3. Polarization and Berry phase

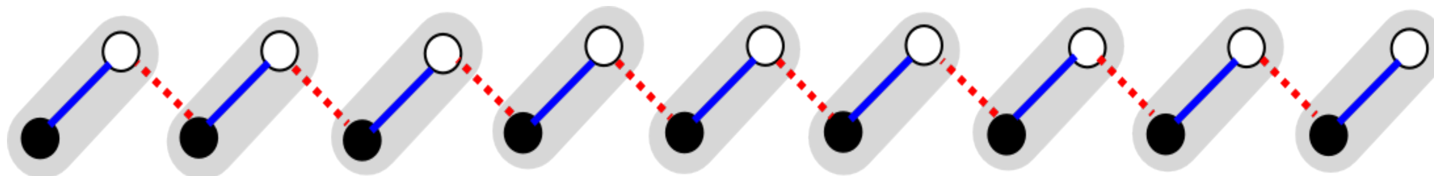
- •Motivation: preparation for charge pumping
- •Toy model: Rice-Mele = SSH+sublattice potential
- •New theory tool: Wannier states
- •Main result: Bulk Polarization as a Berry phase (Zak phase)

$$P_{\text{electric}} = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \langle u(k) | \partial_k | u(k) \rangle$$

- •Corollaries: Inversion symmetry quantizes polarization
  Chiral symmetry quantizes polarization

Rice-Mele model: SSH model+sublattice potential. Breaks chiral & inversion symmetry → ...charge pumping

Toy model:
Rice-Mele =
SSH+sublattice
 potential

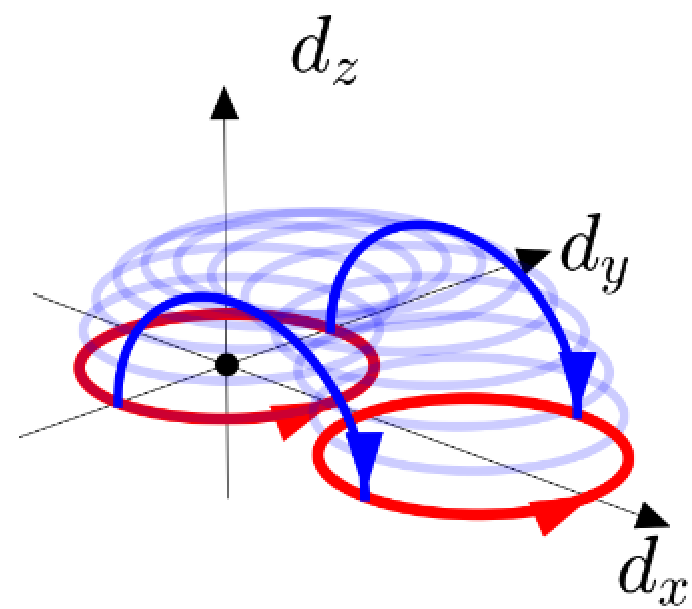


$$\hat{H} = v \sum_{m=1}^{N} |m, A\rangle\langle m, B| + h.c. + w \sum_{m=1}^{N-1} |m+1, B\rangle\langle m, A| + h.c.$$

$$+u \sum_{m=1}^{N} |m, A\rangle\langle m, A| - |m, B\rangle\langle m, B|$$

$$H(k) = \begin{pmatrix} u & v + we^{-ik} \\ v + we^{ik} & -u \end{pmatrix}$$

$$= u\sigma_z + (v + w\cos k)\sigma_x + w \sin k \sigma_y$$



Used in Chapter 1 to break chiral symmetry

Don't confuse plane wave eigenstates $|\Psi_n(k)\rangle$ with internal space states $|u_n(k)\rangle$

Eigenstates of bulk Hamiltonian: plane waves delocalized over whole lattice

$$|\Psi_n(k)\rangle = |k\rangle \otimes |u_n(k)\rangle \qquad \langle \Psi_n(k')|\Psi_n(k)\rangle = \delta_{k',k}$$

Fourier transform,
unit cell single coordinate $$|k\rangle = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{imk}|m\rangle$$

amplitude of plane wave: $\big|u_n(k)\big\rangle$ $$\langle u_n(k')|u_n(k)\rangle \neq \delta_{k',k}$$

Example, Rice-Mele:

$$\hat{H}(k) = u\hat{\sigma}_z + (v + w\cos k)\hat{\sigma}_x + w\sin k\hat{\sigma}_y$$

$$\hat{H}(k)|u_n(k)\rangle = E_n(k)|u_n(k)\rangle$$

Wannier states are a set of tightly localized basis states that span the occupied band

$$\hat{P} = \sum_k |\Psi(k)\rangle\langle\Psi(k)|$$

projector to occupied subspace

$\langle w(j') \,\|\, w(j)\rangle = \delta_{j'j}$	Orthonormal set	(3.8a)
$\sum_{j=1}^{N} \|w(j)\rangle \langle w(j)\| = \hat{P}$	Span the occupied subspace	(3.8b)
$\langle m+1 \,\|\, w(j+1)\rangle = \langle m \,\|\, w(j)\rangle$	Related by translation	(3.8c)
$\lim_{N\to\infty} \langle w(N/2)\| (\hat{x} - N/2)^2 \|w(N/2)\rangle < \infty$	Localization	(3.8d)

$$|w(j)\rangle = \frac{1}{\sqrt{N}} \sum_{k=\delta_k}^{N\delta_k} e^{-ijk} e^{i\alpha(k)} |\Psi(k)\rangle$$

Wannier states are obtained by Fourier transform, with arbitrary gauge function α(k)

$$|w(j)\rangle = \frac{1}{\sqrt{N}} \sum_{k=\delta_k}^{N\delta_k} e^{-ijk} e^{i\alpha(k)} |\Psi(k)\rangle$$

gauge function α(k) can be used to make
Wannier function tightly localized
(1D: can be exponentially localized)

Wannier center $\langle w(j)|\hat{x}|w(j)\rangle$ ≈position of charge
= Berry phase of $|u(k)\rangle$

$$\langle w(j)|\hat{x}|w(j)\rangle = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\,\langle u(k)|\,\partial_k u(k)\rangle + j$$

obtained by partial integration
j∈$\mathbb{Z}$ gauge dependent (bulk polarization defined mod 1)
Agrees with intuitive result

$$P_{\text{electric}} = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\langle u(k)|\partial_k|u(k)\rangle$$

Useful numerical tool to calculate Wannier centers is Resta's unitary position operator $\hat{X} = e^{i\delta_k \hat{x}}$.

Definition: $$\hat{X} = e^{i\delta_k \hat{x}}.$$

Respects periodic boundary condition
Unitary operator that shifts momentum

Connection to position:

$$\langle x \rangle = \frac{N}{2\pi} \log \langle \Psi | \hat{X} | \Psi \rangle$$

(see discussion in quantum optics on "phase operator")

Eigenvalues of the projected unitary position operator give the Wannier centers

$$\hat{X} = e^{i\delta_k \hat{x}}.$$

$$\hat{P} = \sum_k |\Psi(k)\rangle\langle\Psi(k)|$$

$$\hat{X}_P = \hat{P}\hat{X}\hat{P}$$

projection kills unitarity, → eigenstates not orthogonal, except N→ ∞

$$\hat{X}_P^N = \underbrace{\langle u(2\pi)|u(2\pi - \delta_k)\rangle \cdot \ldots \cdot \langle u(2\delta_k)|u(\delta_k)\rangle\langle u(\delta_k)|u(2\pi)\rangle}_{W=|W|e^{i\phi}} \hat{P}$$

W Wilson loop, Φ is Berry phase

eigenvalues λ of X_P give Wannier centers

$$\lambda_n = e^{in\delta_k + \log(W)/N} = |W|^{1/N} e^{i(\phi + n\delta_k)/N}$$

Chiral symmetry quantizes bulk polarization

$$\hat{H}(k)|u(k)\rangle = -E(k)|u(k)\rangle$$

$$\hat{H}(k)|v(k)\rangle = E(k)|v(k)\rangle$$

$$|v(k)\rangle = e^{i\phi_k}\hat{\Gamma}|u(k)\rangle$$

Berry phase of lower band = Berry phase of upper band:

Chiral symmetry quantizes bulk polarization

$$\hat{H}(k)|u(k)\rangle = -E(k)|u(k)\rangle \qquad \hat{H}(k)|v(k)\rangle = E(k)|v(k)\rangle$$

$$|v(k)\rangle = e^{i\phi_k}\hat{\Gamma}|u(k)\rangle$$

Berry phase of lower band = Berry phase of upper band:

$$\begin{aligned} |W|\, e^{i\phi_-} &= \langle u(2)|u(1)\rangle\langle u(1)|u(0)\rangle\langle u(0)|u(-1)\rangle\langle u(-1)|u(2)\rangle \\ &= \langle u(2)|\hat{\Gamma}\hat{\Gamma}|u(1)\rangle\langle u(1)|\hat{\Gamma}\hat{\Gamma}|u(0)\rangle \ldots \langle u(-1)|\hat{\Gamma}\hat{\Gamma}|u(2)\rangle \\ &= \langle v(2)|v(1)\rangle\langle v(1)|v(0)\rangle\langle v(0)|v(-1)\rangle\langle v(-1)|v(2)\rangle = |W|\, e^{i\phi_+} \end{aligned}$$

Elementary properties of Berry phase: $e^{i\phi_+}e^{i\phi_-} = 1$

Two options: bulk polarization 0 or ½