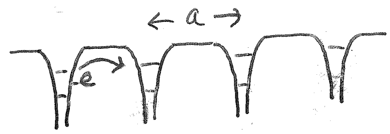
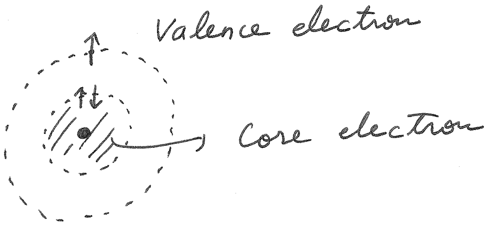
Band structure of solid

1D





$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \qquad \text{with} \qquad V(x) = V(x+a)$$

Solid: Broken translation symmetry

Invariant over discrete translations by $x \to x+a$

$$\hat{T}_a = e^{i\hat{p}a/\hbar} \quad , \quad [\hat{H}, \hat{T}_a] = 0.$$

$$\hat{T}_a \psi(x) = e^{i\hat{p}a/\hbar}\psi(x) = \psi(x+a) = \lambda\psi(x)$$

$$\hat{T}_a^{\,N}\psi(x) = \psi(x+Na) = \psi(x) \qquad \text{imposing PBC}$$

$$= \lambda^N \psi(x)$$

$$\therefore \lambda^N = 1 \qquad \lambda = e^{ika} \to e^{ikaN} = 1 \qquad \therefore ka = \frac{2n\pi}{N}$$

$$n = -\frac{N}{2}, \cdots, \frac{N}{2} \leftarrow n = 1, 2, \cdots N$$

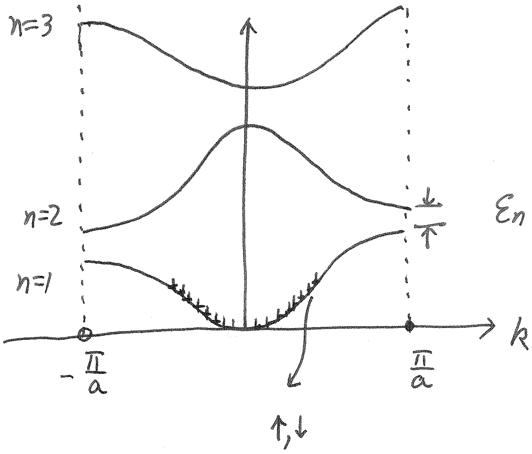
$\hbar k$: crystal momentum (good QN)

Bloch th$^{\underline{m}}$

$$\psi_k(x+a) = e^{ika}\psi_k(x)$$

or $\quad \psi_k(x) = e^{ikx}u_k(x) \quad$ with $\quad u_k(x+a) = u_k(x)$

$$H\psi_k = E(k)\psi_k$$



Group velocity: $v_k = \frac{1}{\hbar}\frac{dE(k)}{dk}$

Energy gap: Forbidden states

Brillouin zone : $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$

Metal: Partially filled band

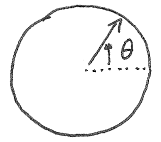
Band insulator : Completely filled band

N_e = even number $\times N$

$BZ \rightarrow U(1)$

$-\pi < ka \leq \pi$

compact variable

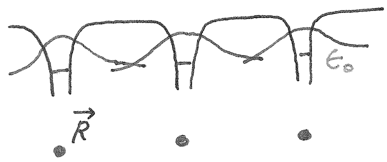


circle

$U^\dagger = U^{-1} \rightarrow |U|^2 = 1 \quad \therefore \quad U = e^{i\theta}$

invariant over $\theta \rightarrow \theta + 2\pi$

• Tight binding method



Wannier function

$$W_{n\vec{R}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{k} \in BZ} e^{-i\vec{k}\cdot\vec{R}} \psi_{n\vec{k}}(\vec{r})$$

$W_{n\vec{R}}$ ↓ quantum number

$\psi_{n\vec{k}}$ ↳ Bloch function, quantum number $\vec{k}$

localized orbital

cf) $W_{n\vec{R}}(\vec{r}) \equiv f(\vec{r} - \vec{R})$

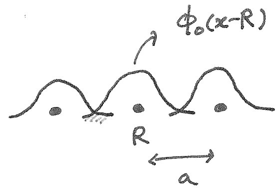
$\langle W_{n\vec{R}} | W_{n\vec{R}'} \rangle = \delta_{\vec{R}\vec{R}'}$

$$\psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} W_{n\vec{R}}(\vec{r})$$

Example) 1D and 1 band case

$$\hat{H} \psi_k(x) = E(k) \psi_k(x)$$

$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ with $V(x) = V(x+a)$.



$$\sum_R e^{ik\cdot R} \hat{H} W_R(x) = \sum_R E(k) e^{ikR} W_R(x)$$

By taking $\langle W_R |$,

$$\sum_{R'} e^{-ik(R-R')} \langle W_R | \hat{H} | W_{R'} \rangle = E(k)$$

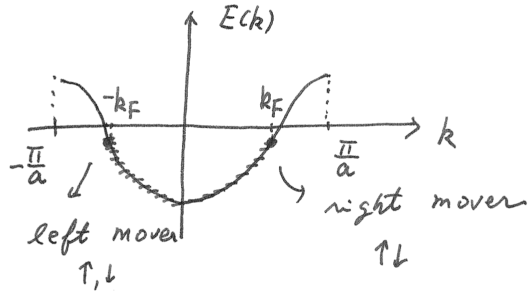
By $W_R(x) \simeq \phi_0(x-R)$ Atomic orbital,

$\epsilon_0 \delta_{RR'} - t(\delta_{R',R+a} + \delta_{R',R-a})$

2 Nearest neighbors.

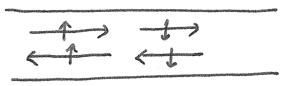
$$t \simeq -\epsilon_0 \int dx\, \phi_0^*(x) \phi_0(x-a)$$

$$\therefore \quad E(k) = \epsilon_0 - 2t \cos ka$$

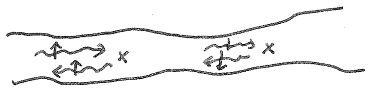


$$v_k = \frac{1}{\hbar} \frac{dE(k)}{dk}$$

• 1D quantum wire

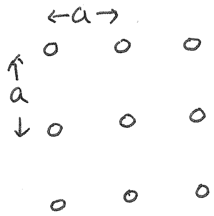


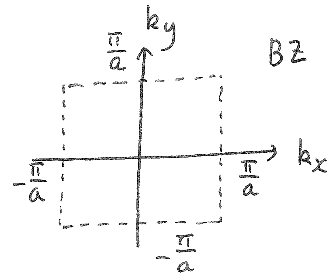
Scattering due to disorder



Strong localization due to backscattering

2D

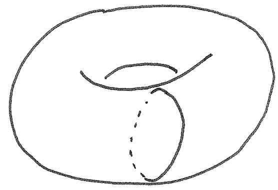




BZ

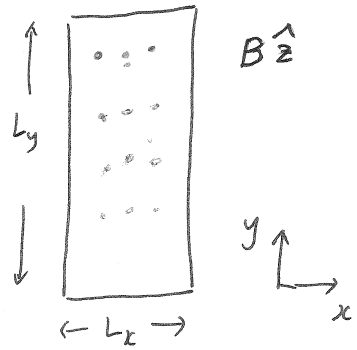
$-\pi < k_x a \leq \pi, \quad -\pi < k_y a \leq \pi$

$\rightarrow$



torus

Quantum Hall Effect



Landau gauge :

$\vec{A}(\vec{r}) = xB\hat{y}$

$\vec{\nabla}\times\vec{A} = B\hat{z}$

$$\hat{H} = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 \quad \text{with } q = -e$$

$$= \frac{1}{2m}\left(P_x^2 + \left(P_y + \frac{eB}{c}x\right)^2\right) \qquad [\hat{H}, P_y] = 0$$

$$\psi_k(x,y) = e^{iky} f_k(x) \qquad \therefore \quad h_k = \frac{1}{2m}P_x^2 + \frac{1}{2m}\left(\hbar k + \frac{eB}{c}x\right)^2$$

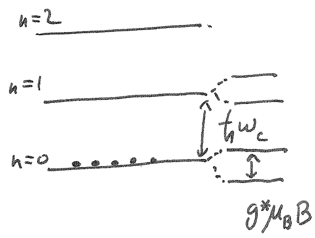
$$h_k f_k(x) = \epsilon_k f_k(x)$$

1D displaced Harmonic oscillator

$$h_k = \frac{1}{2m}P_x^2 + \frac{1}{2}m\omega_c^2(x + kl^2)^2 \quad \text{with } \omega_c \equiv \frac{eB}{mc}, \; l = \sqrt{\frac{\hbar c}{eB}}$$

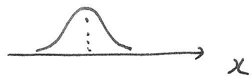
$$\epsilon_{kn} = \left(n + \frac{1}{2}\right)\hbar\omega_c$$

independent of k.



$$\psi_{nk}(\vec{r}) = \frac{1}{\sqrt{L_y}} e^{iky} \underbrace{H_n(x + kl^2)}_{\text{Hermite polynomial}} e^{-\frac{1}{2l^2}(x+kl^2)^2}$$

PBC along $\hat{y}$: $k = \dfrac{2n\pi}{L_y}$



$X_k = -k\ell^2$ $\qquad \Delta X_k = \dfrac{2\pi \ell^2}{L_y}$

Total number of states : $N = \dfrac{L_x}{\Delta X_k} = \dfrac{A}{2\pi \ell^2}$ $\qquad 2\pi\ell^2 = \dfrac{hc}{eB}$

$= \dfrac{\Phi}{\Phi_0} = N_\Phi$ $\qquad \Phi_0 = \dfrac{hc}{e}$

Quantum unit of flux

At the lowest Landau level,

$$\psi_k(\vec{r}) = \frac{1}{\sqrt{\pi^{1/2} L_y \ell}}\, e^{iky}\, e^{-\frac{1}{2\ell^2}(x+k\ell^2)^2}$$ KE quenched to $\epsilon_k = \frac{1}{2}\hbar\omega_c$

Uniform $\vec{E}$-field along $\hat{x}$ direction : $V(\vec{r}) = eEx$

$[\hat{H}, P_y] = 0$ $\qquad h_k = \dfrac{1}{2m}P_x^2 + \dfrac{1}{2}m\omega_c^2(x+k\ell^2)^2 + eEx$

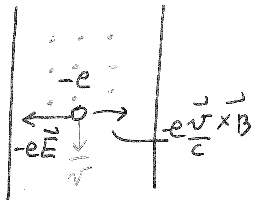
$$= \frac{1}{2m}P_x^2 + \frac{1}{2}m\omega_c^2 (x - X_k)^2$$

with $X_k = -k\ell^2 - \dfrac{eE}{m\omega_c^2}$

$$\epsilon_k = \frac{1}{2}\hbar\omega_c + eEX_k + \frac{1}{2}m\bar{v}^2$$ with $\bar{v} = -c\dfrac{E}{B}$

$$\frac{1}{\hbar}\frac{\partial \epsilon_k}{\partial k} = \frac{eE}{\hbar}\frac{\partial X_k}{\partial k} = -c\frac{E}{B} = \bar{v}$$

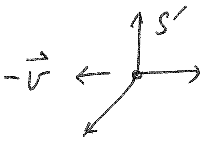
$\therefore \langle J_y \rangle = -e\bar{v}$

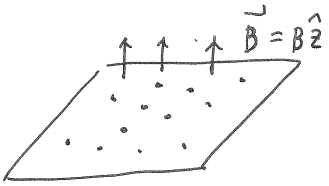


$c\,\vec{E}\times\vec{B}/B^2$

drift

In the absence of any impurity, 2DEG is translationally invariant! No preferred frame!



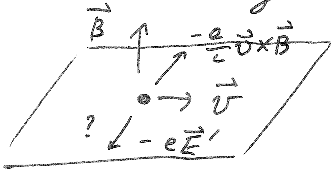


$\vec{E} = 0$ $\qquad$ In the Lab frame

In S', $\quad \vec{E} = -\dfrac{1}{c}\vec{v}\times\vec{B}$

$\vec{B} = B\hat{z}$

Lorentz transformation



$\vec{E}' = -\dfrac{1}{c}\vec{v}\times\vec{B}$

Since $\vec{J} = -ne\vec{v}$, $\qquad \vec{E} = \frac{B}{nec} \vec{J} \times \hat{B}$.

Resistivity tensor $\qquad E^{\mu} = \rho_{\mu\nu} J^{\nu} \qquad \mu, \nu = x, y$

$$\therefore \tilde{\rho} = \frac{B}{nec} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

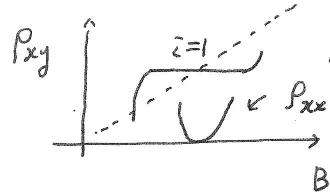
Conductivity tensor $\qquad J^{\mu} = \sigma_{\mu\nu} E^{\nu}, \quad \tilde{\sigma} = \frac{nec}{B} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

QH insulator. $\qquad \sigma_{xx} = 0$ yet $\rho_{xx} = 0 \quad \because \quad \sigma_{xy} = -\frac{nec}{B} \neq 0$.

(In ordinary insulator, $\rho_{xx} = \sigma_{xx}^{-1} \to \infty$)

$$\rho_{xy} = \frac{B}{nec}$$

↳ carrier density

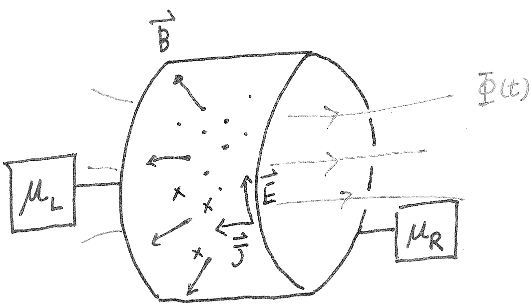


plateau : 2D anderson localization

$$N = N_{\Phi} = \frac{BA}{\Phi_0} \qquad \therefore n \equiv \frac{N}{A} = \left(\frac{hc}{e}\right)^{-1} B$$

$$\therefore \rho_{xy} = \frac{h}{e^2}$$

Laughlin's gauge argument: $\qquad$ quantum pump



Faraday induction: $\qquad \oint_{\Gamma} d\vec{l} \cdot \vec{E} = -\frac{1}{c} \frac{\partial \Phi}{\partial t}$

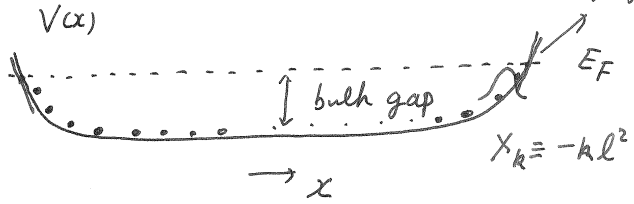
$$\rho_{xy} \frac{\partial Q}{\partial t} = -\frac{1}{c} \frac{\partial \Phi}{\partial t}$$

$$-\rho_{xy} e = -\frac{\Phi_0}{c} \qquad \therefore \rho_{xy} = \frac{1}{ce} \cdot \frac{hc}{e} = \frac{h}{e^2}$$

Quantum Hall Edge states

gapless edge state

$$\hat{H} = \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 + \underbrace{V(x)}_{\text{confining potential}}$$



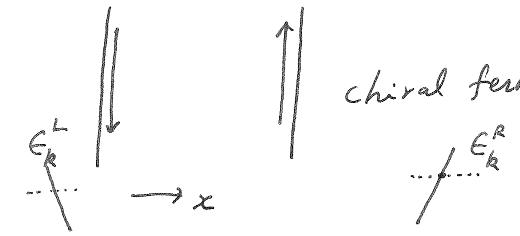
Smoothly varying: Semiclassical approxim.

$$\epsilon_k = \frac{1}{2}\hbar\omega_c + V(X_k)$$

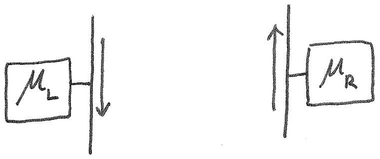
Spatially separated

Group velocity: $\vec{v}_k = \frac{1}{\hbar}\frac{\partial \epsilon_k}{\partial k}\hat{y}$

chiral fermion



$\epsilon_k^L \cong -\hbar v k$ $\epsilon_k \cong \hbar v k$



Occupation number

$$I = -\frac{e}{L_y}\sum_k n_k v_k = -\frac{e}{L_y}\int_{-\infty}^{\infty} dk \frac{L_y}{2\pi}\frac{1}{\hbar}\frac{\partial \epsilon_k}{\partial k} n_k$$

$$= -\frac{e}{h}(\mu_L - \mu_R) \qquad \mu_R - \mu_L \equiv eV_H$$

$$\therefore \quad I = -\frac{e^2}{h}V_H \qquad \therefore \sigma_{xy} = -\frac{e^2}{h} \quad \text{and } \sigma_{xx} = 0$$

$\because$ I flows $\perp$ to V

'Chiral edge states'

Topological insulator : Stable conducting edge states

since back scattering is strongly suppressed.

$\therefore$ Quantum Hall states : topological matter

characterized by n : $\begin{cases} \text{\# of edge states} \\ \text{Quantize Hall resistance} \end{cases}$

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

- $C = \frac{1}{2\pi i}\int_{k \in BZ} d^2k \, \vec{\nabla}_k \times \vec{A}(k_x, k_y) \in \mathbb{Z}$ (cf) TKNN number (Thouless-Kohmoto-Nightingale-den Nijs)

$\vec{A}(k_x, k_y) = \langle u_{\vec{k}} | \vec{\nabla}_k | u_{\vec{k}} \rangle$: first Chern number

Time reversal symmetry and Kramers th$^{\underline{m}}$

$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$ → complex conjugation and $t \to -t$

$= E\psi$ $\quad i\hbar \frac{\partial \psi^*}{\partial t} = \hat{H}^* \psi^* = E\psi^*$ $\hat{H}$ is a Hermitian.

For real Hamitonian, ψ^* is a solution with the same E.
↳ time reversed stste

$T = K_0 \alpha$ with $\alpha = -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ for $s=\frac{1}{2}$ particle.
↳ complex conjugstion

$T\vec{P}T^{-1} = -\vec{P}$, $T\vec{L}T^{-1} = -\vec{L}$ $\quad \therefore \; T\vec{\sigma}T^{-1} = -\vec{\sigma}$

$T\vec{r}T^{-1} = \vec{r}$ $\quad \therefore \; \alpha$ introduced!

$$H = \frac{\vec{P}^2}{2m} + V(\vec{r}) + \underbrace{\frac{\hbar}{4m^2c^2}\vec{\sigma} \times \vec{\nabla}V(\vec{r}) \cdot \vec{P}}_{H_{so}}$$

↳ spin-orbit interaction

$TH_{so}T^{-1} = H_{so}$ $\quad \therefore$ invariant over T!

Magnetic field → $(\vec{p} - \frac{q}{c}\vec{A})^2$ → $\vec{p}\cdot\vec{A}$

$T\vec{p}\cdot\vec{A}T^{-1} = -\vec{p}\cdot\vec{A}$

Broken time reversal symmetry.

For TRI Hamitonian, $\quad THT^{-1} = H$

$H\psi_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma}\psi_{\vec{k}\sigma}$

$TH\psi_{\vec{k}\sigma} = HT\psi_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma}T\psi_{\vec{k}\sigma}$ $\quad \therefore \; T\psi_{\vec{k}\sigma}$ is also a solution with $\epsilon_{\vec{k}\sigma}$.

Kramers th$^{\underline{M}}$

For $s=\frac{1}{2}$ particle, $\langle\psi|T\psi\rangle = 0$ $\quad \therefore$ Kramers pair

Proof) Consider $\langle T\psi | T\phi \rangle = \langle K_0(-i\sigma_y)\psi | (-i\sigma_y) K_0 \phi \rangle$ $\quad \because [-i\sigma_y, K_0] = 0$

$$= \langle K_0\psi | (i\sigma_y)(-i\sigma_y) K_0 \phi \rangle = \langle K_0 \psi | K_0 \phi \rangle$$

$$= \langle \phi | \psi \rangle$$

$$T^2 \psi = (-i\sigma_y)(-i\sigma_y)\psi = -\psi$$

$$\therefore \langle \psi | T\psi \rangle = \langle T^2\psi | T\psi \rangle = -\langle \psi | T\psi \rangle \qquad \therefore \langle \psi | T\psi \rangle = 0.$$

$\therefore$ $\hat{H}\psi_{\vec{k}\sigma} = E_{\vec{k}\sigma}\psi_{\vec{k}\sigma}$, then $T\psi_{\vec{k}\sigma} = \psi_{-\vec{k}-\sigma}$

$$\therefore \quad E_{\vec{k}\sigma} = E_{-\vec{k}-\sigma}$$

Space Inversion symmetry ($\vec{r} \to -\vec{r}$) : $E_{\vec{k}\sigma} = E_{-\vec{k}\sigma}$

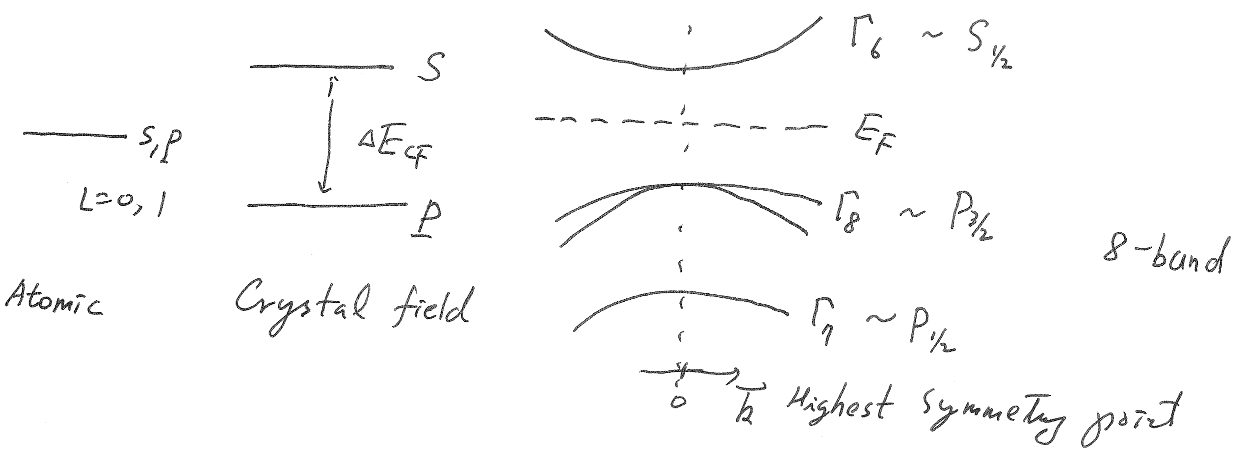
For a system with SI and TRI, $E_{\vec{k}\sigma} = E_{\vec{k}-\sigma}$

$\therefore$ Maximum 4-fold degenerate.

Quantum Spin Hall effect (HgTe quantum well)

$$H = \frac{\vec{p}^2}{2m} + V(\vec{r}) + \underbrace{\frac{\hbar}{4m^2c^2}\vec{\sigma} \times \vec{\nabla} V(\vec{r}) \cdot \vec{p}}_{H_{SO}}$$

For weak H_{so}, $Hg_{0.38}Cd_{0.62}Te \equiv$ 'CdTe' $\Delta E_{CF} \gg \Delta E_{so}$



$$H_{so} = \frac{2A}{\hbar}\vec{S}\cdot\vec{L} \qquad \vec{J} = \vec{L}+\vec{S}$$

$$= A[j(j+1) - l(l+1) - \tfrac{3}{4}]$$

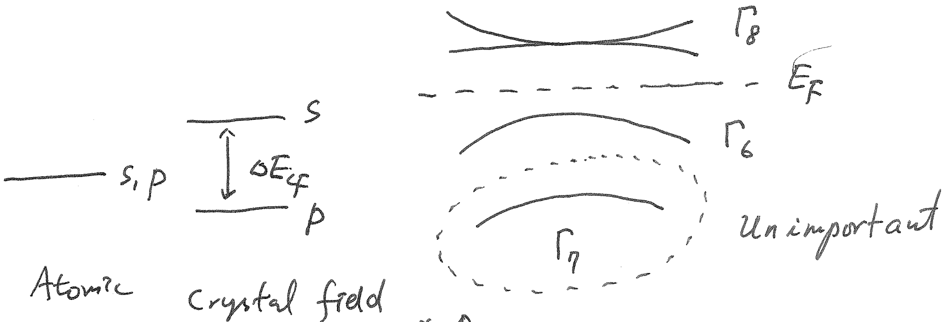
s, p orbital $\therefore$ $L = 0, 1$, $s = \frac{1}{2}$

$1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$

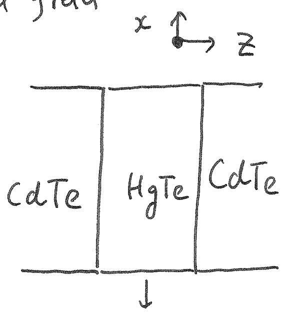
$0 \otimes \frac{1}{2} = \frac{1}{2}$

$$\therefore \quad E_{so} = \begin{cases} A & P_{3/2} \sim \Gamma_8 \\ 0 & S_{1/2} \sim \Gamma_6 \\ -2A & P_{1/2} \sim \Gamma_7 \end{cases}$$

For HgTe, $\Delta E_{so} \gg \Delta E_{CF}$!



6 band model



Grown along [001] : axial symmetry + Inversion sym in xy plane.

$\hat{J}_z$: Good quantum #

$\therefore m_J$

$|E1, m_J = \frac{1}{2}\rangle \cong |\Gamma_6\ m_J = \frac{1}{2}\rangle + |\Gamma_8\ m_J = \frac{1}{2}\rangle$ $\qquad |L1\rangle$: unimportant.

$|H1, m_J = \frac{3}{2}\rangle = |\Gamma_8\ m_J = \frac{3}{2}\rangle$

also for $m_J = -\frac{1}{2}$ and $-\frac{3}{2}$

- Tight-binding approximation $\qquad \hat{z}$: quantum confined

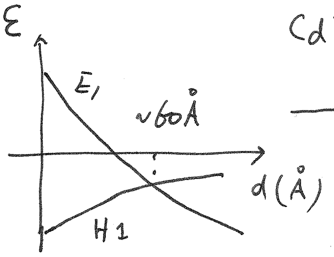
Near Γ point, $H_{eff}(k_x, k_y) = \begin{pmatrix} \boxed{H(k)} & 0 \\ 0 & \boxed{H^*(-k)} \end{pmatrix}$ → spin ↑ ; $k \to -k$ → spin ↓ : Time reversed

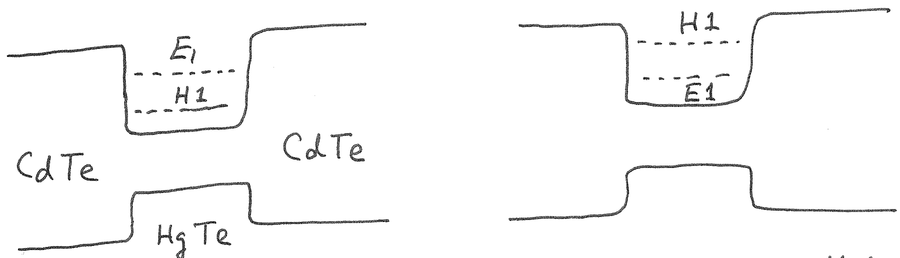
($\vec{k}\cdot\vec{p}$ perturbation)

$H(\vec{k}) = \vec{d}(\vec{k})\cdot\vec{\sigma}$ $\qquad$ $\vec{\sigma}$: Pauli spin matrices

$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\vec{d}(\vec{k}) = (\hbar v k_x, \hbar v k_y, M)$, $d_z = M = \varepsilon(E_1) - \varepsilon(H_1)$ at Γ point!





$M>0$ $\qquad$ $d<d_c$ $\qquad$ $d>d_c$ $\qquad$ $M<0$

Inverted quantum well

$d_c \sim 60\text{Å}$

$\hat{H} = v\,\vec{\sigma}_{\parallel}\cdot\vec{p} + M\sigma_3$ $\qquad$ 2+1 D Dirac Hamiltonian

$\vec{p} = \frac{\hbar}{i}\vec{\nabla}$

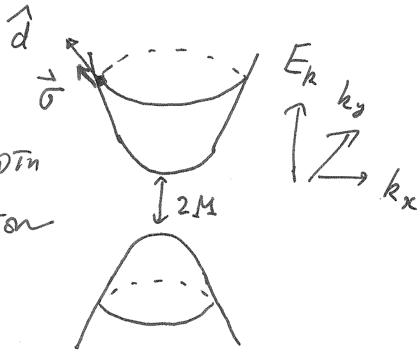
$\vec{\sigma}_{\parallel} = (\sigma_1, \sigma_2)$

$\hat{H}\chi = E\chi$

$[\hat{H}, \vec{p}] = 0$ $\quad \therefore \quad \chi = e^{i\vec{k}\cdot\vec{r}}\phi$ $\quad \therefore \quad \hat{H}(\vec{k})\phi = \vec{d}(\vec{k})\cdot\vec{\sigma}\,\phi$

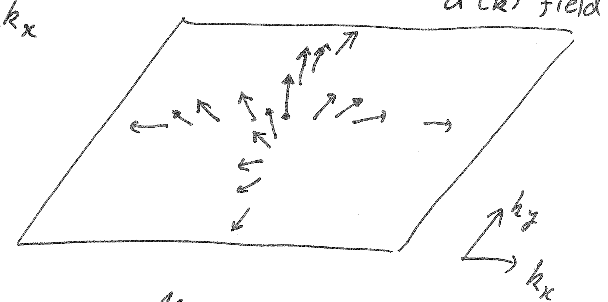
$E_k = \pm|\vec{d}| = \pm\sqrt{\hbar^2 v^2|\vec{k}|^2 + M^2}$ $\qquad$ Helicity: $\hat{\Sigma} = \vec{\sigma}\cdot\hat{d}$

Good quantum #.



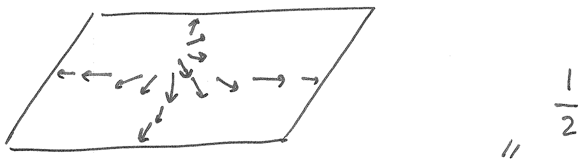
Pseudo spin direction

For $M>0$, $\hat{d}(\vec{k})$-field



Meron

For $M<0$,



$$\sigma^s_{xy} = -\frac{1}{8\pi^2}\int d^2k \;\hat{d}\cdot\partial_x\hat{d}\times\partial_y\hat{d}\cdot\left[\frac{e^2}{h}\right]$$

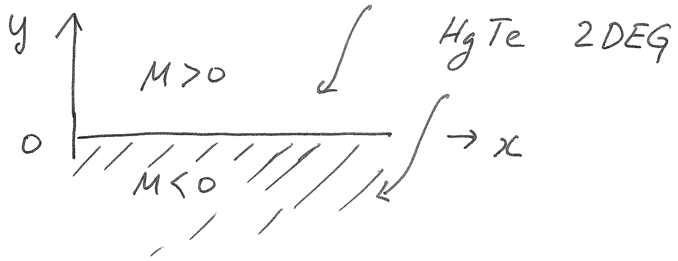
[X.L. Qi et. al., Phys. Rev. B 74, 085308 (2006)]

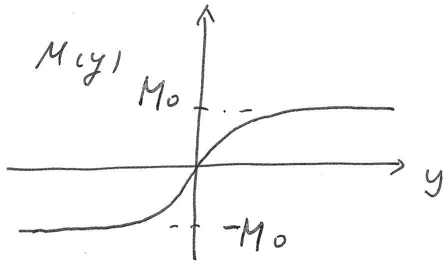
$$\Delta\sigma^s_{xy} = \overset{\uparrow,\downarrow}{2}\,\frac{e^2}{h}$$

a pair of edge states

Z_2 odd topological

distinct from a fully gapped conventional insulator.





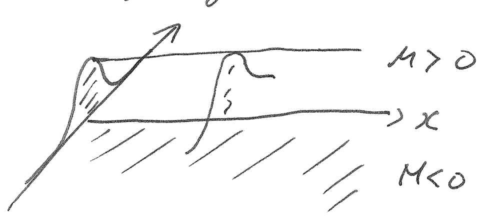
$$\hat{H} = v\,\vec{\sigma}_{\parallel}\cdot\vec{p} + M(y)\,\sigma_3 \qquad \hat{H}\,\phi_k(x,y) = E_k\,\phi_k(x,y)$$

$$[\hat{H}, P_x] = 0 \qquad \phi_k(x,y) = e^{ikx}\,\chi_k(y)$$

Jackiw and Rebbi solition :

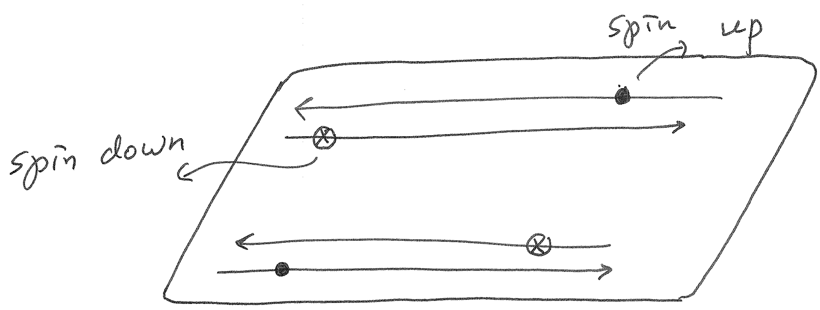
$$\phi_k(x,y) = \begin{pmatrix}1\\-1\end{pmatrix} e^{-\frac{1}{\hbar v}\int_0^y M(y')\,dy'}$$

$$E_k = -\hbar v k$$



for spin ↑

$$\vec{v}_k = \frac{1}{\hbar}\frac{dE_k}{dk}\hat{x} = -v\hat{x}$$



$$\sigma_{xy}^{s} = \frac{2e^2}{h}$$