac{1}{2} \rangle$	$ \frac{3}{2}, \frac{1}{2} \rangle$	$ \frac{3}{2}, -\frac{1}{2} \rangle$	$ \frac{3}{2}, -\frac{3}{2} \rangle$	$ \frac{1}{2}, -\frac{1}{2} \rangle$	$ \frac{3}{2}, -\frac{1}{2} \rangle$

5. (cont.) Now let us look at the spin-orbit energies. The HH and LH states have identical energies, while the SO states are offset by a constant Δ . We now see that strain mixes the LH and SO states, breaking this degeneracy. Ignoring the constant offset Δ , the HH state is altered by β , the LH by $\frac{\beta}{3}$, and the SO by $\frac{2}{3}\beta$.

Generally, this system will follow the usual optical selection rules. However, due to the mixing between the $| \frac{3}{2}, \frac{1}{2} \rangle$ state and the $| \frac{1}{2}, \frac{1}{2} \rangle$ state, there will be some additional transitions allowed from the LH and SO states.