Física de Semiconductores

Lección 15

The K point hamiltonian I

- The whole hamiltonian is

$$H_K = \begin{pmatrix} H_0 + H_z & H_x - iH_y \\ H_x + iH_y & H_0 - H_z \end{pmatrix}$$

$$H_0 = \varepsilon_p - 3V_2 \cos\alpha$$

$$H_x = -\frac{\sqrt{3}V_{pp\pi}a}{2} q_x$$

$$H_y = -\frac{\sqrt{3}V_{pp\pi}a}{2} q_y$$

$$H_z = \Delta_p - 3\sqrt{3}V_2 \sin\alpha$$

- or

$$H_K = \begin{pmatrix} \varepsilon_p - 3V_2\cos\alpha + \Delta_p - 3\sqrt{3}V_2\sin\alpha & -\frac{\sqrt{3}V_{pp\pi}a}{2}\left(q_x - iq_y\right) \\ -\frac{\sqrt{3}V_{pp\pi}a}{2}\left(q_x + iq_y\right) & \varepsilon_p - 3V_2\cos\alpha - \Delta_p + 3\sqrt{3}V_2\sin\alpha \end{pmatrix}$$

K- point hamiltonian II

- Or

$$H_K = -\frac{\sqrt{3}V_{pp\pi}a}{2}\times$$

$$\begin{pmatrix} -2\frac{\varepsilon_p - 3V_2\cos\alpha + \Delta_p - 3\sqrt{3}V_2\sin\alpha}{\sqrt{3}V_{pp\pi}a} & \left(q_x - iq_y\right) \\ \left(q_x + iq_y\right) & -2\frac{\varepsilon_p - 3V_2\cos\alpha - \Delta_p + 3\sqrt{3}V_2\sin\alpha}{\sqrt{3}V_{pp\pi}a} \end{pmatrix}$$

- We then change the zero of energy so that

$$H_K = -\frac{\sqrt{3}V_{pp\pi}a}{2}\begin{pmatrix} -2\frac{+\Delta_p - 3\sqrt{3}V_2\sin\alpha}{\sqrt{3}V_{pp\pi}a} & \left(q_x - iq_y\right) \\ \left(q_x + iq_y\right) & -2\frac{-\Delta_p + 3\sqrt{3}V_2\sin\alpha}{\sqrt{3}V_{pp\pi}a} \end{pmatrix}$$

K and K’ point hamiltonian

- We then define a “mass” so that

$$H_K = -\frac{\sqrt{3}V_{pp\pi}a}{2}\begin{pmatrix} m & q_x - iq_y \\ q_x + iq_y & -m \end{pmatrix} = \hbar v_F \begin{pmatrix} m & q_x - iq_y \\ q_x + iq_y & -m \end{pmatrix}$$

- A similar analysis for the K’ point gives

$$H_{K'} = -\frac{\sqrt{3}V_{pp\pi}a}{2}\begin{pmatrix} m & q_x + iq_y \\ q_x - iq_y & -m \end{pmatrix} = \hbar v_F \begin{pmatrix} m & q_x + iq_y \\ q_x - iq_y & -m \end{pmatrix}$$

Spherical coordinates

- We define

$$m = k\cos\theta$$
$$q_x = k\sin\theta\cos\varphi$$
$$q_y = k\sin\theta\sin\varphi$$

- Then we get

$$H_K = \hbar v_F k \begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix}$$

$$H_{K'} = \hbar v_F k \begin{pmatrix} \cos\theta & \sin\theta e^{i\varphi} \\ \sin\theta e^{-i\varphi} & -\cos\theta \end{pmatrix}$$

Eigenvectors and eigenvalues

- The eigenvalues of our hamiltonians are

$$\varepsilon_{\pm} = \pm \hbar k v_{F}$$

- and the eigenvector for the filled band:

$$u_{-} = \begin{pmatrix} -\sin\dfrac{\theta}{2} \\ e^{i\varphi}\cos\dfrac{\theta}{2} \end{pmatrix}$$

Singularity

- The eigenvector $u_- = \left(-\sin\frac{\theta}{2}, e^{i\varphi}\cos\frac{\theta}{2}\right)$ is singular for θ =0.
- The equivalent eigenvector $u_- = \left(-e^{-i\varphi}\sin\frac{\theta}{2}, \cos\frac{\theta}{2}\right)$ is singular for θ =π. We then choose

$$u_-^S = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix}; \quad u_-^N = \begin{pmatrix} -e^{-i\varphi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}$$

Berry connection I

- We now calculate the Berry connection in spherical coordinates for the south pole eigenvectors.

$$\mathcal{A}_{H}^{S} = i\left\langle u_{-}^{S}\right|\frac{\partial}{\partial k}\left|u_{-}^{S}\right\rangle = 0$$

$$\mathcal{A}_{\theta}^{S} = i\left\langle u_{-}^{S}\right|\frac{1}{k}\frac{\partial}{\partial \theta}\left|u_{-}^{S}\right\rangle = \left(-\sin\frac{\theta}{2}, e^{-i\varphi}\cos\frac{\theta}{2}\right)\frac{1}{k}\frac{\partial}{\partial \theta}\begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix}$$

$$= \frac{i}{k}\left(-\sin\frac{\theta}{2}, e^{-i\varphi}\cos\frac{\theta}{2}\right)\begin{pmatrix} -\frac{1}{2}\cos\frac{\theta}{2} \\ -\frac{1}{2}e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} = 0$$

Berry connection II

$$\mathcal{A}_{\varphi}^{S} = i\left\langle u_{-}^{S}\right|\frac{1}{k\sin\theta}\frac{\partial}{\partial\varphi}\left|u_{-}^{S}\right\rangle = i\left(-\sin\frac{\theta}{2}, e^{-i\varphi}\cos\frac{\theta}{2}\right)\frac{1}{k\sin\theta}\frac{\partial}{\partial\varphi}\begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix}$$

$$= \frac{i}{k\sin\theta}\left(-\sin\frac{\theta}{2}, e^{-i\varphi}\cos\frac{\theta}{2}\right)\begin{pmatrix} 0 \\ ie^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix} = -\frac{\cos^{2}\left(\frac{\theta}{2}\right)}{k\sin\theta}$$

Berry curvature for K point

- For the Berry curvature we use the curl in spherical coordinates, knowing that the connection only has a ϕ component. Then

$$\boldsymbol{\Omega}_K = \nabla \times \mathcal{A} = \frac{1}{k\sin\theta}\frac{\partial}{\partial\theta}\left(\mathcal{A}_\varphi \sin\theta\right)\hat{\boldsymbol{e}}_k - \frac{1}{k}\frac{\partial}{\partial k}\left(k\mathcal{A}_\varphi\right)\hat{\boldsymbol{e}}_\theta$$

$$= \frac{1}{k\sin\theta}\frac{\partial}{\partial\theta}\left(-\frac{1}{k}\cos^2\left(\frac{\theta}{2}\right)\right)\hat{\boldsymbol{e}}_k - \frac{1}{k}\frac{\partial}{\partial k}\left(\frac{\cos^2\left(\frac{\theta}{2}\right)}{\sin\theta}\right)\hat{\boldsymbol{e}}_\theta$$

$$-\frac{1}{k^2\sin\theta}\frac{\partial}{\partial\theta}\left(\cos^2\left(\frac{\theta}{2}\right)\right)\hat{\boldsymbol{e}}_k = -\frac{1}{k^2\sin\theta}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) = -\frac{\hat{\boldsymbol{e}}_k}{2k^2}$$

Berry curvature for K' point

- For the K' point, the only change is $\varphi \rightarrow -\varphi$, an this changes the sign of the connection and the curvature, so

$$\boldsymbol{\Omega}_{K'} = \frac{\hat{\boldsymbol{e}}_k}{2k^2}$$

Chern number

- The Chern number is defined as the surface integral of the Berry curvature over the BZ. - is for K point, + for K' point:

$$\mathcal{C} = \frac{1}{2\pi} \oiint_{BZ} dq_x \, dq_y \Omega_z = \frac{1}{2\pi} \oiint_{BZ} dq_x \, dq_y \frac{\pm\left(\hat{\boldsymbol{e}}_k\right)_z}{2k^2}$$

$$= \pm \frac{1}{4\pi} \oiint_{BZ} dq_x \, dq_y \frac{\cos\theta}{\left(q^2 + m^2\right)} = \pm \frac{1}{4\pi} \oiint_{BZ} dq_x \, dq_y \frac{m}{\left(q^2 + m^2\right)^{3/2}}$$

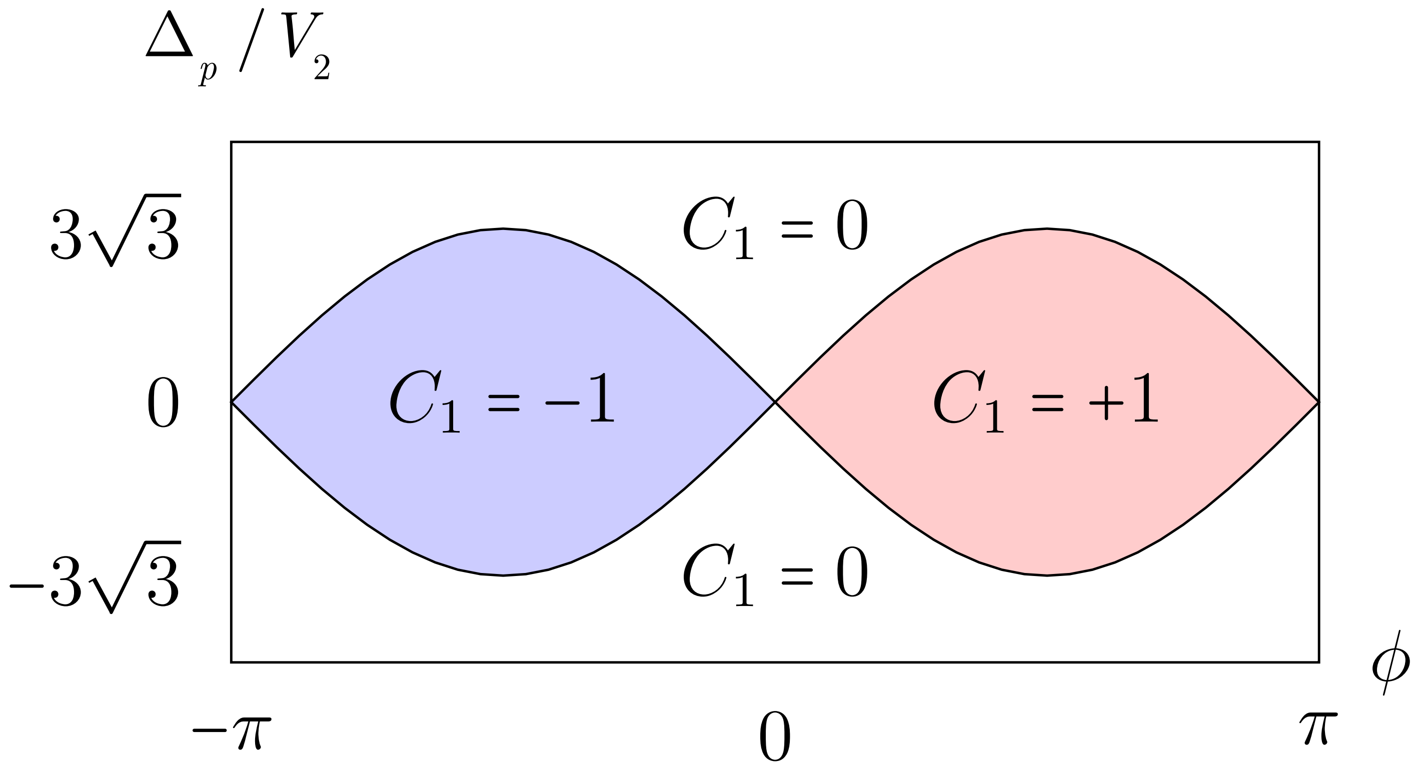
$$= \pm \frac{2\pi}{4\pi} m \int_0^\infty \frac{q\,dq}{\left(q^2 + m^2\right)^{3/2}} = \pm \frac{1}{4} m \int_{m^2}^\infty \frac{du}{u^{3/2}} = \frac{1}{4} m \left(-2u^{-1/2}\right)\Big|_{m^2}^\infty$$

$$= \pm \frac{1}{2} \frac{m}{\left|m\right|} = \pm \frac{1}{2} \operatorname{sgn}\left(m\right)$$

Phase diagram

- For
$$m_K > 0, m_{K'} > 0$$
$$\mathcal{C}_K + \mathcal{C}_{K'} = -\frac{1}{2} + \frac{1}{2} = 0$$
- For
$$m_K < 0, m_{K'} > 0$$
$$\mathcal{C}_K + \mathcal{C}_{K'} = +\frac{1}{2} + \frac{1}{2} = 1$$
- For
$$m_K > 0, m_{K'} < 0$$
$$\mathcal{C}_K + \mathcal{C}_{K'} = -\frac{1}{2} - \frac{1}{2} = -1$$
- For
$$m_K < 0, m_{K'} < 0$$
$$\mathcal{C}_K + \mathcal{C}_{K'} = \frac{1}{2} - \frac{1}{2} = 0$$

Phase diagram



Periodicity of energy function

- The energy function is periodic in k-space:

$$E_n\left(\boldsymbol{k}\right) = E_n\left(\boldsymbol{k} + \boldsymbol{K}\right)$$

- Therefore

$$E_n\left(\boldsymbol{k}\right) = \sum_{\boldsymbol{R}} E_n\left(\boldsymbol{R}\right) e^{i\boldsymbol{R}\cdot\boldsymbol{k}}$$

- Now consider operator $E_n\left(-i\boldsymbol{\nabla}\right)$

$$E_n\left(-i\boldsymbol{\nabla}\right)\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) = \sum_{\boldsymbol{R}} E_n\left(\boldsymbol{R}\right) e^{\boldsymbol{R}\cdot\boldsymbol{\nabla}}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$= \sum_{\boldsymbol{R}} E_n\left(\boldsymbol{R}\right)\left[1 + \boldsymbol{R}\cdot\boldsymbol{\nabla} + \tfrac{1}{2}\left(\boldsymbol{R}\cdot\boldsymbol{\nabla}\right)^2 + \ldots\right]\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

$$= \sum_{\boldsymbol{R}} E_n\left(\boldsymbol{R}\right)\psi_{n\boldsymbol{k}}\left(\boldsymbol{r} + \boldsymbol{R}\right) = \sum_{\boldsymbol{R}} E_n\left(\boldsymbol{R}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right) = E_{n\boldsymbol{k}}\psi_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)$$

- so that the Bloch function is an eigenfunction of this operator with eigenvalue $E_n\left(\boldsymbol{k}\right)$

Bloch hamiltonian plus perturbation

- Consider $\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - e\phi(\boldsymbol{r})\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$
- Ansatz
  $$\psi = \sum_{n\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$
- Then

$$\sum_{n\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - e\phi(\boldsymbol{r})\right]\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$\sum_{n\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\left[E_{n\boldsymbol{k}} - e\phi(\boldsymbol{r})\right]\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_{n\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\left[E_n(-i\boldsymbol{\nabla}) - e\phi(\boldsymbol{r})\right]\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$= i\hbar\frac{\partial\psi}{\partial t}$$

Weak perturbation approx

- If the perturbation is weak enough not to mix different bands

$$\psi \simeq \sum_{\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

- then, since the square bracket is indep of k.

$$\sum_{\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\left[E_n(-i\boldsymbol{\nabla}) - e\phi(\boldsymbol{r})\right]\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \left[E_n(-i\boldsymbol{\nabla}) - e\phi(\boldsymbol{r})\right]\sum_{\boldsymbol{k}} c_{n\boldsymbol{k}}(t)\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$= \left[E_n(-i\boldsymbol{\nabla}) - e\phi(\boldsymbol{r})\right]\psi$$

- So

$$\left[E_n(-i\boldsymbol{\nabla}) - e\phi(\boldsymbol{r})\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Effective mass theory I

- Let us assume

$$E_n(k) = E_0 + \frac{\hbar^2 k^2}{2m^*}; \quad \psi_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \simeq u_{n\boldsymbol{0}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \psi_{n\boldsymbol{0}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

- Then

$$\psi \simeq \sum_{\boldsymbol{k}} c_{n\boldsymbol{k}}(t) \psi_{n\boldsymbol{k}}(\boldsymbol{r}) \simeq \sum_{\boldsymbol{k}} c_{n\boldsymbol{k}}(t) \psi_{n\boldsymbol{0}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} =$$

$$= \psi_{n\boldsymbol{0}}(\boldsymbol{r}) \sum_{\boldsymbol{k}} c_{n\boldsymbol{k}}(t) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = F_n(\boldsymbol{r}, t)\, \psi_{n\boldsymbol{0}}(\boldsymbol{r})$$

- where *F* is called an envelope function.

Effective mass theory II

- Let us now compute

$$E_n\left(-i\boldsymbol{\nabla}\right)F_n\left(\boldsymbol{r},t\right)\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)=\sum_{\boldsymbol{R}}E_n\left(\boldsymbol{R}\right)F_n\left(\boldsymbol{r}+\boldsymbol{R},t\right)\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}+\boldsymbol{R}\right)$$

$$=\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)\sum_{\boldsymbol{R}}E_n\left(\boldsymbol{R}\right)F_n\left(\boldsymbol{r}+\boldsymbol{R},t\right)=\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)\sum_{\boldsymbol{R}}E_n\left(\boldsymbol{R}\right)e^{\boldsymbol{R}\cdot\boldsymbol{\nabla}}F_n\left(\boldsymbol{r},t\right)$$

$$=\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)E_n\left(-i\boldsymbol{\nabla}\right)F_n\left(\boldsymbol{r},t\right)$$

- Then

$$\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)E_n\left(-i\boldsymbol{\nabla}\right)F_n\left(\boldsymbol{r},t\right)-e\phi\left(\boldsymbol{r}\right)\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)F_n\left(\boldsymbol{r},t\right)=i\hbar\psi_{n\boldsymbol{0}}\left(\boldsymbol{r}\right)\frac{\partial F_n\left(\boldsymbol{r},t\right)}{\partial t}$$

- which gives

$$\left[-\frac{\hbar^2\nabla^2}{2m^*}+E_0-e\phi\left(\boldsymbol{r}\right)\right]F_n\left(\boldsymbol{r},t\right)=i\hbar\frac{\partial F_n\left(\boldsymbol{r},t\right)}{\partial t}$$

Quantum wells

- The corresponding equation is

$$\left[-\frac{\hbar^2\nabla^2}{2m^*\left(x\right)}+E_0\left(x\right)\right]F_n\left(\boldsymbol{r},t\right)=i\hbar\frac{\partial F_n\left(\boldsymbol{r},t\right)}{\partial t}$$

- The boundary conditions are complicated. A common choice

$$F_n^-\left(x=0\right)=F_n^+\left(x=0\right)$$

$$\left.\frac{1}{m^{*-}}\frac{\partial F_n^-}{\partial x}\right|_{x=0}=\left.\frac{1}{m^{*+}}\frac{\partial F_n^+}{\partial x}\right|_{x=0}$$

Edge states IV

- We now apply EMT to our Haldane hamiltonian

$$\hbar v_F \begin{pmatrix} m & q_x - iq_y \\ q_x + iq_y & -m \end{pmatrix} \Rightarrow \hbar v_F \begin{pmatrix} m(y) & -i\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \\ -i\frac{\partial}{\partial x} + \frac{\partial}{\partial y} & -m(y) \end{pmatrix}$$

- We propose a solution

$$\Psi(x,y)\begin{pmatrix} 1 \\ -1 \end{pmatrix} = e^{iq_x x} \exp\left(-\int_0^y m(y')\,dy'\right)\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

- Then, using

$$\frac{\partial \Psi(x,y)}{\partial x} = iq_x \Psi(x,y); \quad \frac{\partial \Psi(x,y)}{\partial y} = -m(y)\Psi(x,y)$$

Edge states V

- Then

$$m(y)\Psi(x,y) - \left(-i\frac{\partial\Psi(x,y)}{\partial x} - \frac{\partial\Psi(x,y)}{\partial y}\right) = E\Psi(x,y)$$

$$m(y)\Psi(x,y) + i\frac{\partial\Psi(x,y)}{\partial x} + \frac{\partial\Psi(x,y)}{\partial y} = E\Psi(x,y)$$

$$m(y)\Psi(x,y) + i(iq_x)\Psi(x,y) - m(y)\Psi(x,y) = E\Psi(x,y)$$

$$-q_x = E$$

$$H \propto \begin{pmatrix} m(y) & -i\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \\ -i\frac{\partial}{\partial x} + \frac{\partial}{\partial y} & -m(y) \end{pmatrix}$$

$$-i\frac{\partial\Psi(x,y)}{\partial x} + \frac{\partial\Psi(x,y)}{\partial y} + m(y)\Psi(x,y) = -E\Psi(x,y)$$

$$-i(iq_x) - m(y) + m(y) = -E$$

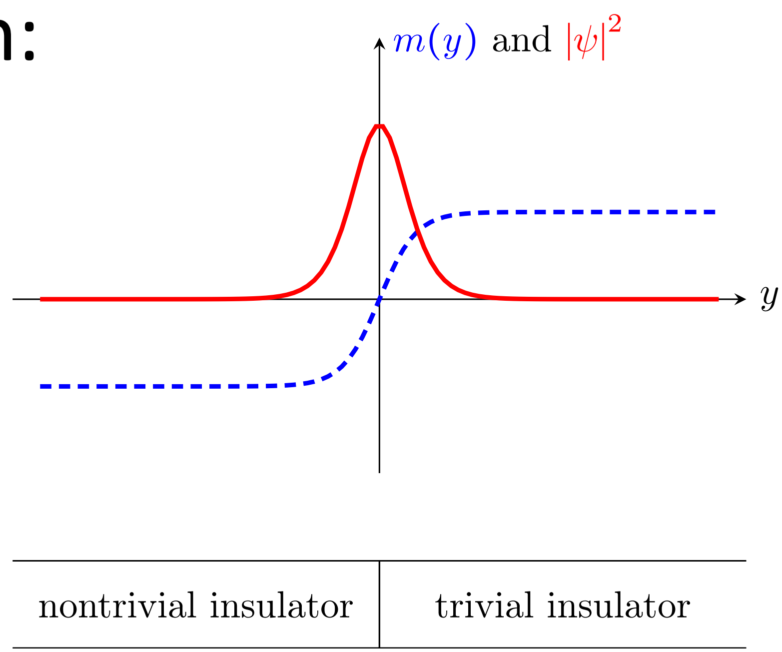
$$q_x = -E$$

Edge states VI

- Restoring units

$$E = -\hbar v_F q_x$$

Wavefunction:



arXiv:1310.0255v2

The other side

- We propose

$$\Psi\left(x,y\right)\begin{pmatrix} 1 \\ 1 \end{pmatrix} = e^{iq_x x}\exp\left(\int_0^y m\left(y'\right)dy'\right)\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\frac{\partial\Psi\left(x,y\right)}{\partial x} = iq_x\Psi\left(x,y\right); \quad \frac{\partial\Psi\left(x,y\right)}{\partial y} = m\left(y\right)\Psi\left(x,y\right)$$

- Then

$$m\left(y\right)\Psi\left(x,y\right) + \left(-i\frac{\partial\Psi\left(x,y\right)}{\partial x} - \frac{\partial\Psi\left(x,y\right)}{\partial y}\right) = E\Psi\left(x,y\right)$$

$$m\left(y\right)\Psi\left(x,y\right) - i\frac{\partial\Psi\left(x,y\right)}{\partial x} - \frac{\partial\Psi\left(x,y\right)}{\partial y} = E\Psi\left(x,y\right)$$

$$m\left(y\right)\Psi\left(x,y\right) - i\left(iq_x\right)\Psi\left(x,y\right) - m\left(y\right)\Psi\left(x,y\right) = E\Psi\left(x,y\right)$$

$$q_x = E$$

$$\Rightarrow E = \hbar v_F q_x$$

The k.p hamiltonian

- In a previous lecture we wrote down the k.p hamiltonian for $\boldsymbol{k} = (0, 0, k_z)$. Allowing for x- and y-components, it is easy to show that

	$\left\|S_a \uparrow\right\rangle$	$\left\|\frac{3}{2},-\frac{3}{2}\right\rangle_b$	$\left\|\frac{3}{2},\frac{1}{2}\right\rangle_b$	$\left\|S_a \downarrow\right\rangle$	$\left\|\frac{3}{2},\frac{3}{2}\right\rangle_b$	$\left\|\frac{3}{2},-\frac{1}{2}\right\rangle_b$
$\left\|S_a \uparrow\right\rangle$	E_0	0	$\frac{i\hbar P k_z}{m}\sqrt{\frac{2}{3}}$	0	$\frac{i\hbar P}{m}\frac{\left(k_x + ik_y\right)}{\sqrt{2}}$	$\frac{i\hbar P}{\sqrt{3}m}\frac{\left(k_x - ik_y\right)}{\sqrt{2}}$
$\left\|\frac{3}{2},-\frac{3}{2}\right\rangle_b$	0	0	0	$\frac{-i\hbar P}{m}\frac{\left(k_x - ik_y\right)}{\sqrt{2}}$	0	0
$\left\|\frac{3}{2},\frac{1}{2}\right\rangle_b$	$-\frac{i\hbar P k_z}{m}\sqrt{\frac{2}{3}}$	0	0	$\frac{-i\hbar P}{\sqrt{3}m}\frac{\left(k_x + ik_y\right)}{\sqrt{2}}$	0	0
$\left\|S_a \downarrow\right\rangle$	0	$\frac{i\hbar P}{m}\frac{\left(k_x + ik_y\right)}{\sqrt{2}}$	$\frac{i\hbar P}{\sqrt{3}m}\frac{\left(k_x - ik_y\right)}{\sqrt{2}}$	E_0	0	$\frac{i\hbar P k_z}{m}\sqrt{\frac{2}{3}}$
$\left\|\frac{3}{2},\frac{3}{2}\right\rangle_b$	$-\frac{i\hbar P}{m}\frac{\left(k_x - ik_y\right)}{\sqrt{2}}$	0	0	0	0	0
$\left\|\frac{3}{2},-\frac{1}{2}\right\rangle_b$	$-\frac{i\hbar P}{\sqrt{3}m}\frac{\left(k_x + ik_y\right)}{\sqrt{2}}$	0	0	$-\frac{i\hbar P k_z}{m}\sqrt{\frac{2}{3}}$	0	0

Heavy hole hamiltonian

- If we make a quantum well and apply effective mass theory, the light holes and heavy holes will approximately decouple, and we get for HH

	$\left\|S_a \uparrow\right\rangle$	$\left\|\frac{3}{2},-\frac{3}{2}\right\rangle_b$	$\left\|S_a \downarrow\right\rangle$	$\left\|\frac{3}{2},\frac{3}{2}\right\rangle_b$
$\left\|S_a \uparrow\right\rangle$	E_0	0	0	$\frac{i\hbar P}{m}\frac{\left(k_x+ik_y\right)}{\sqrt{2}}$
$\left\|\frac{3}{2},-\frac{3}{2}\right\rangle_b$	0	0	$\frac{-i\hbar P}{m}\frac{\left(k_x-ik_y\right)}{\sqrt{2}}$	0
$\left\|S_a \downarrow\right\rangle$	0	$\frac{i\hbar P}{m}\frac{\left(k_x+ik_y\right)}{\sqrt{2}}$	E_0	0
$\left\|\frac{3}{2},\frac{3}{2}\right\rangle_b$	$-\frac{i\hbar P}{m}\frac{\left(k_x-ik_y\right)}{\sqrt{2}}$	0	0	0

Reorder:

	$\left\| S_a \uparrow \right\rangle$	$\left\| \frac{3}{2}, \frac{3}{2} \right\rangle$	$\left\| S_a \downarrow \right\rangle$	$\left\| \frac{3}{2}, -\frac{3}{2} \right\rangle$
$\left\| S_a \uparrow \right\rangle$	E_0	$\frac{i\hbar P}{m}\frac{\left(k_x + ik_y\right)}{\sqrt{2}}$	0	0
$\left\| \frac{3}{2}, \frac{3}{2} \right\rangle$	$\frac{-i\hbar P}{m}\frac{\left(k_x - ik_y\right)}{\sqrt{2}}$	0	0	0
$\left\| S_a \downarrow \right\rangle$	0	0	E_0	$\frac{i\hbar P}{m}\frac{\left(k_x + ik_y\right)}{\sqrt{2}}$
$\left\| \frac{3}{2}, -\frac{3}{2} \right\rangle$	0	0	$-\frac{i\hbar P}{m}\frac{\left(k_x - ik_y\right)}{\sqrt{2}}$	0

Pauli matrices

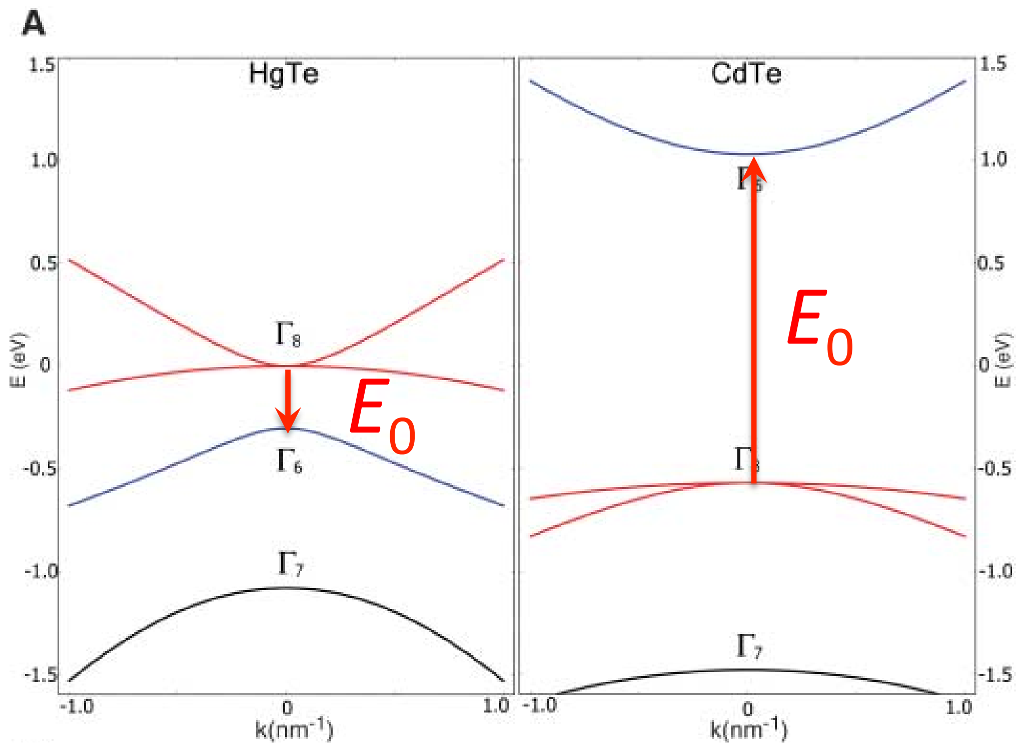
- This has the form

$$H = \begin{pmatrix} H(\boldsymbol{k}) & 0 \\ 0 & H^*(-\boldsymbol{k}) \end{pmatrix} \qquad H(\boldsymbol{k}) = E(\boldsymbol{k}) + \sum_{\alpha} d_{\alpha} \sigma_{i}$$

- With

$$d_x = \frac{i\hbar P}{\sqrt{2m}}; \quad d_y = -\frac{i\hbar P}{\sqrt{2m}}; \quad d_z = \frac{E_0}{2}$$

The bands



We see that E_0 is positive for CdTe and negative for HgTe. so we can get the same "mass" reversal we had in the Haldane model. The fact that HgTe is a semimetal, not a semiconductor, can be "fixed" by applying strain, which lifts the degeneracy at the G point. So by making strained layer HgTe-CdTe superlattices one can obtain topological phases akin to the Haldane model.