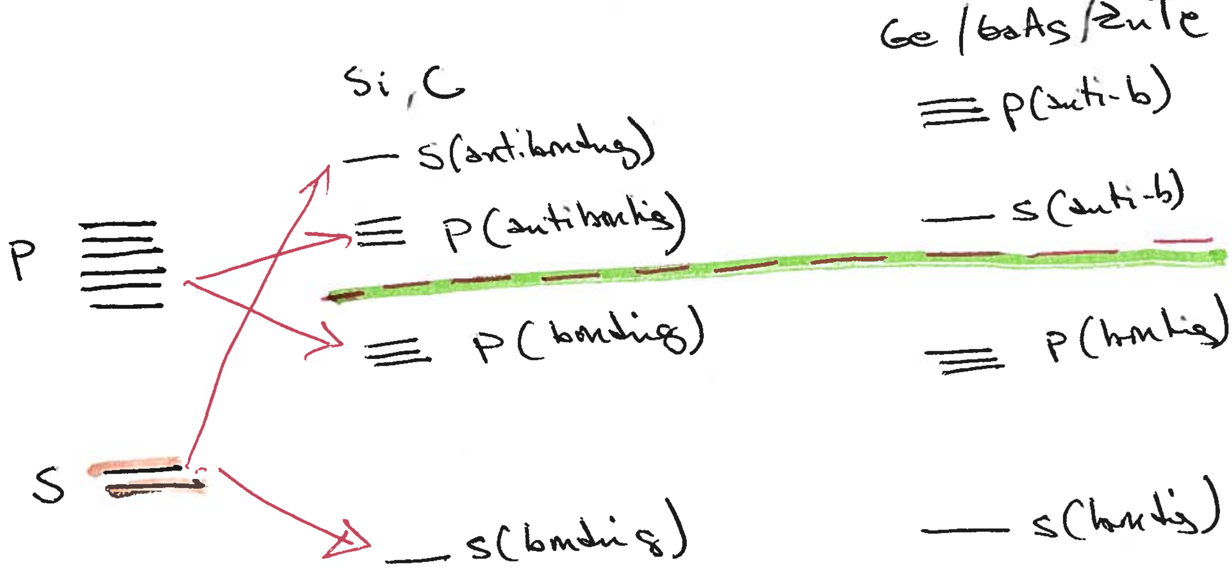
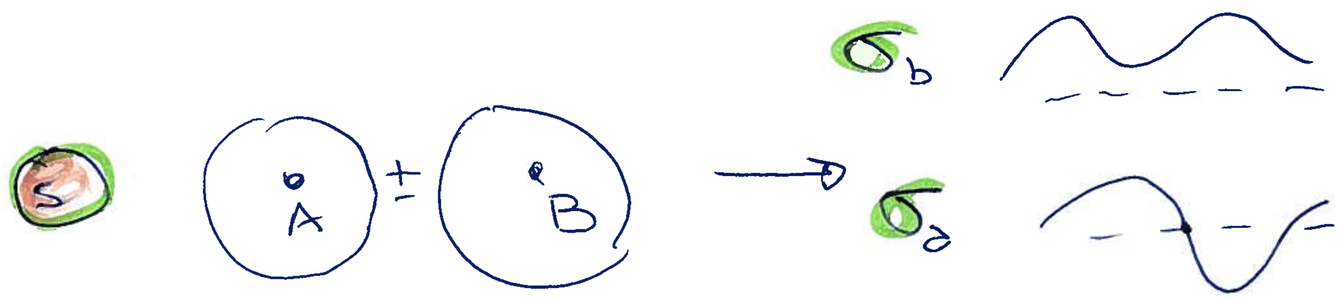
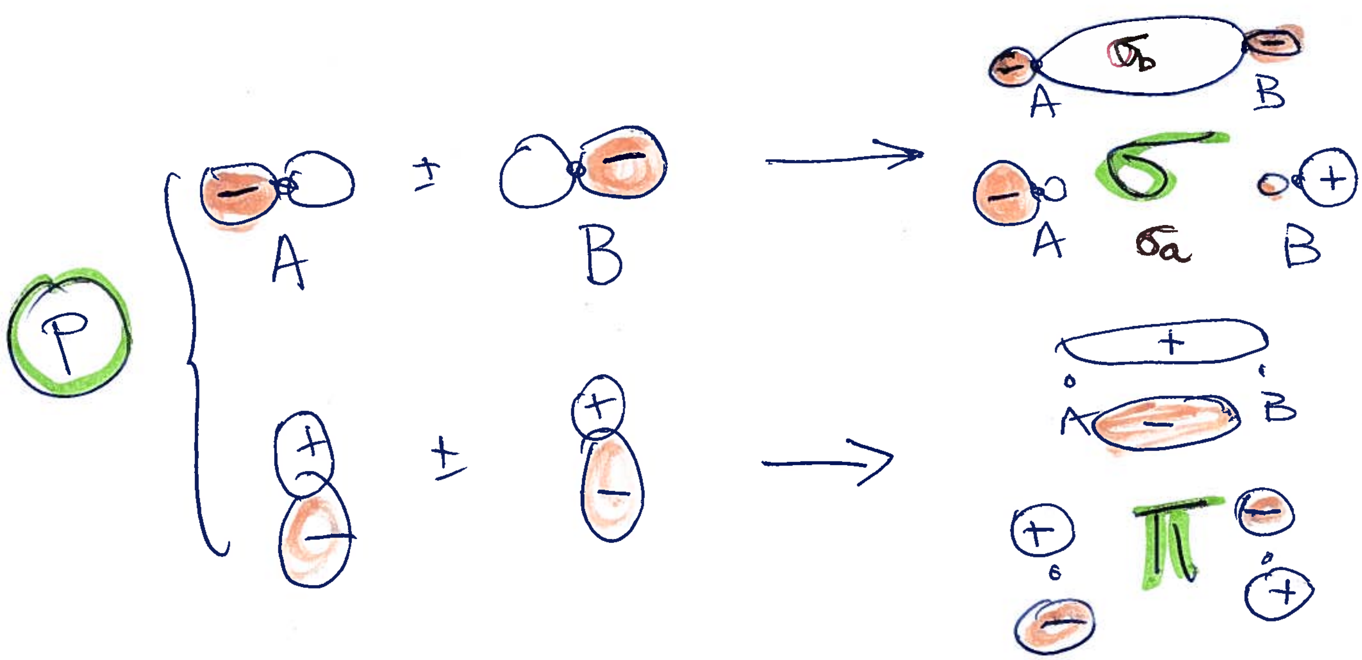
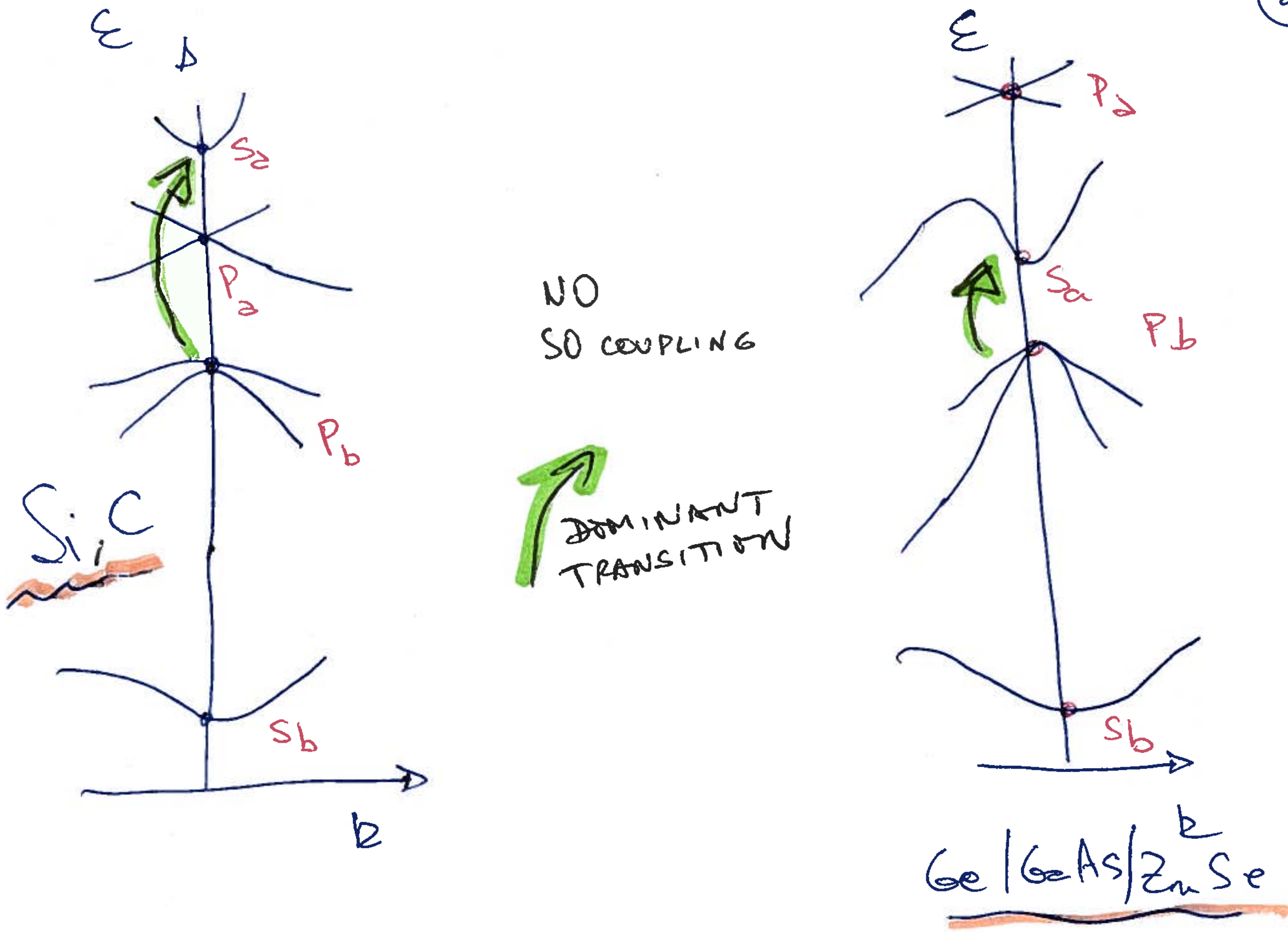
Diamond / Zinc-Blende Semiconductors

GOAL: DETERMINE THE MATRIX ELEMENT $\langle s' | \vec{p} | s \rangle$?









IF WE WERE DEALING WITH ATOMS OR MOLECULES, IT WOUD BE RELATIVELY SIMPLE TO FIND OUT THE OPTICAL SELECTION RULES. STILL +/- TRUE IN SOLIDS

IN SOLIDS, IT IS VERY USEFUL TO USE THE SO-CALLED $k \cdot p$ METHOD

IN THIS METHOD, ONE ASSUMES THAT THE EXACT WAVEFUNCTIONS ARE KNOWN AT $k=0$, AND USE PERT. THEORY TO FIND ψ_k @ $k \neq 0$

THE SOLUTIONS ARE OF THE FORM

$$\psi_{n\vec{k}} = e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})$$

PLUG INTO SCHRODINGER'S EQS. GIVES

$$\left[\frac{p^2}{2m} + \underbrace{\frac{\hbar\,\vec{k}\cdot\vec{p}}{m} + \frac{\hbar^2 k^2}{2m}}_{\text{PERTURBATION}} + \underbrace{V(\vec{r})}_{\text{PERIODIC}}\right] u_{n\vec{k}} = E_{n\vec{k}}\, u_{n\vec{k}}$$

ASSUME WE KNOW $\{u_{nk=0}\}$ COMPLETE SET

LOWEST ORDER OF PERTURBATION THEORY GIVES

$$u_{n\vec{k}} \simeq u_{nk=0} + \frac{\hbar}{m}\sum_{n'\neq n} \frac{\langle u_{nk=0} | k\cdot p | u_{n'} \rangle}{E_{n0} - E_{n'0}} \times u_{n'k=0}$$

UP TO SECOND ORDER:

$$E_{nk} \simeq E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\sum_{n'\neq n} \frac{|\langle u_{n0} | \vec{k}\cdot\vec{p} | u_{n'0} \rangle|^2}{E_{n0} - E_{n'0}}$$

- OPTICAL MATRIX ELEMENT ENTERS IN PERTURBATION
- WEIGHT DEPENDS ON $E_{n0} - E_{n'0}$

IF WE FOCUS OUR ATTENTION ON THE S-LIKE BANDS (NON-DEGENERATE

$\Rightarrow E_{nk} \approx E_{n0} + \frac{\hbar^2 k^2}{2m^*}$ effective mass

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m k^2} \sum_{n' \neq n} \frac{|\langle u_{n0} | k \cdot p | u_{n'0} \rangle|^2}{E_n - E_{n'0}}$$

THE DOMINANT CONTRIBUTION FOR THE S_a-LIKE BAND IS THAT OF THE P_b-LIKE BAND

$$\Rightarrow \frac{1}{m_c^*} \approx \frac{1}{m} + \frac{2 |\langle S_a | \hat{P} | P_b \rangle|^2}{m^2 E_{GAP}}$$

RELATIONSHIP BETWEEN m_c^* & E_{GAP} FROM WHERE $\langle |\hat{p}| \rangle$ CAN BE DETERMINED

AS IT TURNS OUT

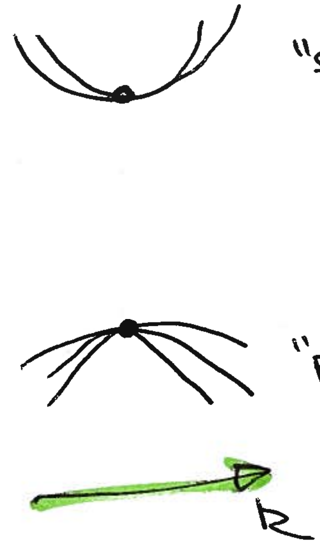
$$\Rightarrow \frac{2 \hat{p}^2}{m} \approx 20 \text{ eV}$$

FOR MOST OF GROUP V, III-V & II-VI COMPOUNDS (HOMEWORK)

WHAT ARE THE EIGENFUNCTIONS?

s ═ 1x2 ⇒ "s"-like

p ≡ 3x2 ⇒ "p"-like



GROUP THEORY USED TO ~~DEFINE~~ CLASSIFY SYMMETRIES AND DEGENERACIES

EXAMPLE

@ k=0 IN ZB SYSTEMS
IGNORING SPIN

$\underbrace{A_1 \quad A_2}_{1} \qquad \underset{2}{E} \qquad \overbrace{F_1 \qquad \underset{x,\,y,\,z}{F_2}}^{3}$

$A_1 \downarrow$ $|S\rangle$ $\qquad$ $F_2 \downarrow$ $|P\rangle$

CUSTOMARY

$|1\rangle$

CUSTOMARY

$|X\rangle$
$|Y\rangle$
$|Z\rangle$

SIMILAR TO ATOMIC p-STATES

But
However, keep in mind that the actual eigenfunctions are periodic;

$$|u_c\rangle \,\hat{=}\, \cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)\cos(2\pi z/a)$$

$$|X\rangle \simeq \sin\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)\cos(2\pi z/a)$$

$$|Y\rangle \simeq \sin\left(\frac{2\pi y}{a}\right)\cos\left(\frac{2\pi x}{a}\right)\cos(2\pi z/a)$$

$$|Z\rangle \simeq \sin\left(\frac{2\pi z}{a}\right)\cos\left(\frac{2\pi x}{a}\right)\cos(2\pi y/a)$$

FREE ELECTRON MODEL

SPIN-ORBIT COUPLING

$$H_{SO} = \frac{\hbar}{4c^2m^2}\left(\vec{\nabla}V \times \hat{p}\right)\cdot\hat{\sigma}$$

BEHAVES AS $\hat{\sigma}\cdot\vec{L}$

~~BY SYMMETRY~~

$$\equiv \frac{\hbar}{4c^2m^2}\Big\{\sigma_x\Big[\overbrace{\partial_y V}^{y} P_z - \overbrace{\partial_z V}^{z} P_y\Big]$$

$$+\sigma_y\Big[\overbrace{\partial_z V}^{z} P_x - \overbrace{\partial_x V}^{x} P_z\Big]$$

$$+\sigma_z\Big[\overbrace{\partial_x V}^{x} P_y - \overbrace{\partial_y V}^{y} P_x\Big]\Big\}$$

TAKE 6 STATES & DIAGONALIZE

SIMILAR AS ATOMIC STATES

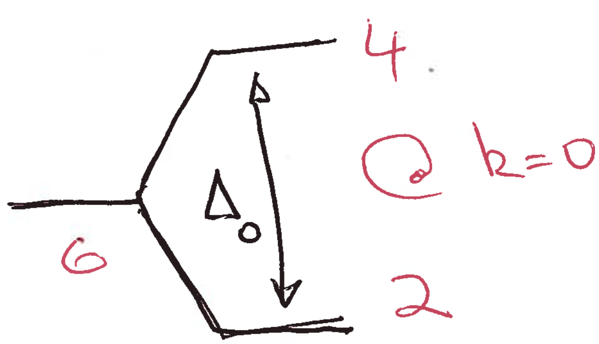
$$\left[\hat{\sigma} + \vec{\nabla} V \times \hat{p}\right]^2 = \sigma^2 + (\vec{\nabla} V \times \vec{p})^2 + 2\,\hat{\sigma}\cdot(\vec{\nabla} V \times \vec{p})$$

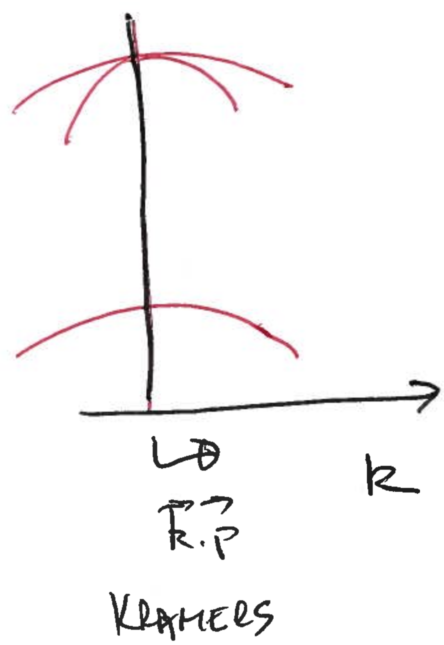
HOMEWORK

AT THE END, WE GET

$$J = 3/2 \begin{cases} 3/2 & 2^{-1/2}\left(|X\rangle + i|Y\rangle\right)\uparrow \\ 1/2 & 6^{-1/2}\left[2|Z\rangle\uparrow + (|X\rangle + i|Y\rangle)\downarrow\right] \\ -1/2 & 6^{-1/2}\left[2|Z\rangle\downarrow + (|X\rangle - i|Y\rangle)\downarrow\right] \\ -3/2 & 2^{-1/2}\left(|X\rangle - i|Y\rangle\right)\downarrow \end{cases}$$

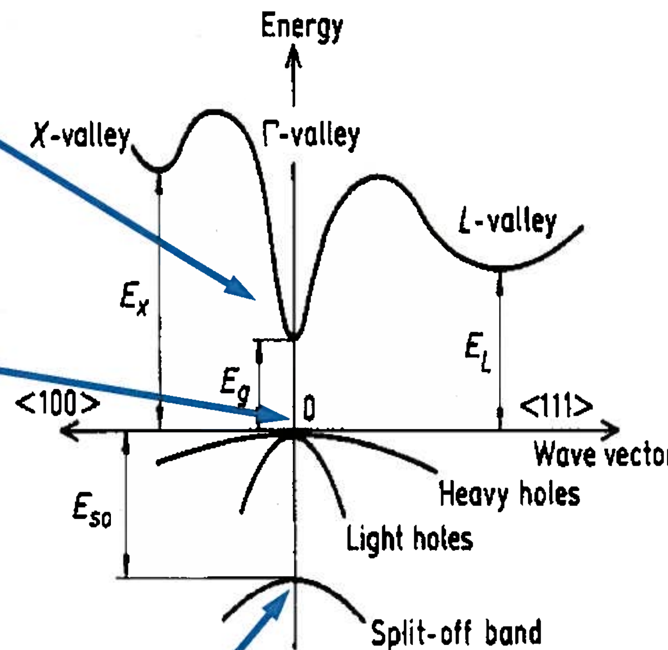
$$J = 1/2 \begin{cases} 1/2 & 3^{-1/2}\left[|Z\rangle\uparrow - (X + iY)\downarrow\right] \\ -1/2 & 3^{-1/2}\left[|Z\rangle\downarrow + (|X\rangle - i|Y\rangle)\uparrow\right] \end{cases}$$





SPIN-ORBIT COUPLING

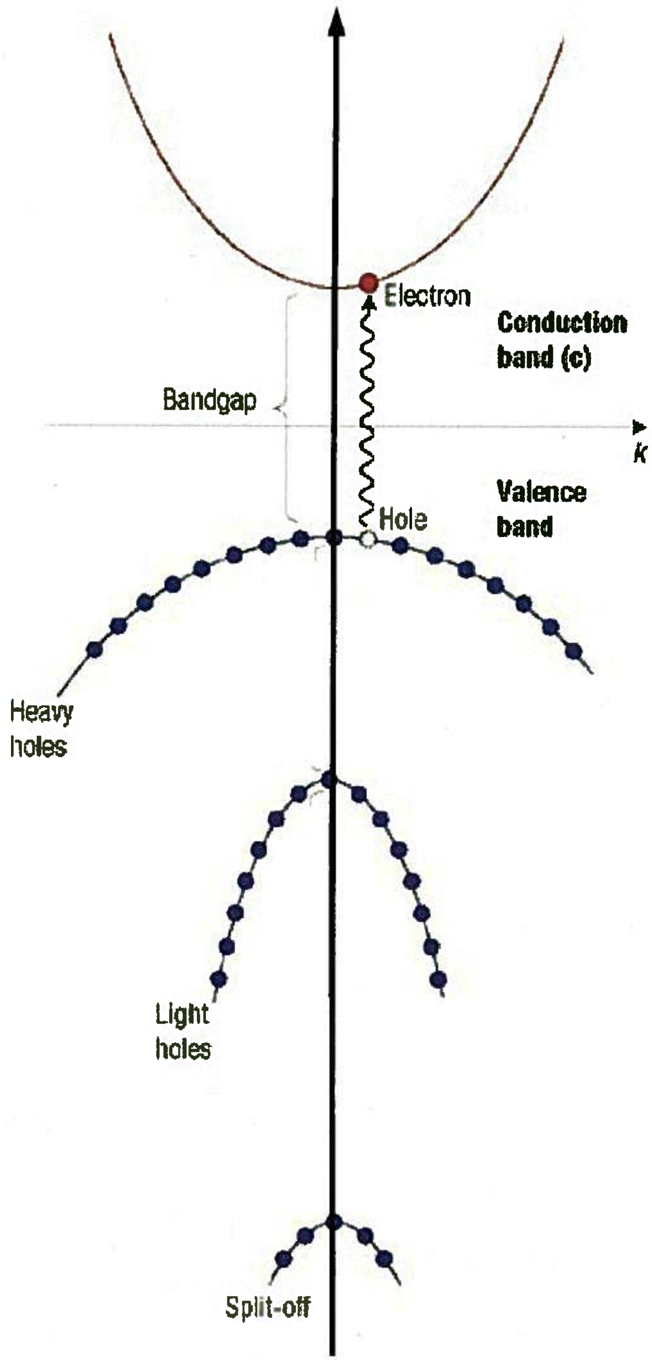
$$\text{conduction band}: \begin{cases} |1\uparrow\rangle \equiv |+1/2\rangle \\ |1\downarrow\rangle \equiv |-1/2\rangle \end{cases}$$



$$\text{'heavy'-hole:} \begin{cases} \frac{1}{\sqrt{2}}|(X+iY)\uparrow\rangle & |J=3/2\,;m_J=+3/2\rangle \\ \frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle & |J=3/2\,;m_J=-3/2\rangle \end{cases}$$

$$\text{'light'-hole:} \begin{cases} \frac{1}{\sqrt{6}}|2Z\downarrow-(X-iY)\uparrow\rangle & |J=3/2\,;m_J=-1/2\rangle \\ \frac{1}{\sqrt{6}}|2Z\uparrow+(X+iY)\downarrow\rangle & |J=3/2\,;m_J=+1/2\rangle \end{cases}$$

$$\text{'split-off'-hole:} \begin{cases} \frac{1}{\sqrt{3}}|Z\uparrow-(X+iY)\downarrow\rangle & |J=1/2\,;m_J=+1/2\rangle \\ \frac{1}{\sqrt{3}}|Z\downarrow+(X-iY)\uparrow\rangle & |J=1/2\,;m_J=-1/2\rangle \end{cases}$$



SPIN-ORBIT COUPLING

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STRESS

(or quantum confinement)

SPIN-ORBIT COUPLING
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UNIAXIAL [001] STRESS
(or quantum confinement)
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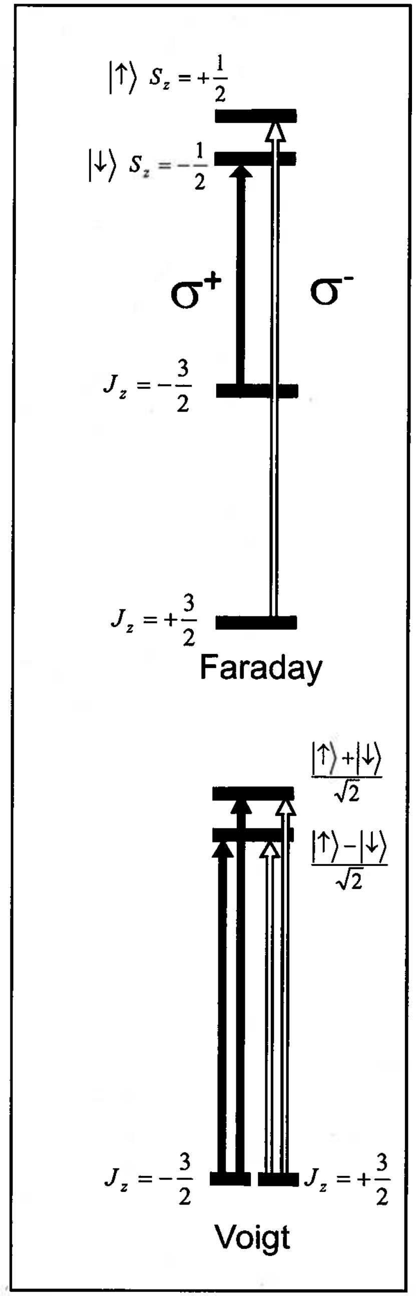
EXTERNAL MAGNETIC FIELD



NOTES:
only heavy-hole states are shown for the valence band
$\sigma^{+/-}$ denote circular polarization

Faraday: **B** parallel to [001]
Voigt: **B** perpendicular to [001]