L18 10/20/2022

$k_z = \pi/2$ (the bottom of the nth band) and the top of the n-th band crosses the n+1 band at $k_z = 0$.

For n odd, the top of the nth band crosses the bottom of the n+1 band at $k_z = 0$ while the bottom of the nth band crosses the top of the n-1st band at $k_z = 0$.

Here n labels the bands and the gaps. The top band ($n = q$) only crosses the band with $n = q-1$ at $k_z = 0$ (q even) or $k_z = \frac{\pi}{q}$ (q odd)

$\Rightarrow$ the Chern numbers I_n are integers determined by the changes of the phases as $\vec{k}$ traverses the degeneracy points. We can compute this using Brillouin-Wigner pert. theory.

For p and q fixed ($B = 2\pi \frac{p}{q}$) the nth band crosses the mth band if $m = n - l_n$ where l_n is the solution of the Diophantine Eqn.

$$n = q s_n + p l_n \quad \text{(TKNN 1982)}$$

$(|l_n| < q/2)$

The Schrödinger Eqn mixes $\psi^{(n)}$ only with $\psi^{(n\pm 1)}$

$\Rightarrow$ it takes l_n orders to mix $\psi^{(n)}$ with $\psi^{(n-l)}$. For $\vec{k}$ close to the degeneracy points will have almost all of their weight in these two states ($\psi^{(n)}$ and $\psi^{(n-l)}$)

$\Rightarrow$ we get an effective Schrödinger Eqn.

$$E_n^{(0)} \psi_n + V_{n,n-l}\, \psi_{n-l} = E\, \psi_n$$

$$V_{n,n-l}\, \psi_n + E_{n-l}^{(0)}\, \psi_{n-l} = E\, \psi_{n-l}$$

$$V_{n,n-l} = V^*_{n-l,n} \cong (-\lambda t e^{-ik_1}) \prod_{r=n-l+1}^{n-1} \frac{(-\lambda e^{-ik_1})}{\frac{1}{2}(E_n^{(0)} + E_{n-l}^{(0)}) - E_r^{(0)}}$$

$$E_n^{(0)}(\vec{k}) = -2t \cos\left(k_2 + 2\pi \frac{p}{q} n\right)$$

$$E^{\pm}(\vec{k}) = \frac{1}{2}\left(E_n^{(0)} + E_{n-l}^{(0)}\right) \pm \sqrt{\frac{(E_n^{(0)} - E_{n-l}^{(0)})^2}{4} + |V_{n,n-l}|^2}$$

$\psi_n^{\pm} = |\psi_n^{\pm}|\, e^{i\theta_n^{\pm}}$, same for ψ_{n-l_n}.

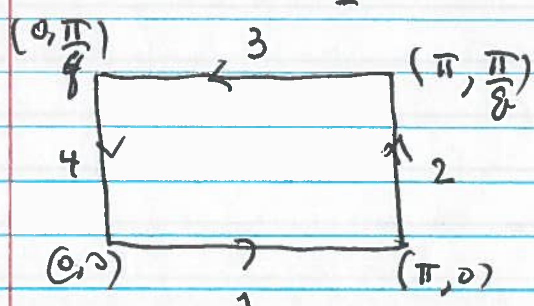
Phases: $\theta_n^+ - \theta_{n-l_n}^+ = \arg(V_{n,n-l_n}) + \pi = -k_1 l_n - (l_n - 2)\pi$

$\theta_n^- - \theta_{n-l_n}^- = \arg(V_{n,n-l_n}) = -k_1 l_n - l_n \pi$

Consider n even (same for n odd). At $k_2 = \pi/2$ the band with n even crosses the band with n+1. At this degeneracy we must choose $E^{(-)}$ for the top of the nth band. At $k_2=0$, the nth band crosses the n-1 band. $\Rightarrow$ we choose $E^{(+)}$ for the bottom of the nth band.

Let us compute the circulation of the Berry connection $A_j^{(n)}(\vec{k})$ for the nth band for $\vec{k} = (k_1, k_2)$ along the contour γ that encloses the MBZ

$$\gamma : (0,0) \xrightarrow{1} (\pi, 0) \xrightarrow{2} \left(\pi, \frac{\pi}{q}\right) \xrightarrow{3} \left(0, \frac{\pi}{q}\right) \xrightarrow{4} (0,0)$$



On the segments 1 and 3 of γ, k_2 is constant and k_1 changes $0 \to \pi$ and $\pi \to 0$

$$\Rightarrow A_1^{(n)}\Big|_{k_2 = \frac{\pi}{q}} = \frac{\partial}{\partial k_1} \arg(V_{n,n-l_n})\Big|_{k_2=\frac{\pi}{q}} = -l_n$$

$$A_1^{(n)}\Big|_{k_2=0} = \frac{\partial}{\partial k_1} \arg\left(V_{n,n-1-l_{n-1}}\right)\Big|_{k_2=0} = -l_{n-1}$$

On segments 2 and 4, $A_2^{(n)}$ has no dependence on k_2 $\Rightarrow$ $A_2^{(n)}\Big|_{k_1=0,\pi} = 0$

$\Rightarrow$ circulation

$$I_n = \frac{1}{2\pi}\oint_\gamma A_j^{(n)}\, dk_j = \int_0^\pi \frac{dk_1}{2\pi}\left[A_1^{(n)}(k_1,0) - A_1^{(n)}\left(k_1,\frac{\pi}{q}\right)\right]$$

$$\Rightarrow \quad I_n = l_n - l_{n-1}$$

$$\Rightarrow \quad \left(\sigma_{xy}\right)^{(n)} = \frac{e^2}{h}\left(l_n - l_{n-1}\right)$$

For r filled bands

$$\sigma_{xy} = \frac{e^2}{h}\sum_{n=1}^{r}\left(l_n - l_{n-1}\right) = \frac{e^2}{h}\left(l_n - l_0\right) \equiv \frac{e^2}{h}\, l_r$$

$$\Rightarrow \quad \sigma_{xy} = \frac{e^2}{h}\, l_r \qquad (\text{since } l_0 = 0)$$

$\Rightarrow$ σ_{xy} is determined by a <u>topological invariant</u>, the Chern number of the band.

$\Rightarrow$ The calculation reduces to the solution of the Diophantine Eqn.

The integers l_n may be positive or negative.

This result reflects the Bragg scattering due to the magnetic unit cells.

Example: $p=11$, $q=7$, we need to find two integers (s_n, l_n)

$$\Rightarrow (-3,2), (-6,4), (2,-1), (-1,1), (7,-4), (4,-2), (1,0)$$

$n=1,\dots,7 \Rightarrow$ bands $n=3,5,6$, $l=-1,-4,-2$ (<0)

$n=1,2,4$, $l=2,4,1$ (>0)

$n=7$, $l=0$

The solution to the Diophantine eqn. is unique for q odd. For q even the band with $n=q/2$ is degenerate. (~~see~~ the Dirac cones).

Topological Band Structures and TI's

(see ch. 16 of EF's FTCMS)

Topological insulators (TI's) are solid state systems with quantized transport properties due to topological properties of their energy bands. Their band structures are characterized by a topological invariant. The existence of these invariants is due to the fact that for these systems the Bloch states are not globally defined on the entire BZ.

We can think of these systems as generalization of TKNN.

Let's reexamine the integer QH effect on lattices from this perspective.

We have M electronic bands with ev's $\{E_m(\vec{k})\}$ $(m = 1, \ldots, M)$. The Bloch states are

$$\psi_m(\vec{k}) = u_m(\vec{k})\, e^{i\vec{k}\cdot\vec{x}}$$

$\vec{k}$: "quasi-momentum" in the 1st BZ

We will assume that $|E_m(\vec{k}) - E_n(\vec{k})| > 0$

(non-degenerate).

Berry connection: $A_j^{(m)}(\vec{k}) = i\langle u_m(\vec{k})| \frac{\partial}{\partial k_j} |u_m(\vec{k})\rangle$

$j = 1, 2$

$$|u_m(\vec{k})\rangle \to e^{i f_m(\vec{k})} |u_m(\vec{k})\rangle$$

$$A_j^{(m)}(\vec{k}) \longrightarrow A_j^{(m)}(\vec{k}) + \frac{\partial}{\partial k_j} f_m(\vec{k})$$

$f_m(\vec{k})$ are continuous and diff. on the BZ.

Only gauge-invariant ~~q~~ quantities matter.

$\Rightarrow$ Berry curvature: $\mathcal{F}_m(\vec{k}) = \varepsilon_{ij} \frac{\partial}{\partial k_i} A_j^{(m)}(\vec{k})$

Γ: boundary of the BZ

$$\Rightarrow \int_{BZ} d^2k\, \mathcal{F}_m(\vec{k}) = \oint_\Gamma d\vec{k} \cdot \vec{A}^{(m)}(\vec{k})$$

Dirac quantization $\Rightarrow$ $\oint_\Gamma d\vec{k} \cdot \vec{A}^{(m)}(\vec{k}) = 2\pi N_m$, $N_m \in \mathbb{Z}$

(Bloch states must be single valued on BZ)

N_m: 1st Chern number

$$H = \oint \sum_{n,m} \int_{BZ} d^2k \; c_n^\dagger(\vec{k})\, \mathcal{H}_{n,m}(\vec{k})\, c_m(\vec{k})$$

If $N_m \neq 0 \Rightarrow$ a smooth change of $\mathcal{H}_{n,m}(\vec{k})$ cannot change N_m unless there is a gap closing

We saw after TKNN that the N_m's determine the Hall conductance.

We will now generalize this perspective.

The Anomalous QH effect

Consider a 2D band insulator (i.e. all bands below E_F are full and all above E_F are empty (no degeneracies)

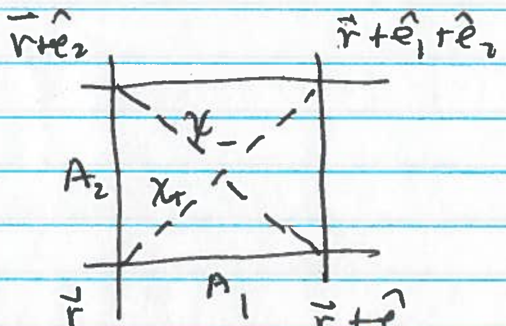
Typically @ $T=0$ a band insulator has a finite dielectric constant and vanishing conductivity. However, if the insulator breaks time-reversal invariance, the Hall conductivity may be $\neq 0$. We will see that in such systems σ_{xy} is quantized.

Two simple models of the AQH effect.

(I) spinless fermions on a square lattice with flux π/plaquette with a flux $\pi/2$ on Δ (i.e. flux phases)

(II) Haldane's modified graphene model.

(I)
$$H = -t \sum_{\vec r, j=1,2} c^\dagger(\vec r)\, e^{iA_j(\vec r)}\, c(\vec r + \hat e_j) + h.c.$$
$$- t' \sum_{\vec r} \left(c^\dagger(\vec r)\, e^{i\chi_+}\, c(\vec r + \hat e_1 + \hat e_2) + c^\dagger(\vec r + \hat e_2)\, e^{+i\chi_-}\, c(\vec r + \hat e_1) + h.c. \right)$$



$A_1 = \pi$, $A_2 = 0$ $\quad x_1$ even

$A_1 = 0$, $A_2 = 0$ $\quad x_1$ odd

$\chi_\pm = \pm \pi/2$

$\Rightarrow$ the flux on each Δ is $\pi/2$ and this adds up to π on the plaquette. This state arises in the MFT. of the chiral spin liquid.

Two bands

$$E_\pm(\vec k) = \pm\left((2t\cos k_1)^2 + (2t\cos k_2)^2 + (4t' \sin k_1 \sin k_2)^2 \right)^{1/2}$$

We will assume that we have 1 fermion / site

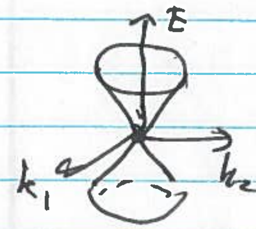
(half-filling) $\Rightarrow E_F = 0$

For $t' = 0$ we have "nodal points" (degeneracies)

at $\left(\frac{\pi}{2}, \frac{\pi}{2}\right)$ (and its reflections in the 3 other

quadrants of the BZ)

$\vec{q}$ measured from the nodal points



$$\Rightarrow E_{\pm}(\vec{q}) = \pm \underset{\uparrow \text{lattice spacing}}{2ta}|\vec{q}| + O(\vec{q}^{\,2})$$

The low energy states (close to $E_F = 0$)

are two Dirac spinors $u_a(\vec{x})$, $v_a(\vec{x})$

($a = 1, 2$)

For $t' \neq 0$ $\quad E_{\pm}(\vec{q}) = \pm\sqrt{v_F^2 \vec{q}^{\,2} + m^2 v_F^4}$

$$v_F = 2ta, \quad m = \frac{t'}{2t^2a^2}$$

v_F : "speed of light" (Fermi velocity)

m: mass $\Rightarrow$ two Dirac equations

$$\left(i\gamma_0 \partial_0 - i v_F \vec{\gamma}\cdot\vec{\nabla} + m v_F^2\right)_{ab} u_b(\vec{x}) = 0$$

$$\left(i\gamma_0 \partial_0 - i v_F \vec{\gamma}\cdot\vec{\nabla} + m v_F^2\right)_{ab} v_b(\vec{x}) = 0$$