Reading note of Bernevig's science

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1 The 6-band bulk Kane model

The 6-band bulk Kane model which involves the Γ_6 and Γ_8 bands but neglects the Γ_7 band. For the last one is far away from the former two. In the basis $(|\Gamma^6, +1/2>, |\Gamma^6, -1/2>, |\Gamma^8, +3/2>, |\Gamma^8, +1/2>, |\Gamma^8, -1/2>, |\Gamma^8, -3/2>)$.

$$H(\mathbf{k}) = \begin{pmatrix} E_c I_{2\times 2} + H_c & T_{2\times 4} \\ T^\dagger_{4\times 2} & E_v I_{4\times 4} + H_v \end{pmatrix}. \tag{1}$$

where E_C and E_V are the offset energy of the conduction band and the valence band respectively. H_c and H_v are the (Luttinger) band Hamiltonian.

$$H_c = \begin{pmatrix} \frac{\hbar^2 k^2}{2m^*} & 0 \\ 0 & \frac{\hbar^2 k^2}{2m^*} \end{pmatrix}; \tag{2}$$

$$H_v = -\frac{\hbar^2}{2m_0}(\gamma_1 + \frac{5}{2}\gamma_2)k^2 + \frac{\hbar^2}{m_0}\gamma_2(\mathbf{k}\cdot\mathbf{S})^2 \tag{3}$$

$T(k)$ is the interaction matrix.

$$T^\dagger = \begin{pmatrix} -\frac{1}{\sqrt{2}}Pk_- & 0 \\ \sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{6}}Pk_- \\ \frac{1}{\sqrt{2}}Pk_- & \sqrt{\frac{2}{3}}Pk_z \\ 0 & -\frac{1}{\sqrt{2}}Pk_- \end{pmatrix}; \tag{4}$$

where, $k_\pm = k_x \pm ik_y$ and $P = -\frac{\hbar}{m_0} < S|p_x|X >$,$S$ is the spin $-3/2$ operator.

2 Envelope function at $\mathbf{k}_\parallel = 0$

The quantum well growth direction is along z, $HgTe$ for $-d/2 < z < d/2$, $CdTe$ for $z > d/2$ and $z < -d/2$.

The wave-function in each region take the gerneral form:

$$H(\mathbf{k})\psi(k_x, k_y, z) = H(k_x, k_y, -i\partial_z)\psi(k_x, k_y, z);$$

$$\psi(k_x, k_y, z) = e^{i(k_x x + k_y y)}\Psi(z) \tag{5}$$

We split the Hamiltonian into one zero in-plane momentum part and the other with finite in-plane momentum.

Fhe first part.

$$H(0,0,-i\partial_z) = \begin{pmatrix} T & 0 & 0 & \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 & 0 \\ 0 & T & 0 & 0 & \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 \\ 0 & 0 & U+V & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 & 0 & U-V & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}}P(-i\partial_z) & 0 & 0 & U-V & 0 \\ 0 & 0 & 0 & 0 & 0 & U+V \end{pmatrix} \tag{6}$$

where $T = E_c(z) + (-\partial_z A(z)\partial_z), U = E_v(z) - (-\partial_z\gamma_1(z)\partial_z), V = 2(-\partial_z\gamma_2(z)\partial_z)$.

A state has the general form under the envelope function approximation:

$$\Psi(k_x,k_y,z) = e^{i(k_x x + k_y y)} \begin{pmatrix} f_1(z) \\ f_2(z) \\ f_3(z) \\ f_4(z) \\ f_5(z) \\ f_6(z) \end{pmatrix} \tag{7}$$

When $k_x = k_y = 0$, f_3 and f_6 components are decoupled from others and from the spin up and spin down states of the H_1 subband. While f_1, f_2, f_4, f_5 components combine together to form the spin up and spin down states of the E_1 and L_1 subbands.

The linear-in-k_z operator $\sqrt{\frac{2}{3}}Pk_z$ requires the $|\Gamma_6, \pm\frac{1}{2} > (z)$ and $|\Gamma_8, \pm\frac{1}{2} > (z)$ of the E_1 to have different symmetry under reflection of z to $-z$. (parity with respect to z.) $|\Gamma_6 >$ band is symmetric, while $|\Gamma_8, \pm\frac{1}{2} >$ band is antisymmetric in z.

3 An ansatz solution at $\mathbf{k}_\parallel = 0$

1 . For the E_1 band, we take the ansatz to be:

$$\Psi_I = \begin{pmatrix} e^{\alpha z}C_1 \\ 0 \\ 0 \\ e^{\alpha z}C_4 \\ 0 \\ 0) \end{pmatrix}, \Psi_{II} = \begin{pmatrix} (e^{\delta z} + e^{-\delta z})V_1 \\ 0 \\ 0 \\ (e^{\delta z} - e^{-\delta z})V_4 \\ 0 \\ 0) \end{pmatrix}, \Psi_{III} = \begin{pmatrix} e^{-\alpha z}C_1 \\ 0 \\ 0 \\ e^{-\alpha z}C_4 \\ 0 \\ 0) \end{pmatrix}, \tag{8}$$

Take them into the Schrodinger equation, we get:

$$\begin{gathered} Tf_1(z) + \sqrt{\tfrac{2}{x}}P(z)(-i\partial_z)f_4(z) = Ef_1(z) \\ \sqrt{\tfrac{2}{x}}P(z)(-i\partial_z)f_1(z) + (U-V)f_4(z) = Ef_4(z) \end{gathered} \tag{9}$$

In region I,

$$\begin{gathered} [E_c^{(Cd)} + (-\partial_z A^{(Cd)}\partial_z)]e^{\alpha z}C_1 + \sqrt{\tfrac{2}{x}}P(-i\partial_z)e^{\alpha z}C_4 = Ee^{\alpha z}C_1 \\ \sqrt{\tfrac{2}{x}}P(-i\partial_z)e^{\alpha z}C_1 + [(E_v(z) - (-\partial_z\gamma_1^{(Cd)}\partial_z) - 2(-\partial_z\gamma_2^{(Cd)}\partial_z))]e^{\alpha z}C_4 = Ee^{\alpha z}C_4 \end{gathered} \tag{10}$$

Simplifying,

$$\begin{gathered} (E_c^{(Cd)} - A^{(Cd)}\alpha^2(E) - E)C_1 = \sqrt{\tfrac{2}{3}}P(i\alpha(z))C_4 \\ \sqrt{\tfrac{2}{3}}P(i\alpha(z))C_1 = (E_v^{(Cd)} - (\gamma_1^{(Cd)} + 2\gamma_2^{(Cd)})\alpha^2(E) - E)C_4 \end{gathered} \tag{11}$$

For the non-trivial case,we get,

$$\frac{E_c^{(Cd)} - A^{(Cd)}\alpha^2(E) - E}{\sqrt{\frac{2}{3}}P(i\alpha(z))C_4} = \frac{\sqrt{\frac{2}{3}}P(i\alpha(z))C_4}{E_v^{(Cd)} - (\gamma_1^{(Cd)} + 2\gamma_2^{(Cd)})\alpha^2(E) - E} = \frac{C_4}{C_1} \tag{12}$$

In region II,

$$\begin{gathered}[E_c^{(Hg)} + (-\partial_z A(z)\partial_z)](e^{\delta z} + e^{-\delta z})V_1 + \sqrt{\tfrac{2}{x}}P(-i\partial_z)(e^{\delta z} - e^{-\delta z})V_4 = E(e^{\delta z} + e^{-\delta z})V_1 \\ \sqrt{\tfrac{2}{3}}P(-i\partial_z)(e^{\delta z} + e^{-\delta z})V_1 + [(E_v(z) - (-\partial_z\gamma_1^{(Hg)}\partial_z) - 2(-\partial_z\gamma_2^{(Hg)}\partial_z))](e^{\delta z} - e^{-\delta z})V_4 = Ee^{\alpha z}(e^{\delta z} - e^{-\delta z})V_4\end{gathered} \tag{13}$$

Simplifying, we can also easily obtain an equation of δ,

$$\frac{E_c^{(Hg)} - A^{(Hg)}\delta^2(E) - E}{\sqrt{\frac{2}{3}}P(i\delta(z))} = \frac{\sqrt{\frac{2}{3}}P(i\delta(z))}{E_v^{(Hg)} - (\gamma_1^{(Hg)} + 2\gamma_2^{(Hg)})\delta^2(E) - E} = \frac{V_4}{V_1} \tag{14}$$

The boundary condition:

$$\begin{aligned}\Psi_I(-d/2) &= \Psi_{II}(-d/2) \\ \partial_z\Psi_I(z)\big|_{z=-\frac{d}{2}} &= \partial_z\Psi_{II}(z)\big|_{z=-\frac{d}{2}}\end{aligned} \tag{15}$$

$$\begin{aligned}f_{I1}(-d/2) &= f_{II1}(-d/2) \\ f_{I4}(-d/2) &= f_{II4}(-d/2)\end{aligned}$$

$$\Longrightarrow \frac{f_{II4}(-d/2)}{f_{II1}(-d/2)} = \frac{f_{I4}(-d/2)}{f_{I1}(-d/2)}$$

$$\Longrightarrow \tanh(\frac{\delta(E)d}{2})\frac{V_4}{V_1} = \frac{C_4}{C_1} \tag{16}$$

Inserting (12) and (14), we arrive at

$$\Longrightarrow -\tanh(\frac{\delta(E)d}{2})\frac{E_c^{(Hg)} - A^{(Hg)}\delta^2(E) - E}{\sqrt{\frac{2}{3}}P(i\delta(z))} = \frac{E_c^{(Cd)} - A^{(Cd)}\alpha^2(E) - E}{\sqrt{\frac{2}{3}}P(i\alpha(z))} \tag{17}$$

$$\Longrightarrow -\tanh(\frac{\delta(E)d}{2})\frac{E_c^{(Hg)} - A^{(Hg)}\delta^2(E) - E}{\delta(z)} = \frac{E_c^{(Cd)} - A^{(Cd)}\alpha^2(E) - E}{\alpha(z)} \tag{18}$$

2 . Derive the H_1 subband follow a similar procedure.
The wave-function in the three regions is

$$\begin{pmatrix}\Psi_I(z) \\ \Psi_{II}(z) \\ \Psi_{III}(z)\end{pmatrix} = \begin{pmatrix}C_3e^{\beta z} \\ V_3\cos(\kappa z) \\ C_3e^{-\beta z}\end{pmatrix} \tag{19}$$

$$(U + V)f_3(z) = Ef_3(z) \tag{20}$$

$$[E_v(z) - (-\partial_z\gamma_1(z)\partial_z) + 2(-\partial_z\gamma_2(z)\partial_z)]f_3(z) = Ef_3(z) \tag{21}$$

Let's look at the surface continuity between the region I and region II.

Perform a small integration near the surface in the z direction.

$$\int_{-d/2-\epsilon}^{-d/2+\epsilon} dz[E_v(z) - (-\partial_z \gamma_1(z)\partial_z) + 2(-\partial_z \gamma_2(z)\partial_z)]f_3(z) = \int_{-d/2-\epsilon}^{-d/2+\epsilon} dz E f_3(z) \tag{22}$$

when $\epsilon \to 0$,

$$\int_{0}^{-d/2+\epsilon} dz[\gamma_1^{(Cd)} - 2\gamma_2^{(Cd)}]\frac{d^2}{dz^2} f_3(z) + \int_{-d/2-\epsilon}^{0} dz[\gamma_1^{(Hg)} - 2\gamma_2^{(Hg)}]\frac{d^2}{dz^2} f_3(z) = \int_{-d/2-\epsilon}^{-d/2+\epsilon} dz[E - E_v(z)]f_3(z) \simeq 0, \epsilon \to 0$$

$$\Longrightarrow [\gamma_1^{(Cd)} - 2\gamma_2^{(Cd)}]\frac{df_3(z)}{dz}|_{z=-d/2} = -[\gamma_1^{(Hg)} - 2\gamma_2^{(Hg)}]\frac{df_3(z)}{dz}|_{z=-d/2} \tag{23}$$

Note that

$$f_{I3}(-d/2) = f_{II3}(-d/2) \tag{24}$$

Combine together (23) and (24), we arrive at the following energy equation,

$$\frac{1}{(\gamma_1^{(Cd)} - 2\gamma_2^{(Cd)})\beta(E)} = \frac{1}{(\gamma_1^{(Hg)} - 2\gamma_2^{(Hg)})\kappa(E)} \cot(\kappa(E)d/2) \tag{25}$$