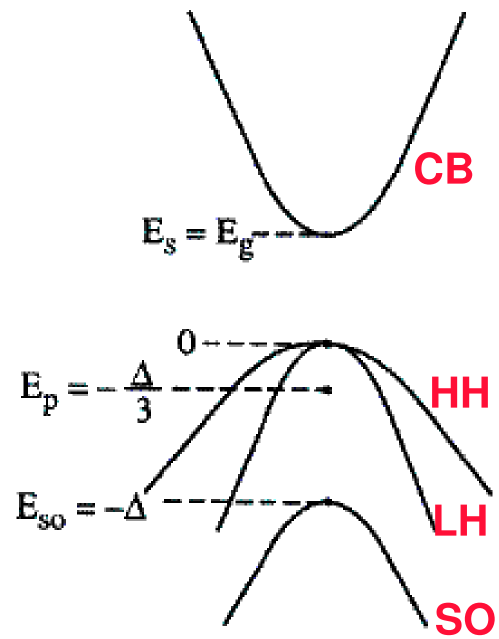
In This Lecture:

- Four-band Kane's Model with Spin-orbit interaction
- Eigenfunctions in Kane's Model

Kane's model : Four-band k·p with Spin-Orbit Interaction

- Four bands: CB, HH, LH, SO
- Double degeneracy with their spin counterparts
- Coupling to any other band is neglected
- These four bands are solved exactly using the matrix formalism based on a convenient basis choice



> Spin-orbit coupling (SOC) is a relativistic effect that scales with the atomic number, *Z*. Thus for se/c containing heavier elements, such as Ge, Ga, As, In, and Sb, one expects the SOC to be significant, and has to be included particularly for states near **k**=0.

The Schrödinger Equation for the cell-periodic fn.

$$H = H_0 + \frac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot\nabla V\times\mathbf{p}$$

$$H_0 = \frac{p^2}{2m_0} + V(\mathbf{r})$$

The Hamiltonian near $\boldsymbol{k}_0=0$

spin-orbit interaction

Components of the Pauli spin matrix:

$$\bar{\bar{\sigma}}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \bar{\bar{\sigma}}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \bar{\bar{\sigma}}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

operating on the spins

$$\uparrow \equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \downarrow \equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

yield

reverse the spinors

$$\bar{\bar{\sigma}}_x\uparrow = \downarrow \qquad \bar{\bar{\sigma}}_y\uparrow = i\downarrow$$

$$\bar{\bar{\sigma}}_x\downarrow = \uparrow \qquad \bar{\bar{\sigma}}_y\downarrow = -i\uparrow$$

preserves the spinors: eigenfn's

$$\bar{\bar{\sigma}}_z\uparrow = \uparrow$$

$$\bar{\bar{\sigma}}_z\downarrow = -\downarrow$$

Ref: Chuang

From the original Schrödinger equation for the Bloch function,

$$\left\{ \frac{p^2}{2m_0} + V(\mathbf{r}) + \frac{\hbar}{4m_0^2c^2}[\nabla V \times \mathbf{p}] \cdot \boldsymbol{\sigma} \right\} \psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) \psi_{n\mathbf{k}}(\mathbf{r})$$

The Schrödinger equation for the cell periodic function $u_{n\mathbf{k}}(\mathbf{r})$ is obtained:

$$\left\{ \frac{p^2}{2m_0} + V(\mathbf{r}) + \frac{\hbar}{m_0}\mathbf{k} \cdot \mathbf{p} + \frac{\hbar}{4m_0^2c^2}[\nabla V \times \mathbf{p}] \cdot \boldsymbol{\sigma} + \boxed{\frac{\hbar^2}{4m_0^2c^2} \nabla V \times \mathbf{k} \cdot \boldsymbol{\sigma}} \right\}$$

$$\times\, u_{n\mathbf{k}}(\mathbf{r}) = E' u_{n\mathbf{k}}(\mathbf{r})$$

$$E' = E_n(\mathbf{k}) - \hbar^2 k^2 / 2m_0$$

to be neglected compared to this term

$\hbar\vec{k}$ is the crystal momentum or the momentum of the envelope, whereas $\vec{p}$ is the actual linear momentum of the *e* which is much greater than $\hbar\vec{k}$ due to $u_{n\vec{k}}(\vec{r})$ part coming from the atomic wavefunction where most of the SO interaction actually occurs.

$$H u_{n\mathbf{k}}(\mathbf{r}) \simeq \left(H_0 + \frac{\hbar}{m_0}\mathbf{k} \cdot \mathbf{p} + \frac{\hbar}{4m_0^2c^2} \nabla V \times \mathbf{p} \cdot \boldsymbol{\sigma} \right) u_{n\mathbf{k}}(\mathbf{r}) = E' u_{n\mathbf{k}}(\mathbf{r})$$

Ref: Chuang

Nature of the Bands Near Bandedges

In semiconductors we are pimarily interested in the valence band and conduction band. Moreover, for most applications we are interested in what happens near the top of the valence band and the bottom of the conduction band. These states originate from the atomic levels of the valence shell in the elements making up the semiconductor.

IV Semiconductors

C $1s^2\underbrace{2s^22p^2}$

Si $1s^22s^22p^6\underbrace{3s^23p^2}$

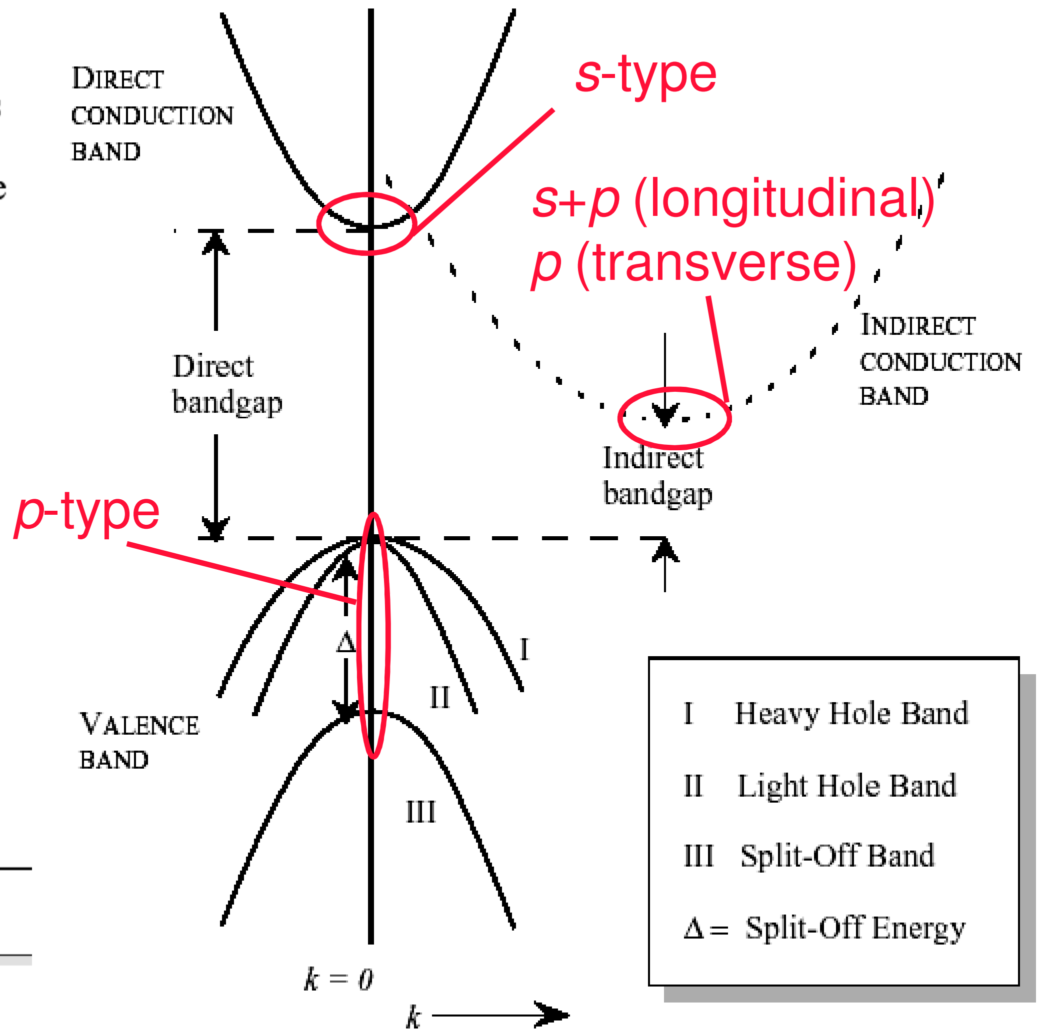
Ge $1s^22s^22p^63s^23p^63d^{10}\underbrace{4s^24p^2}$

III-V Semiconductors

Ga $1s^22s^22p^63s^23p^63d^{10}\underbrace{4s^24p^1}$

As $1s^22s^22p^63s^23p^63d^{10}\underbrace{4s^24p^3}$

Outermost atomic levels are either *s*-type or *p*-type.



Ref: Singh

Recall the *s,p,d*-type Spherical Harmonics

$\ell = 0$ (s orbit)

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$\ell = 1$ (p orbits)

$$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \equiv |Z\rangle$$

$$Y_{1\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi} = \mp\sqrt{\frac{3}{8\pi}}\frac{x \pm iy}{r}$$

$$\equiv \mp\frac{1}{\sqrt{2}}|X \pm iY\rangle$$

$\ell = 2$ (d orbits)

$$Y_{20}(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right) = \sqrt{\frac{5}{16\pi}}\left(\frac{3z^2}{r^2} - 1\right)$$

$$Y_{2\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\varphi} = \mp\sqrt{\frac{15}{8\pi}}\frac{(x \pm iy)z}{r^2}$$

$$Y_{2\pm 2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\varphi} = \sqrt{\frac{15}{32\pi}}\frac{(x \pm iy)^2}{r^2}$$

$$Y_{\ell m}(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\,(-1)^{(m+|m|)/2}P_\ell^{|m|}(\cos\theta)\, e^{im\varphi}$$

and

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}|Y_\ell^m(\theta,\varphi)|^2\sin\theta\, d\theta\, d\varphi = 1$$

Ref: Chuang

The Convenient Basis Choice and the Corresponding Hamiltonian Matrix

We look for the eigenvalue E' with corresponding eigenfunction

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{n'} a_{n'} u_{n'0}(\mathbf{r})$$

The band-edge functions $u_{n0}(\mathbf{r})$ are

Conduction band: $|S\uparrow\rangle$, $|S\downarrow\rangle$ with corresponding eigenenergy E_s

Valence band: $|X\uparrow\rangle$, $|Y\uparrow\rangle$, $|Z\uparrow\rangle$, $|X\downarrow\rangle$, $|Y\downarrow\rangle$, $|Z\downarrow\rangle$ with eigenenergy E_p

They deviate from a totally spherical function *f(r)* by:

X(x,y,z)=-X(-x,y,z); odd fn of *x* but even wrt *y* & *z*

similarly for

Ref: Chuang

However, it is convenient to switch to the following linear combinations:

$$|u_1\rangle = |iS\downarrow\rangle$$

$$|u_2\rangle = \left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle = |Y_{1\,-1}\uparrow\rangle$$

$$|u_3\rangle = |Z\downarrow\rangle = |Y_{1\,0}\downarrow\rangle$$

$$|u_4\rangle = \left|-\frac{X+iY}{\sqrt{2}}\uparrow\right\rangle = |Y_{1\,1}\uparrow\rangle$$

$$|u_5\rangle = |iS\uparrow\rangle$$

$$|u_6\rangle = \left|-\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle = |Y_{1\,1}\downarrow\rangle$$

$$|u_7\rangle = |Z\uparrow\rangle = |Y_{1\,0}\uparrow\rangle$$

$$|u_8\rangle = \left|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle = |Y_{1\,-1}\downarrow\rangle$$

The first four basis fn's are degenerate with the last four

Ref: Chuang

Using this basis, expansion coefficients and the eigenenergies are determined from the the following 8x8 Hamiltonian Matrix

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{n'} a_{n'} u_{n'0}(\mathbf{r})$$

$$\begin{bmatrix} \overline{\overline{\mathbf{H}}} & 0 \\ 0 & \overline{\overline{\mathbf{H}}} \end{bmatrix}$$

$$Hu_{n\mathbf{k}}(\mathbf{r}) \simeq \left(H_0 + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar}{4m_0^2c^2}\nabla V \times \mathbf{p}\cdot\boldsymbol{\sigma} \right) u_{n\mathbf{k}}(\mathbf{r}) = E' u_{n\mathbf{k}}(\mathbf{r})$$

$$\overline{\overline{\mathbf{H}}} = \begin{bmatrix} E_s & 0 & kP & 0 \\ 0 & E_p - \frac{\Delta}{3} & \sqrt{2}\Delta/3 & 0 \\ kP & \sqrt{2}\Delta/3 & E_p & 0 \\ 0 & 0 & 0 & E_p + \frac{\Delta}{3} \end{bmatrix}$$

assuming $\mathbf{k} = k\hat{z}$

Don't worry, this will be relaxed later on

where

$$P \equiv -\mathrm{i}\frac{\hbar}{m_0}\langle S|p_z|Z\rangle$$ Kane's parameter

$$\Delta \equiv \frac{3\hbar \mathrm{i}}{4m_0^2c^2}\langle X|\frac{\partial V}{\partial x}p_y - \frac{\partial V}{\partial y}p_x|Y\rangle$$ SO split off energy

Ref: Chuang

Kane's Hamiltonian (cont'd)

➢Analysis of the matrix entries

Recall

- *X(x,y,z)=-X(-x,y,z)*; odd fn of *x* but even wrt *y* & *z, etc.*
- $\langle \downarrow | \sigma_x | \downarrow \rangle = \langle \downarrow | \sigma_y | \downarrow \rangle = 0$

$$H_{11} = \langle iS\downarrow | H_0 + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar}{4m_0^2c^2}\sigma\cdot\nabla V\times\mathbf{p} | iS\downarrow\rangle$$

$$= \langle S\downarrow | H_0 | S\downarrow\rangle + \frac{\hbar}{m_0}\langle S\downarrow | \mathbf{k}\cdot\mathbf{p} | S\downarrow\rangle$$

$$+ \langle S\downarrow | \frac{\hbar}{4m_0^2c^2}\sigma_z\left(\frac{\partial V}{\partial x}p_y - \frac{\partial V}{\partial y}p_x\right) | S\downarrow\rangle$$

$$= E_S$$

$$\sigma\cdot\nabla V\times\mathbf{p} = \sigma_x(\nabla V\times\mathbf{p})_x + \sigma_y(\nabla V\times\mathbf{p})_y + \sigma_z(\nabla V\times\mathbf{p})_z$$

$$\langle S\downarrow | \mathbf{p} | S\downarrow\rangle = \langle S | \mathbf{p} | S\rangle = \int S(r)\frac{\hbar}{i}\nabla S(r)\,\mathrm{d}^3 r = 0$$

The σ_z term vanishes as this term changes sign when x↔y whereas the xtal is invariant under this xformation

As an exercise, obtain the remaining matrix elements!

Ref: Chuang

Solutions of Kane's Hamiltonian

Define the reference energy so that: $E_p = -\Delta/3$, and $E_s = E_g$

$$\overline{\overline{\mathbf{H}}} = \begin{bmatrix} E_g & 0 & kP & 0 \\ 0 & -\frac{2\Delta}{3} & \sqrt{2}\Delta/3 & 0 \\ kP & \sqrt{2}\Delta/3 & \frac{-\Delta}{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$E' = 0$ Decoupled from the rest

$$E'(E'-E_g)(E'+\Delta) - k^2P^2\left(E' + \tfrac{2}{3}\Delta\right) = 0$$

Band edge ***k***=0

$E' = E_g$, $E' = 0$ and $E' = -\Delta$

Ref: Chuang

Solutions for small k

Let $E' = E_g + \varepsilon(k^2)$ where $\varepsilon \ll \Delta$ and E_g → $\varepsilon \simeq \dfrac{k^2P^2(E_g + 2\Delta/3)}{E_g(E_g + \Delta)}$

Let $E' = 0 + \varepsilon(k^2)$ → $\varepsilon \simeq -\dfrac{2k^2P^2}{3E_g}$

Let $E' = -\Delta + \varepsilon(k^2)$ → $\varepsilon = -\dfrac{k^2P^2}{3(E_g + \Delta)}$

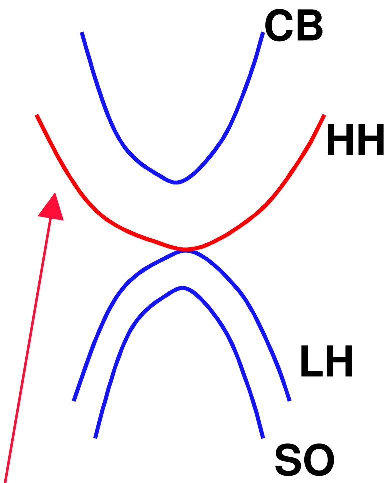
Since $E' = E_n(k) - \hbar^2k^2/2m_0$

$n = c \qquad E_c(k) = E_g + \dfrac{\hbar^2k^2}{2m_0} + \dfrac{k^2P^2(E_g + 2\Delta/3)}{E_g(E_g + \Delta)}$

$n = \mathrm{hh} \qquad E_{\mathrm{hh}}(k) = \dfrac{\hbar^2k^2}{2m_0}$

$n = l\mathrm{h} \qquad E_{l\mathrm{h}}(k) = \dfrac{\hbar^2k^2}{2m_0} - \dfrac{2k^2P^2}{3E_g}$

$n = \mathrm{so} \qquad E_{\mathrm{so}}(k) = -\Delta + \dfrac{\hbar^2k^2}{2m_0} - \dfrac{k^2P^2}{3(E_g + \Delta)}$



HH band concave up with free-e mass ☹

To be fixed by the LK Hamiltonian

Ref: Chuang

Kane's Model: Eigenvectors

The eigenvectors are obtained by substituting each eigenvalue into the eigenequation

$$\begin{bmatrix} E_g - E'_n & 0 & kP \\ 0 & \frac{-2\Delta}{3} - E'_n & \sqrt{2}\,\frac{\Delta}{3} \\ kP & \sqrt{2}\,\frac{\Delta}{3} & -\frac{\Delta}{3} - E'_n \end{bmatrix} \begin{bmatrix} a_n \\ b_n \\ c_n \end{bmatrix} = 0$$

and then normalizing such that $(a_n^2 + b_n^2 + c_n^2)^{1/2} = 1$.

The results in the limit $k^2 \to 0$ give

$$\begin{aligned} n &= c & a &\cong 1, & b &\cong 0, & c &\simeq 0 \\ n &= lh & a &\simeq 0, & b &= \frac{1}{\sqrt{3}}, & c &= \sqrt{\frac{2}{3}} \\ n &= \text{so} & a &\simeq 0, & b &= \sqrt{\frac{2}{3}}, & c &= -\sqrt{\frac{1}{3}} \end{aligned}$$

$$\begin{bmatrix} \overline{\overline{\mathbf{H}}} & 0 \\ 0 & \overline{\overline{\mathbf{H}}} \end{bmatrix}$$

where, for upper 4x4 matrix:

$$\phi_{hh,\alpha} = \left| -\left(\frac{X + iY}{\sqrt{2}}\right)\uparrow \right\rangle \qquad \text{hh band}$$

$$\phi_{n,\alpha} = a_n|iS\downarrow\rangle + b_n\left|\frac{X - iY}{\sqrt{2}}\uparrow\right\rangle + c_n|Z\downarrow\rangle \qquad n = c, lh, \text{so}$$

and from lower 4x4 matrix:

$$\phi_{hh,\beta} = \left|\frac{X - iY}{\sqrt{2}}\downarrow\right\rangle \qquad \text{hh band}$$

$$\phi_{n,\beta} = a_n|iS\uparrow\rangle + b_n\left|-\frac{X + iY}{\sqrt{2}}\downarrow\right\rangle + c_n|Z\uparrow\rangle \qquad n = c, lh, \text{so}$$

Ref: Chuang

Summary of Kane's model

Conduction band

$$E_c(k) = E_g + \frac{\hbar^2 k^2}{2m_0} + \frac{k^2 P^2}{3}\frac{(3E_g + 2\Delta)}{E_g(E_g+\Delta)} \left(\equiv E_g + \frac{\hbar^2 k^2}{2m_e^*} \right)$$

$$\phi_{c,\alpha} = |iS\downarrow\rangle$$

$$\phi_{c,\beta} = |iS\uparrow\rangle$$

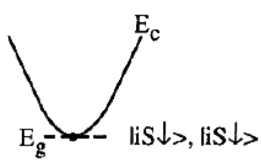
Valence band

Heavy hole

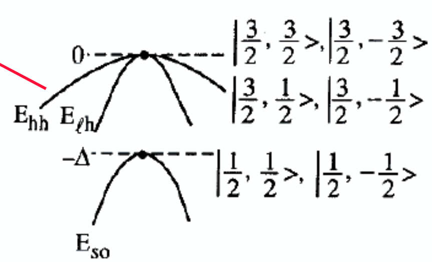
$$E_{hh}(k) = \frac{\hbar^2 k^2}{2m_0} \quad \left(\text{should be } -\frac{\hbar^2 k^2}{2m_{hh}^*} \right)$$

$$\phi_{hh,\alpha} = \frac{-1}{\sqrt{2}}|(X+iY)\uparrow\rangle \equiv \left|\frac{3}{2},\frac{3}{2}\right\rangle$$

$$\phi_{hh,\beta} = \frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle \equiv \left|\frac{3}{2},-\frac{3}{2}\right\rangle$$



with corrected HH curvature (LK)



Light hole

$$E_{lh}(k) = \frac{\hbar^2 k^2}{2m_0} - \frac{2k^2P^2}{3E_g} \left(\equiv -\frac{\hbar^2 k^2}{2m_{lh}^*} \right)$$

$$\phi_{lh,\alpha} = \frac{1}{\sqrt{6}}|(X-iY)\uparrow\rangle + \sqrt{\frac{2}{3}}|Z\downarrow\rangle \equiv \left|\frac{3}{2},-\frac{1}{2}\right\rangle$$

$$\phi_{lh,\beta} = -\frac{1}{\sqrt{6}}|(X+iY)\downarrow\rangle + \sqrt{\frac{2}{3}}|Z\uparrow\rangle \equiv \left|\frac{3}{2},\frac{1}{2}\right\rangle$$

Spin-orbit split-off band

$$E_{so}(k) = -\Delta + \frac{\hbar^2 k^2}{2m_0} - \frac{k^2P^2}{3(E_g+\Delta)} \left(\equiv -\Delta - \frac{\hbar^2 k^2}{2m_{so}^*} \right)$$

$$\phi_{so,\alpha} = \frac{1}{\sqrt{3}}|(X-iY)\uparrow\rangle - \frac{1}{\sqrt{3}}|Z\downarrow\rangle \equiv \left|\frac{1}{2},\frac{-1}{2}\right\rangle$$

$$\phi_{so,\beta} = \frac{1}{\sqrt{3}}|(X+iY)\downarrow\rangle + \frac{1}{\sqrt{3}}|Z\uparrow\rangle \equiv \left|\frac{1}{2},\frac{1}{2}\right\rangle$$

Ref: Chuang

The Journey of the Eigenfunctions

For the unperturbed H, eigenfn's at the band edge we anticipated them to be of *s* and *p* type orbital symmetry: $|S,\uparrow\rangle, |S,\downarrow\rangle, |X,\uparrow\rangle, |X,\downarrow\rangle, |Y,\uparrow\rangle, |Y,\downarrow\rangle, |Z,\uparrow\rangle, |Z,\downarrow\rangle$

$$|u_1\rangle = |iS\downarrow\rangle$$

$$|u_2\rangle = \left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle = |Y_{1\,-1}\uparrow\rangle$$

$$|u_3\rangle = |Z\downarrow\rangle = |Y_{1\,0}\downarrow\rangle$$

$$|u_4\rangle = \left|-\frac{X+iY}{\sqrt{2}}\uparrow\right\rangle = |Y_{1\,1}\uparrow\rangle$$

$$|u_5\rangle = |iS\uparrow\rangle$$

$$|u_6\rangle = \left|-\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle = |Y_{1\,1}\downarrow\rangle$$

$$|u_7\rangle = |Z\uparrow\rangle = |Y_{1\,0}\uparrow\rangle$$

$$|u_8\rangle = \left|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle = |Y_{1\,-1}\downarrow\rangle$$

Perturbation: SO+k.P

Kane's band edge eigenfn's

$$u_{10}(\mathbf{r}) = \left|\frac{3}{2},\frac{3}{2}\right\rangle = \frac{-1}{\sqrt{2}}|(X+iY)\uparrow\rangle$$

$$u_{20}(\mathbf{r}) = \left|\frac{3}{2},\frac{1}{2}\right\rangle = \frac{-1}{\sqrt{6}}|(X+iY)\downarrow\rangle + \sqrt{\frac{2}{3}}|Z\uparrow\rangle$$

$$u_{30}(\mathbf{r}) = \left|\frac{3}{2},\frac{-1}{2}\right\rangle = \frac{1}{\sqrt{6}}|(X-iY)\uparrow\rangle + \sqrt{\frac{2}{3}}|Z\downarrow\rangle$$

$$u_{40}(\mathbf{r}) = \left|\frac{3}{2},\frac{-3}{2}\right\rangle = \frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle$$

$$u_{50}(\mathbf{r}) = \left|\frac{1}{2},\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}|(X+iY)\downarrow\rangle + \frac{1}{\sqrt{3}}|Z\uparrow\rangle$$

$$u_{60}(\mathbf{r}) = \left|\frac{1}{2},\frac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}|(X-iY)\uparrow\rangle - \frac{1}{\sqrt{3}}|Z\downarrow\rangle$$

Refreshment on Addition of Angular Momenta

Spin-orbit coupling: Nonzero angular momentum state *e*'s (i.e., other than *s*-type wf's) generate a magnetic field through which they interact with the spin of the *e*. Particulary important for the VB (*p*-like states).

Because of this coupling neither spin nor orbital angular momentum but the total angular momentum becomes a good quantum number.

Consider two angular momentum operators which commute with each other (J_1, J_2), we wish to determine the eigenstates of the total angular momentum operator $J = J_1 + J_2$

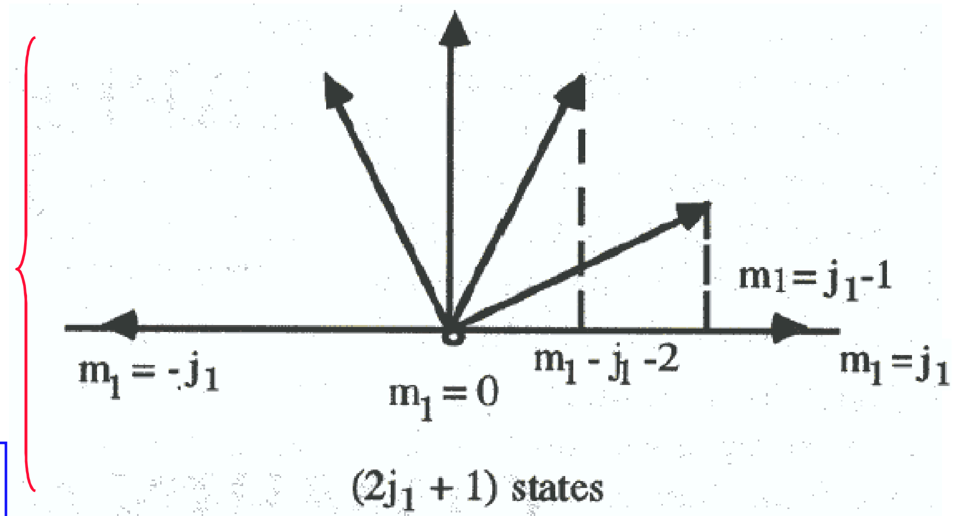
$$\left| j, m \right\rangle = \sum a_{m_1 m_2} \left| \underbrace{j_1, m_1}_{\text{orbital}} ; \underbrace{j_2, m_2}_{\text{spin}} \right\rangle$$

Clebsch-Gordan coefficients: $a_{m_1 m_2}$

There are ($2J_1+1$) and ($2J_2+1$) states corresponding to J_1 and J_2

Refreshment on total Angular Momentum (cont'd)

A schematic representation of the angular momentum states



J=L+S

$j=l+s=3/2$, $m_j=3/2,\ldots,-3/2$

$j=l-s=1/2$ $m_j=1/2,-1/2$

Clebsch-Gordan coefficients for $J_1=1$ and $J_2=1/2$

$j_1 = 1 \quad j_2 = \frac{1}{2}$:

$\lvert l,s\rangle$ \ $\lvert j,m\rangle$	$\frac{3}{2}\ \frac{3}{2}$	$\frac{3}{2}\ \frac{1}{2}$	$\frac{1}{2}\ \frac{1}{2}$	$\frac{3}{2}\ -\frac{1}{2}$	$\frac{1}{2}\ -\frac{1}{2}$	$\frac{3}{2}\ -\frac{3}{2}$
$1\ \frac{1}{2}$	1					
$1\ -\frac{1}{2}$		$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$			
$0\ \frac{1}{2}$		$\sqrt{\frac{2}{3}}$	$-\sqrt{\frac{1}{3}}$			
$0\ -\frac{1}{2}$				$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	
$-1\ \frac{1}{2}$				$\sqrt{\frac{1}{3}}$	$-\sqrt{\frac{2}{3}}$	
$-1\ -\frac{1}{2}$						1

Be ware, different phase choices exist as in LK

Ref: Singh

Extraction of Kane's parameter from experimental data

$$E_c(k) - E_g = \frac{\hbar^2 k^2}{2m_0} + \frac{k^2 P^2 \left(E_g + \frac{2}{3}\Delta\right)}{E_g(E_g + \Delta)} = \frac{\hbar^2 k^2}{2m_e^*}$$

$$P^2 = \left(1 - \frac{m_e^*}{m_0}\right) \frac{\hbar^2 E_g (E_g + \Delta)}{2m_e^* (E_g + 2\Delta/3)}$$

So, by feeding three parameters from experiment, Kane's parameter can be extracted. This parameter, *P* plays a key role in any optical property regarding the over-the-band gap excitations

Ref: Chuang

General *k* direction

Up to now, we have assumed: $\mathbf{k} = k\hat{z}$

For a general case: $\mathbf{k} = k\sin\theta\cos\varphi\,\hat{x} + k\sin\theta\sin\varphi\,\hat{y} + k\cos\theta\,\hat{z}$

The following transformations can be used to find the basis functions in the general coordinate system:

$$\begin{bmatrix} \uparrow' \\ \downarrow' \end{bmatrix} = \begin{bmatrix} e^{-i\phi/2}\cos\frac{\theta}{2} & e^{i\phi/2}\sin\frac{\theta}{2} \\ -e^{-i\phi/2}\sin\frac{\theta}{2} & e^{i\phi/2}\cos\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \uparrow \\ \downarrow \end{bmatrix}$$

$$\begin{bmatrix} X' \\ Y' \\ Z' \end{bmatrix} = \begin{bmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix}$$

Ref: Chuang

k·p and Similar Band Edge Techniques

Brief Highlights

- Single- and two-band **k·p**
  - Coupling to other bands accounted perturbatively
  - Predicts an analytical <u>effective</u> mass tensor (heavier/lighter than m_0)
- Kane's Hamiltonian
  - 8 bands (CB+3 VB with spin) treated <u>exactly</u>
  - Coupling with the other bands neglected
  - HH band comes out with wrong sign and value (due above approximation)
  - No warping predicted (i.e., isotropic) for finite **k**
- Luttinger-Kohn Hamiltonian (for degenerate bands with spin-orbit)
  - 6 VBs treated exactly; can be extended to include CBs as well
  - Other bands are included via Löwdin's technique
  - Warping of the VBs is predicted
- Pikus-Bir Hamiltonian
  - Just like LK Hamiltonian, but includes the effects of strain in the xtal