LECTURE 2 2015-01-08

- Berry phase and the Chern invariant

Bloch eq. (1) is invariant under the transformation

$$|u(\vec{k})\rangle \rightarrow e^{i\phi(\vec{k})}|u(\vec{k})\rangle \qquad (2)$$

reminiscent of an electromagnetic gauge transformation.

This invites a definition of the "vector potential" or "Berry connection"

$$\vec{A}(\vec{k}) = -i\langle u(\vec{k})|\vec{\nabla}_k|u(\vec{k})\rangle$$

Under transf. (2) it transforms as $\vec{A}(\vec{k}) \rightarrow \vec{A}(\vec{k}) + \vec{\nabla}_k\phi(\vec{k})$.

Although $\vec{A}(\vec{k})$ is gauge dependent, we may define a GAUGE INVARIANT Berry phase

$$\gamma_c = \oint_c \vec{A}\cdot d\vec{k} = \int_S \vec{\mathcal{F}}\cdot d\vec{S} \quad \leftarrow \text{specializing to 3D}$$

where $\vec{\mathcal{F}} = \vec{\nabla}_k \times \vec{A}$ is the Berry curvature.

- Chern invariant (Chern number)

$$\frac{1}{2\pi}\int_S \vec{\mathcal{F}}\cdot d\vec{S} = n \in \mathbb{Z} \quad \text{for any } \underline{\text{closed surface } S}.$$

See e.g. H. Nakahara: "Geometry, Topology and Physics" for proof. | Textbook sec. 3.6

Example : 2-level Hamiltonian

$$H(\vec{k}) = \vec{d}(\vec{k})\cdot\vec{\sigma} + \varepsilon(\vec{k})\mathbb{1}$$

$\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ Pauli matrices

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

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$$

$$\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k + \delta_{ij}$$

- neglect $\varepsilon(\vec{k})$ as it does not affect the eigen-vectors

$$H(\vec{k}) = \begin{pmatrix} d_z & d_x - id_y \\ d_x + id_y & -d_z \end{pmatrix}$$

Energy spectrum:

$$H^2 = d_i\sigma_i d_j\sigma_j = d_i d_j(\sigma_i\sigma_j) = d_i d_j(\delta_{ij} + i\varepsilon_{ijk}\sigma_k)$$

$$= \vec{d}\cdot\vec{d}$$

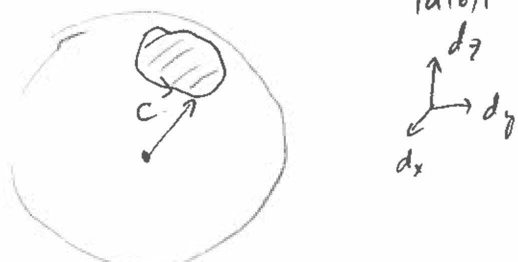
$$E(\vec{k}) = \pm\sqrt{\vec{d}(\vec{k})\cdot\vec{d}(\vec{k})} = \pm|\vec{d}(\vec{k})|$$

Berry's phase:

$$\hat{d}(\vec{k}) = \frac{\vec{d}(\vec{k})}{|d(\vec{k})|}$$

$$\gamma_c = \frac{1}{2}\Omega$$

↑ solid angle swept by $\hat{d}(\vec{k})$



Berry curvature can be expressed as

$$\mathcal{F}_{ij} = \frac{1}{2}\,\hat{d}\cdot(\partial_i\hat{d}\times\partial_j\hat{d})$$

• POLARIZATION AND TOPOLOGY IN ONE DIMENSION

(INSULATORS)

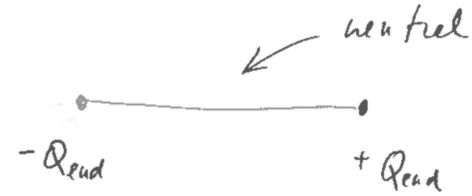
Electric polarization $\vec{P}$: dipole moment per unit volume

leads to: - bulk bound charges $\rho_b = -\vec{\nabla}\cdot\vec{P}$

- surface charge $\sigma_b = \vec{P}\cdot\vec{n}$

In 1D:

$P \equiv Q_{end}$



"Ferroelectricity"

Modern theory of Ferroelectricity relates P to the Berry phase:

$$\boxed{P = \frac{e}{2\pi}\sum_{n\in occ}\oint_{BZ} A_n(k)\,dk}$$

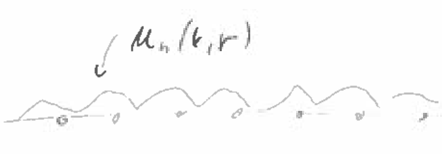
$$A_n(k) = -i\langle u_n(k)|\,\partial_k u_n(k)\rangle$$

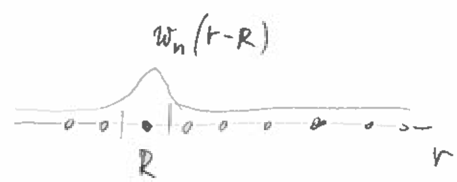
Simplest example of the bulk-boundary correspondence

PROOF: Introduce Wannier functions

$$w_n(r-R) = \frac{\sqrt{N}L}{2\pi}\int_{BZ} dk\, e^{ik(r-R)}\, u_n(k,r)$$

$$u_n(k,r) = \frac{1}{\sqrt{N}}\sum_R e^{-ik(r-R)}\, w_n(r-R)$$





$$A_n(k) = -i \frac{1}{N} \sum_{R,R'} \int_{cell} dr \; e^{ik(r-R)} (-i)(r-R') e^{-ik(r-R')} w_n^*(r-R) w_n(r-R')$$

$$\int \frac{dk}{2\pi} e^{-ik(R-R')} = \frac{1}{a} \delta_{RR'}$$

$$P = \frac{e}{Na} \sum_{n \in occ} \sum_R \int_{cell} dr \; (r-R) |w_n(r-R)|^2$$

$$= \frac{e}{L} \sum_{n \in occ} \int dr \; r \, |w_n(r)|^2 \quad \checkmark \quad \leftarrow$$

dipole moment per unit length $\Rightarrow$ polarization 1D.

- Polarization ambiguity

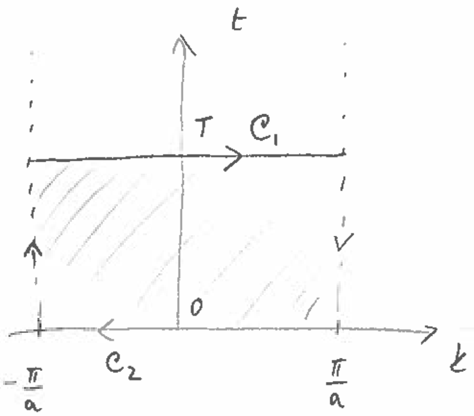
- P is defined only modulo ne because one can always add an electron to the end without changing the bulk
- Berry phase has the same ambiguity under gauge transf $|u(k)\rangle \to e^{i\phi(k)} |u(k)\rangle$ with $\phi(\frac{\pi}{a}) - \phi(-\frac{\pi}{a}) = 2\pi n$ we have $P \to P + ne$.

• Thouless charge pump

Imagine Hamiltonian also depends on time t, slowly, so that $H(k, t+T) = H(k,t)$ (period T)

Change in polarization:

$$\Delta P = P_{t=T} - P_{t=0} = \frac{e}{2\pi}\left[\oint_{C_1} - \oint_{C_2}\right] \mathcal{A}\, dk = \frac{e}{2\pi}\oint_C \mathcal{A}\, dk$$



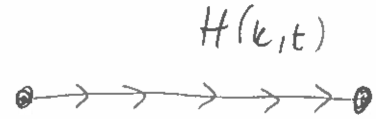
$$= \frac{e}{2\pi}\int_S \mathcal{F}_{kt}\, dk\, dt = \boxed{en}$$

↑ Chern number.

$$\vec{\mathcal{A}} = \langle u(k,t) | \nabla_{\vec{k}}\, u(k,t) \rangle$$

$$\mathcal{F}_{kt} = \partial_k \mathcal{A}_t - \partial_t \mathcal{A}_k = \left(\vec{\nabla}_{\vec{k}} \times \vec{\mathcal{A}}_k\right)_3$$

$$\vec{k} = (k,t) \qquad \text{2D vector}$$



<u>Result</u>: by adiabatically changing the Hamiltonian in a periodic fashion one can pump charge in 1D insulating system with $\Delta Q = ne$ per cycle from one end to the other.