LECTURE 12

Topological insulators with inversion symmetry

[Fu & Kane, PRB 76, 045302 (2007)]

Main idea: The $\mathbb{Z}_2$ invariant can be evaluated simply when $\mathcal{P}$ is present in addition to $\mathcal{T}$.

$$\vec{A}(\vec{k}) = -i \sum_n{}' \langle u_{nk} | \vec{\nabla}_k | u_{nk} \rangle$$

Consider Berry curvature $\mathcal{F}_{xy}(\vec{k}) = \partial_x A_y(\vec{k}) - \partial_y A_x(\vec{k})$

- We showed previously that in $\mathcal{T}$-inv. system

$$\mathcal{F}_{xy}(\vec{k}) = -\mathcal{F}_{xy}(-\vec{k}) \qquad (\Rightarrow \text{Chern } \# = 0)$$

- One can similarly show that in a $\mathcal{P}$-inv. system

$$\mathcal{F}_{xy}(\vec{k}) = \mathcal{F}_{xy}(-\vec{k}) \qquad [\text{Check!}]$$

Thus, when both $\mathcal{P}$ and $\mathcal{T}$ are present

$$\mathcal{F}_{xy}(\vec{k}) = -\mathcal{F}_{xy}(\vec{k}) = 0 \qquad [\text{Haldane, 2004}]$$

Since $\mathcal{F}_{xy}(\vec{k}) = 0$ one should be able to choose a gauge where

$$\vec{A}(\vec{k}) = 0$$

Define a matrix

$$v_{mn}(\vec{k}) = \langle u_{mk} | P\Theta | u_{nk} \rangle$$

- v is unitary and antisymmetric [Check!].

$$v^{+}v = 1 \,, \qquad v^{T} = -v \qquad \Rightarrow \quad v^{*} = -v^{+}$$

$$\mathrm{Tr}\left[v^{+}(\vec{k})\, \nabla_k\, v(\vec{k})\right] = \sum_{n,m} \left[v^{+}\right]_{nm} \left[\langle \vec{\nabla}_k u_{mk} | P\Theta\, u_{nk} \rangle + \langle u_{mk} | P\Theta\, \nabla_k u_{nk} \rangle\right]$$

$$\left[v^{*}\right]_{mn} = \langle u_{mk} | P\Theta\, u_{nk} \rangle^{*} = \langle P\Theta\, u_{nk} | u_{mk} \rangle$$

$$\left[v^{+}\right]_{mn} = \langle P\Theta\, u_{mk} | u_{nk} \rangle$$

$$\stackrel{(=)}{} \; 2 \sum_{n,m} \langle P\Theta\, u_{nk} \overbrace{| u_{mk} \rangle \langle u_{mk} |}^{1} P\Theta\, \vec{\nabla}_k u_{nk} \rangle$$

$$= 2 \sum_{n} \langle P\Theta\, u_{nk} | P\Theta\, \vec{\nabla}_k u_{nk} \rangle = -2 \sum_{n} \langle u_{nk} | \vec{\nabla}_k | u_{nk} \rangle$$

One can show, as before for $w(\vec{k})$, that

$$\vec{A}(\vec{k}) = -\frac{i}{2}\, \mathrm{Tr}\left[v^{+}(\vec{k})\, \vec{\nabla}_k\, v(\vec{k})\right] = -i\, \vec{\nabla}_k \ln \mathrm{Pf}\left[v(\vec{k})\right]$$

- We adjust the phase of u_{nk} to make $\mathrm{Pf}\left[v(\vec{k})\right] = 1$ and hence $\vec{A}(\vec{k}) = 0$.

N.B. This can be done by a transf.

$$|u_{nk}\rangle \to \begin{cases} e^{i\theta_k}|u_{nk}\rangle & \text{for } n=1 \\ |u_{nk}\rangle & \text{for } n\neq 1 \end{cases}$$

$$\det[v(\vec{k})] \to \det[v(\vec{k})]\, e^{-i(\theta_k+\theta_{-k})}$$

$$\mathrm{Pf}[v(\vec{k})] \to \mathrm{Pf}[v(\vec{k})]\, e^{-i\theta_k}$$

Important: in this gauge, the problem of continuing $\sqrt{\det[w(\vec{k})]}$ is eliminated because $\det[w(\vec{k})]=1$.

<u>Proof:</u> $$v(-\vec{k}) = w(\vec{k})\, v^*(\vec{k})\, w^T(\vec{k}) \qquad [\text{Check!}]$$

$$\underbrace{\mathrm{Pf}[v(-\vec{k})]}_{1} = \mathrm{Pf}[w(\vec{k})\, v^*(\vec{k})\, w^T(\vec{k})] = \det[w(\vec{k})]\, \underbrace{\mathrm{Pf}[v^*(\vec{k})]}_{1}$$

$$\Rightarrow \boxed{\det[w(\vec{k})]=1}$$

Calculate the ν invariant

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

$$w_{mn}(\vec{\Gamma}_i) = \langle u_{m\Gamma_i}|\theta|u_{n\Gamma_i}\rangle = \langle \psi_{m\Gamma_i}|\overset{P^2=1}{\vee}\theta|\psi_{n\Gamma_i}\rangle$$

$$= \langle P\psi_{m\Gamma_i}|P\theta|\psi_{n\Gamma_i}\rangle$$

Since $[H, P] = 0$, $|\psi_{n\Gamma_i}\rangle$ is an eigenstate of P with eigenvalue $\xi(\Gamma_i) = \pm 1$

$$w_{mn}(\vec{\Gamma}_i) = \xi_m(\vec{\Gamma}_i)\, v_{mn}(\vec{\Gamma}_i)$$

$$\mathrm{Pf}^2[w] = \det[w] = \det[v] \prod_n{}' \xi_n$$

Due to Kramers degeneracy at $\vec{\Gamma}_i$, distinct states $|u_{2m\Gamma_i}\rangle$ and $|u_{2m+1\Gamma_i}\rangle = \theta|u_{2m\Gamma_i}\rangle$ share the same parity eigenvalue $[P, \theta] = 0$.

$$\mathrm{Pf}[w] = \mathrm{Pf}[v] \prod_{m=1}^{N} \xi_{2m}$$

$$\downarrow$$

$$1$$

$$\mathrm{Pf}[w(\Gamma_i)] = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) \equiv \delta_i$$

$$\boxed{(-1)^\nu = \prod_{i=1}^{4} \delta_i} \leftarrow \text{Fu-Kane parity eigenvalue criterion.}$$