CH. 4: TOPOLOGICAL BAND THEORY IN THREE DIMENSIONS

(1) Semiclassical electron dynamics

What are the equations of motion for an electron moving in an electromagnetic field?

1.1 Crystal with space inversion and time-reversal symmetries

Electron in band n w/ crystal momentum $\hbar\vec{k}$ and energy $E_{\vec{k}n}$:

velocity: $$\vec{v}_{\vec{k}n} = \frac{\partial E_{\vec{k}n}}{\partial \vec{k}} \frac{1}{\hbar}$$

force: $$\hbar\dot{\vec{k}} = -e\vec{E} - e\,\vec{v}_{\vec{k}n} \times \vec{B}$$

These equations help understand electronic transport properties.

1.2 Anomalous velocity

Contribution from Berry curvature to $\vec{v}_{\vec{k}n}$.

For simplicity, ignore magnetic field ($\vec{B} = 0$), but allow for an electric field $\vec{E}$ (uniform and dc)

Change of $\vec{v}_{\vec{k}n}$ due to $\vec{E}$:

$$\delta \vec{v}_{\vec{k}n} = \delta \left(\langle \psi_{\vec{k}n} | \underbrace{\vec{v}}_{\text{velocity operator}} | \psi_{\vec{k}n} \rangle \right)$$

$$= \left(\delta \langle \psi_{\vec{k}n} |\right) \vec{v} \,|\psi_{\vec{k}n}\rangle$$

$$+ \langle \psi_{\vec{k}n} | \left(\delta \vec{v}\right) | \psi_{\vec{k}n}\rangle$$

$$+ \langle \psi_{\vec{k}n} | \vec{v} \left(\delta | \psi_{\vec{k}n}\rangle\right)$$

$$= \langle \psi_{\vec{k}n} | \vec{v} \, \delta | \psi_{\vec{k}n}\rangle + c.c.$$

lec. 13

$\delta \vec{v} = 0$

$$\delta |\psi_{\vec{k}n}\rangle = \sum_{\substack{n' \\ (n' \neq n)}} |\psi_{\vec{k}n'}\rangle \frac{\langle \psi_{\vec{k}n'} | e\vec{E}\cdot\vec{r} | \psi_{\vec{k}n}\rangle}{E_{\vec{k}n} - E_{\vec{k}n'}}$$

$$= i\hbar e E_\beta \sum_{n'} |\psi_{\vec{k}n'}\rangle \frac{\langle \psi_{\vec{k}n'} | v_\beta | \psi_{\vec{k}n}\rangle}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

lec. 13

(sum over $\beta \in \{x, y, z\}$)

Then,

$\in \{x, y, z\}$

$$\delta\left(\langle \psi_{\vec{k}n} | v_{\alpha} | \psi_{\vec{k}n} \rangle\right) =$$

$$= i\hbar e E_{\beta} \sum_{n'} \frac{\langle \psi_{\vec{k}n} | v_{\alpha} | \psi_{\vec{k}n'} \rangle \langle \psi_{\vec{k}n'} | v_{\beta} | \psi_{\vec{k}n} \rangle}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

$$+ \text{c.c.}$$

$$= -2e\hbar E_{\beta} \, \mathrm{Im} \sum_{n'} \frac{\langle \psi_{\vec{k}n} | v_{\alpha} | \psi_{\vec{k}n'} \rangle \langle \psi_{\vec{k}n'} | v_{\beta} | \psi_{\vec{k}n} \rangle}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

$$=$$

lec. 13

$$-2e\hbar E_\beta \;\mathrm{Im} \sum_{n'} \frac{\langle u_{\vec{k}n} | \frac{\partial h}{\hbar \partial k_\alpha} | u_{\vec{k}n'} \rangle \langle u_{\vec{k}n'} | \frac{\partial h}{\hbar \partial k_\beta} | u_{\vec{k}n} \rangle}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

where we used

$$|\psi_{\vec{k}n}\rangle = e^{i\vec{k}\cdot\vec{r}}\, |u_{\vec{k}n}\rangle$$

$$h(\vec{k}) = e^{i\vec{k}\cdot\vec{r}}\, \mathcal{H}\, e^{-i\vec{k}\cdot\vec{r}}$$

full Hamiltonian.

$$= \frac{e}{\hbar} E_\beta \underbrace{\epsilon_{\alpha\beta\gamma}}_{\uparrow\ \text{Levi-Civita}} \underbrace{B_{n,\gamma}(\vec{k})}_{\uparrow\ \text{component } \gamma \text{ of Berry curvature vector (hw \# 1)}}$$

$$= \frac{e}{\hbar} \left(\vec{E} \times \vec{B}_n(\vec{k}) \right)_\alpha$$

Therefore,

$$\vec{v}_{\vec{k}n} = \frac{1}{\hbar} \frac{\partial E_{\vec{k}n}}{\partial \vec{k}} + \underbrace{\frac{e}{\hbar} \vec{E} \times \vec{B}_n(\vec{k})}_{\uparrow\ \text{anomalous velocity}}$$

(nonzero if the crystal break SIS or TRS)

In a magnetic field, this changes to

$$\vec{v}_{\vec{k}n} = \frac{1}{\hbar} \frac{\partial E_{\vec{k}n}}{\partial \vec{k}} - \dot{\vec{k}} \times \vec{B}_n(\vec{k})$$

* Physical consequence :

$\vec{j}$ = current density =

$$= \frac{-e}{V} \sum_{\vec{k}n} \vec{v}_{\vec{k}n} f_{\vec{k}n}$$

volume of crystal

$$= -\frac{e}{V} \sum_{\vec{k}n} \frac{1}{\hbar} \frac{\partial E_{\vec{k}n}}{\partial \vec{k}} f_{\vec{k}n}$$

$$+ \frac{1}{V} \frac{e}{\hbar} \vec{E} \times \underbrace{\sum_{\vec{k}n} \vec{B}_{\vec{k}n} f_{\vec{k}n}}_{\text{sum of Berry curvature over occupied states}}$$

$\sum_{\vec{k}n} \vec{B}_{\vec{k}n} f_{\vec{k}n} \neq 0$ if the system breaks TRS.

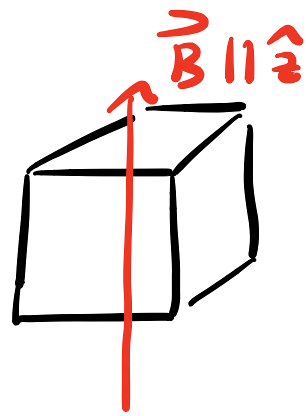
$$\left(\text{TRS:} \quad \begin{cases} E_{-\vec{k}} = E_{\vec{k}} \\ \Rightarrow f_{-\vec{k}} = f_{\vec{k}} \\ \vec{B}_{\vec{k}} = -\vec{B}_{-\vec{k}} \end{cases} \right)$$

Anomalous velocity leads to anomalous Hall effect.

Review paper: D. Xiao, M. C. Chang and Q. Niu, RMP 82, 1959 (2010).

(2) 3D quantum Hall effect

Generalisation of 2D QHE to 3D?



* Essential signatures:

(i) ρ_{xy} = Hall resistivity = quantized.

(ii) $\rho_{xx} = \rho_{yy}$ = longitudinal resistivity = 0.

* Conceptual difficulties:

(i) In 2D, BZ is a 2-torus (a closed 2D surface).

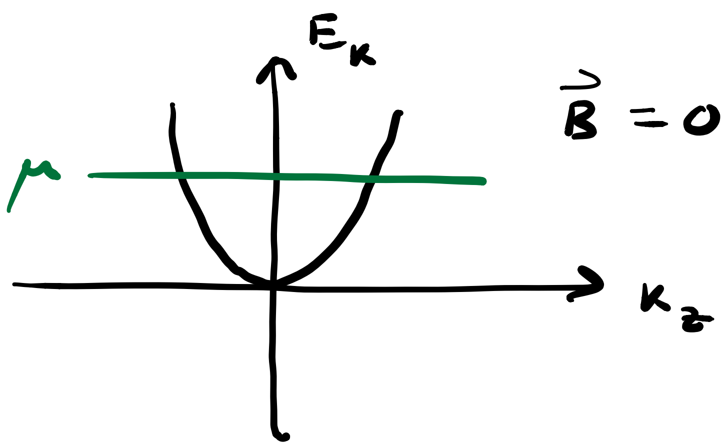
$\sigma_{xy} \sim$ flux of $\vec{B}_{\vec{k}}$ over BZ

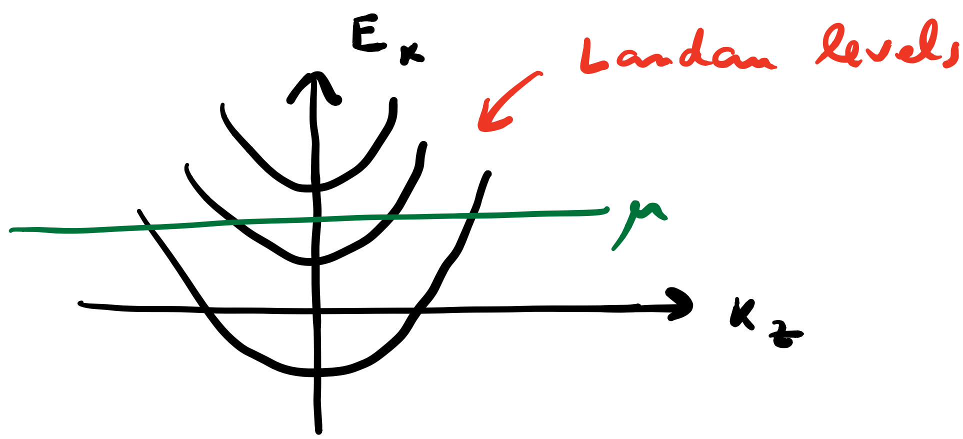
$\rightarrow$ quantized. (Chern #).

In 3D, BZ is a 3-torus (a closed 3D surface).

Integral of $\vec{B}_{\vec{k}}$ over 3D surface is not quantized.

(ii) Unlike in 2D, in 3D a magnetic field does not typically "transform" a metal in an insulator.





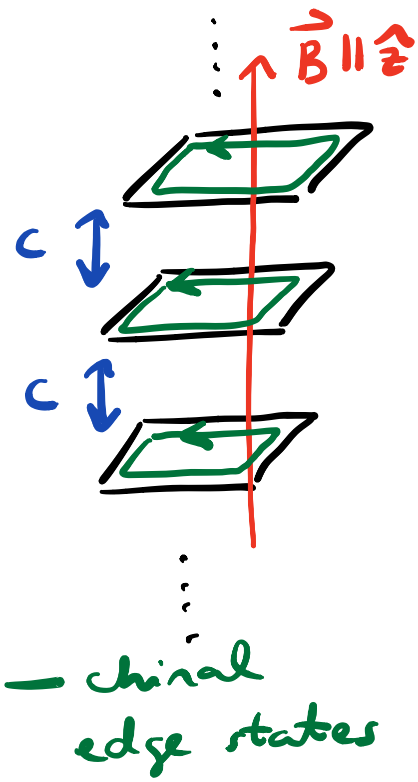
$$E_{k_z n} = \hbar \omega_c \left(n + \frac{1}{2} \right) + \frac{\hbar^2 k_z^2}{2m}$$

yet, a bulk gap is <u>needed</u> to have $\rho_{xx} = \rho_{yy} = 0$.

* "Layer construction":

stack of 2D QH systems.

Decoupled layers:



Each layer behaves as a 2D QH insulator:

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

$$\sigma_{xy}^{3D} = \frac{1}{L} \sum_{k_z} \sigma_{xy}^{2D}(k_z)$$

length of system along z

$$= \int_{-\frac{\pi}{c}}^{\frac{\pi}{c}} \frac{dk_z}{2\pi} \sigma_{xy}^{2D}(k_z)$$

$$= \frac{1}{c} \sigma_{xy}^{2D}$$

for decoupled layers, $\sigma_{xy}^{2D}(k_z)$ is independent of k_z

$$= \frac{1}{c} \frac{e^2}{h} \nu = \sigma_{xy}^{3D}$$

Let's add some interlayer coupling, $t_\perp$. If $t_\perp$ does not close the bulk gap, we expect to have chiral surface states on surfaces parallel to $\hat{z}$ axis. Then, it can be shown that

$$\sigma_{xy}^{3D} = \frac{1}{c} \frac{e^2}{h} \times \text{integer}$$

is still true.

[B. Halperin, Jpn. J. Appl. Phys. 26, 1913 (1987)]

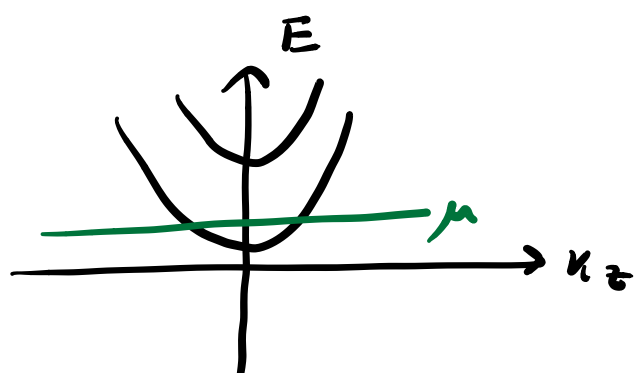
But, this is not a genuine 3D topological phase, b/c it is adiabatically connected to a stack of decoupled QH layers.

* Experimental discovery:

F. Tang et al., Nature 569, 537 (2019).

$ZrTe_5$: 3D material (not layered)

Under high magnetic field, only lowest LL is occupied.



There's a charge-density-wave instability that opens a gap at μ

* Open questions:

(1) Thermal Hall effect in $ZrTe_5$?

(2) Any 3D generalisation to the QAH insulator ?