In This Lecture:

- Eigenfunctions in Kane's Model
- Luttinger-Kohn Model

Kane’s Model: Eigenvectors

The eigenvectors are obtained by substituting each eigenvalue into the eigenequation

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

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

$$n = c \qquad a \cong 1, \qquad b \cong 0, \qquad c \simeq 0$$

$$n = lh \qquad a \simeq 0, \qquad b = \frac{1}{\sqrt{3}}, \qquad c = \sqrt{\frac{2}{3}}$$

$$n = \mathrm{so} \qquad a \simeq 0, \qquad b = \sqrt{\frac{2}{3}}, \qquad c = -\sqrt{\frac{1}{3}}$$

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

where, for upper 4x4 matrix:

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

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

and from lower 4x4 matrix:

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

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

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

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

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

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

Light hole

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

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

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

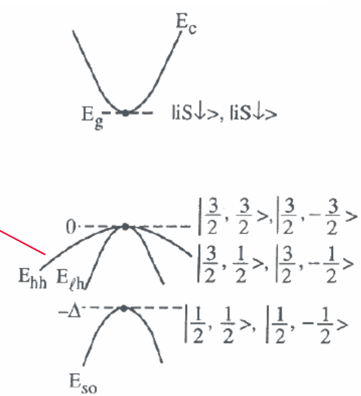
Spin-orbit split-off band

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

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

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

with corrected HH curvature (LK)



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: $\left|S,\uparrow\right\rangle,\left|S,\downarrow\right\rangle,\left|X,\uparrow\right\rangle,\left|X,\downarrow\right\rangle,\left|Y,\uparrow\right\rangle,\left|Y,\downarrow\right\rangle,\left|Z,\uparrow\right\rangle,\left|Z,\downarrow\right\rangle$

$$\left|u_1\right\rangle=\left|iS\downarrow\right\rangle$$
$$\left|u_2\right\rangle=\left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle=\left|Y_{1\,-1}\uparrow\right\rangle$$
$$\left|u_3\right\rangle=\left|Z\downarrow\right\rangle=\left|Y_{1\,0}\downarrow\right\rangle$$
$$\left|u_4\right\rangle=\left|-\frac{X+iY}{\sqrt{2}}\uparrow\right\rangle=\left|Y_{1\,1}\uparrow\right\rangle$$
$$\left|u_5\right\rangle=\left|iS\uparrow\right\rangle$$
$$\left|u_6\right\rangle=\left|-\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle=\left|Y_{1\,1}\downarrow\right\rangle$$
$$\left|u_7\right\rangle=\left|Z\uparrow\right\rangle=\left|Y_{1\,0}\uparrow\right\rangle$$
$$\left|u_8\right\rangle=\left|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle=\left|Y_{1\,-1}\downarrow\right\rangle$$

Perturbation:
SO+k.P

Kane's band edge eigenfn's

$$u_{10}(\mathbf{r})=\left|\frac{3}{2},\frac{3}{2}\right\rangle=\frac{-1}{\sqrt{2}}\left|(X+\mathrm{i}Y)\uparrow\right\rangle$$
$$u_{20}(\mathbf{r})=\left|\frac{3}{2},\frac{1}{2}\right\rangle=\frac{-1}{\sqrt{6}}\left|(X+\mathrm{i}Y)\downarrow\right\rangle+\sqrt{\frac{2}{3}}\left|Z\uparrow\right\rangle$$
$$u_{30}(\mathbf{r})=\left|\frac{3}{2},\frac{-1}{2}\right\rangle=\frac{1}{\sqrt{6}}\left|(X-\mathrm{i}Y)\uparrow\right\rangle+\sqrt{\frac{2}{3}}\left|Z\downarrow\right\rangle$$
$$u_{40}(\mathbf{r})=\left|\frac{3}{2},\frac{-3}{2}\right\rangle=\frac{1}{\sqrt{2}}\left|(X-\mathrm{i}Y)\downarrow\right\rangle$$
$$u_{50}(\mathbf{r})=\left|\frac{1}{2},\frac{1}{2}\right\rangle=\frac{1}{\sqrt{3}}\left|(X+\mathrm{i}Y)\downarrow\right\rangle+\frac{1}{\sqrt{3}}\left|Z\uparrow\right\rangle$$
$$u_{60}(\mathbf{r})=\left|\frac{1}{2},\frac{-1}{2}\right\rangle=\frac{1}{\sqrt{3}}\left|(X-\mathrm{i}Y)\uparrow\right\rangle-\frac{1}{\sqrt{3}}\left|Z\downarrow\right\rangle$$

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 <u>total angular momentum</u> 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 $J = J_1 + J_2$

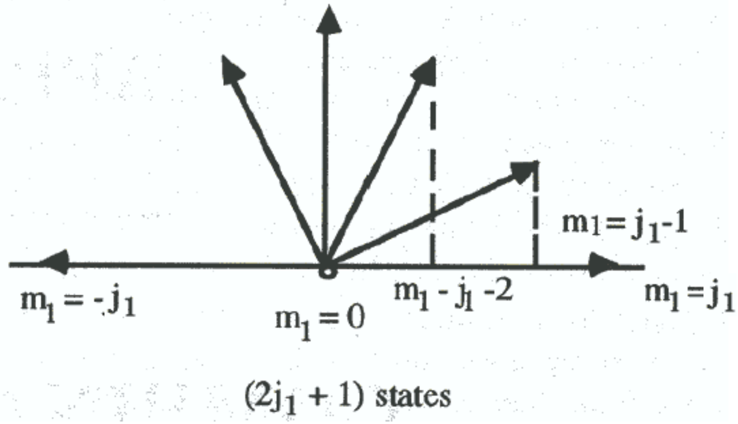
$$\left| j,m \right\rangle = \sum a_{m_1 m_2} \left| \overbrace{j_1, m_1}^{\text{orbital}} ; \overbrace{j_2, m_2}^{\text{spin}} \right\rangle$$

Clebsch-Gordan coefficients

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 $J_2=1/2$

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

$$
\begin{array}{c|c}
|l,s\rangle \backslash |j,m\rangle & \begin{array}{cccccc} \frac{3}{2},\frac{3}{2} & \frac{3}{2},\frac{1}{2} & \frac{1}{2},\frac{1}{2} & \frac{3}{2},-\frac{1}{2} & \frac{1}{2},-\frac{1}{2} & \frac{3}{2},-\frac{3}{2} \end{array} \\
\hline
\begin{array}{c} 1\ \frac{1}{2} \\ 1\ -\frac{1}{2} \\ 0\ \frac{1}{2} \\ 0\ -\frac{1}{2} \\ -1\ \frac{1}{2} \\ -1\ -\frac{1}{2} \end{array} &
\begin{bmatrix}
1 & & & & & \\
 & \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} & & & \\
 & \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{3}} & & & \\
 & & & \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} & \\
 & & & \sqrt{\frac{1}{3}} & -\sqrt{\frac{2}{3}} & \\
 & & & & & 1
\end{bmatrix}
\end{array}
$$

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 effective mass tensor (heavier/lighter than m_0)
- Kane's Hamiltonian
  - 8 bands (CB+3 VB with spin) treated exactly
  - 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

Luttinger-Kohn Hamiltonian

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Motion of Electrons and Holes in Perturbed Periodic Fields

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A new method of developing an "effective-mass" equation for electrons moving in a perturbed periodic structure is discussed. This method is particularly adapted to such problems as arise in connection with impurity states and cyclotron resonance in semiconductors such as Si and Ge. The resulting theory generalizes the usual effective-mass treatment to the case where a band minimum is not at the center of the Brillouin zone, and also to the case where the band is degenerate. The latter is particularly striking, the usual Wannier equation being replaced by a set of coupled differential equations.

Begin with the total Hamiltonian for the cell-periodic fn's dropping their band indices for convenience:

$$Hu_{\mathbf{k}}(\mathbf{r}) = E(\mathbf{k})u_{\mathbf{k}}(\mathbf{r})$$

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

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

$$H' = \frac{\hbar}{m_0}\mathbf{k} \cdot \Pi$$

Neglect compared to

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

Ref: Chuang

Expand any cell-periodic wfn in terms of the **k**=0 basis:

$$u_{\mathbf{k}}(\mathbf{r}) = \sum_{j'}^{A} a_{j'}(\mathbf{k}) u_{j'0}(\mathbf{r}) + \sum_{\gamma}^{B} a_{\gamma}(\mathbf{k}) u_{\gamma 0}(\mathbf{r})$$

where, from Kane's model we learned that **k**=0 solutions are of the form:

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

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

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

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

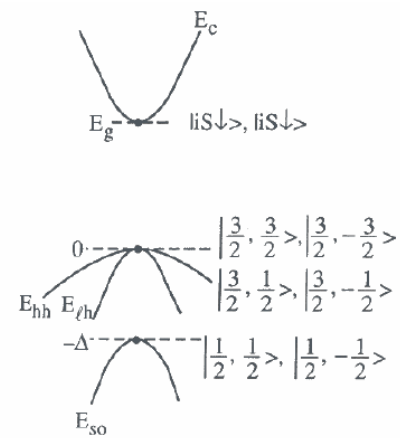
$$u_{50}(\mathbf{r}) = \left|\frac{1}{2}, \frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}} |(X + \mathrm{i}Y)\downarrow\rangle + \frac{1}{\sqrt{3}} |Z\uparrow\rangle$$

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

Ref: Chuang

Also recall that at **k**=0, band edge fn's satisy:

$$H(\mathbf{k}=0)u_{j0}(\mathbf{r}) = E_j(0)u_{j0}(\mathbf{r})$$



$$E_j(0) = E_p + \frac{\Delta}{3} = 0 \qquad \text{for } j = 1,2,3,4$$

$$E_j(0) = E_p - \frac{2\Delta}{3} = -\Delta \qquad \text{for } j = 5,6$$

where $E_p = -\Delta/3$

Now, apply Löwdin's method:

$$\sum_{j'}^{A}\left(U_{jj'}^{A} - E\delta_{jj'}\right)a_{j'}(\mathbf{k}) = 0$$

Effect of remote bands are here

Ref: Chuang

where

$$U_{jj'}^{A} = H_{jj'} + \sum_{\gamma \neq j,\, j'}^{B} \frac{H_{j\gamma} H_{\gamma j'}}{E_0 - E_\gamma} = H_{jj'} + \sum_{\gamma \neq j,\, j'}^{B} \frac{H'_{j\gamma} H'_{\gamma j'}}{E_0 - E_\gamma}$$

$$H_{jj'} = \langle u_{j0} | H | u_{j'0} \rangle = \left[E_j(0) + \frac{\hbar^2 k^2}{2m_0} \right] \delta_{jj'} \qquad (j, j' \in A)$$

$$H'_{j\gamma} = \langle u_{j0} | \frac{\hbar}{m_0} \mathbf{k} \cdot \overset{\mathbf{p}}{\mathbf{\Pi}} | u_{\gamma 0} \rangle \cong \sum_{\alpha} \frac{\hbar k_\alpha}{m_0} p_{j\gamma}^{\alpha} \qquad (j \in A, \gamma \notin A)$$

where we note that $\Pi_{jj'} = 0$, for $j, j' \in A$, and $\Pi_{j\gamma}^{\alpha} \simeq p_{j\gamma}^{\alpha}$ for $j \in A$ and $\gamma \notin A$. Since $\gamma \neq j$, adding the unperturbed part to the perturbed part in $H'_{j\gamma}$ does not affect the results, i.e., $H_{j\gamma} = H'_{j\gamma}$. We thus obtain

$$U_{jj'}^{A} = \left[E_j(0) + \frac{\hbar^2 k^2}{2m_0} \right] \delta_{jj'} + \frac{\hbar^2}{m_0^2} \sum_{\gamma \neq j,\, j'}^{B} \sum_{\alpha,\, \beta} \frac{k_\alpha k_\beta p_{j\gamma}^{\alpha} p_{\gamma j'}^{\beta}}{E_0 - E_\gamma}$$

Change of notation; let $U_{jj'}^{A} \equiv D_{jj'}$

Ref: Chuang

$$D_{jj'} = E_j(0)\,\delta_{jj'} + \sum_{\alpha,\beta} D_{jj'}^{\alpha\beta} k_\alpha k_\beta$$

where $$D_{jj'}^{\alpha\beta} = \frac{\hbar^2}{2m_0}\left[\delta_{jj'}\delta_{\alpha\beta} + \sum_{\gamma}^{B} \frac{p_{j\gamma}^{\alpha} p_{\gamma j'}^{\beta} + p_{j\gamma}^{\beta} p_{\gamma j'}^{\alpha}}{m_0(E_0 - E_\gamma)}\right]$$

For *j=j’*, similar to single-band effective mass tensor

To write the matrix elements explicity, define:

$$A_0 = \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0^2}\sum_{\gamma}^{B} \frac{p_{x\gamma}^{x} p_{\gamma x}^{x}}{E_0 - E_\gamma}$$

$$B_0 = \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0^2}\sum_{\gamma}^{B} \frac{p_{x\gamma}^{y} p_{\gamma x}^{y}}{E_0 - E_\gamma}$$

$$C_0 = \frac{\hbar^2}{m_0^2}\sum_{\gamma}^{B} \frac{p_{x\gamma}^{x} p_{\gamma y}^{y} + p_{x\gamma}^{y} p_{\gamma y}^{x}}{E_0 - E_\gamma}$$

Luttinger parameters

$$-\frac{\hbar^2}{2m_0}\gamma_1 = \frac{1}{3}(A_0 + 2B_0)$$

$$-\frac{\hbar^2}{2m_0}\gamma_2 = \frac{1}{6}(A_0 - B_0)$$

$$-\frac{\hbar^2}{2m_0}\gamma_3 = \frac{C_0}{6}$$

Ref: Chuang

In terms of Luttinger parameters, the LK Hamiltonian becomes:

$$\overline{\overline{\mathbf{H}}}^{\mathrm{LK}} = -\left[\begin{array}{cccccc} P+Q & -S & R & 0 & -S/\sqrt{2} & \sqrt{2}R \\ -S^{+} & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{3/2}\,S \\ R^{+} & 0 & P-Q & S & \sqrt{3/2}\,S^{+} & \sqrt{2}Q \\ 0 & R^{+} & S^{+} & P+Q & -\sqrt{2}R^{+} & -S^{+}/\sqrt{2} \\ -S^{+}/\sqrt{2} & -\sqrt{2}Q^{+} & \sqrt{3/2}\,S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^{+} & \sqrt{3/2}\,S^{+} & \sqrt{2}Q^{+} & -S/\sqrt{2} & 0 & P+\Delta \end{array}\right]\begin{array}{l} \text{HH} \\ \text{LH} \\ \text{LH} \\ \text{HH} \\ \text{SO} \\ \text{SO} \end{array}$$

complex conjugate

where

$$P = \frac{\hbar^2\gamma_1}{2m_0}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$Q = \frac{\hbar^2\gamma_2}{2m_0}\left(k_x^2 + k_y^2 - 2k_z^2\right)$$

$$R = \frac{\hbar^2}{2m_0}\left[-\sqrt{3}\,\gamma_2\left(k_x^2 - k_y^2\right) + i2\sqrt{3}\,\gamma_3 k_x k_y\right]$$

$$S = \frac{\hbar^2\gamma_3}{m_0}\sqrt{3}\,(k_x - ik_y)k_z$$

Ref: Chuang

So, essentially we have solved the Hamiltonian

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

where

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r}) \qquad u_{n\mathbf{k}}(\mathbf{r}) = \sum_{j=1}^{6} a_j(\mathbf{k})\,u_{j0}(\mathbf{r})$$

For the expansion eigenvectors and eigenvalues:

$$\sum_{j'=1}^{6} H_{jj'}^{\mathrm{LK}}a_{j'}(\mathbf{k}) = Ea_j(\mathbf{k}) \qquad\qquad E_n(\mathbf{k}) = E$$

Ref: Chuang