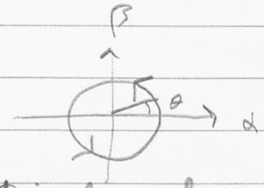
P_{bulk} evaluated from boxed eqn. for our TB chain model with PBCs is in perfect agreement with previous results obtained for finite chain ✓

Berry-phase theory of pumping cycle



Previous fig.:

$$\Delta\phi^{(cycle)} \equiv \phi(\theta=2\pi) - \phi(\theta=0) = \begin{cases} 0 & \text{trivial cycle} \\ -2\pi & \text{non-trivial} \end{cases}$$

$$\phi(\theta) = i\int_0^{2\pi/a} dk \langle u_k(\theta) | \partial_k u_k(\theta)\rangle$$

$$= \int_0^{2\pi/a} dk\, A_k(\theta)$$

Write $\Delta\phi^{(cycle)} = \int_0^{2\pi} d\theta \dfrac{d\phi}{d\theta}$

$$\Delta\phi^{(cycle)} = \int_0^{2\pi} d\theta \int_0^{2\pi/a} dk \left[i\langle \partial_\theta u | \partial_k u\rangle + i\langle u | \partial^2_{\theta k} u\rangle \right]$$

$$i\langle u | \partial^2_{\theta k} u\rangle = \partial_k \underbrace{\left(i\langle u | \partial_\theta u\rangle \right)}_{\equiv A_\theta(k)} - i\langle \partial_k u | \partial_\theta u\rangle$$

$$\Rightarrow \Delta\phi^{(cycle)} = \int_0^{2\pi} d\theta \int_0^{2\pi/a} dk\, i\left[\langle \partial_\theta u | \partial_k u\rangle - c.c. \right]$$

$$+ \underbrace{\int_0^{2\pi} d\theta \int_0^{2\pi/a} dk\, \partial_k A_\theta(k)}$$

$A_\theta(k=2\pi/a) - A_\theta(k=0) = 0$ in per. gauge:

$$A_\theta(k+2\pi/a) = i\langle u_k | \cancel{e^{+i\frac{2\pi}{a}x}}\, \partial_\theta \left(\cancel{e^{-i\frac{2\pi}{a}x}} |u_k\rangle \right) = A_\theta(k) \checkmark$$

$$\Rightarrow \Delta\phi^{(cycle)} = \int_0^{2\pi} d\theta \int_0^{2\pi/a} dk \left[-2\,\mathrm{Im}\langle \partial_\theta u | \partial_k u\rangle \right]$$

$$\boxed{F_{\theta k} = -2\,\mathrm{Im}\langle \partial_\theta u | \partial_k u\rangle} = -F_{k\theta}$$

Berry curvature

$$\Delta\phi^{(\text{cycle})} = \int_0^{2\pi} d\theta \int_0^{2\pi/a} dk\,(-F_{k\theta}) = \begin{cases} 0 & \text{trivial cycle} \\ -2\pi & \text{non-trivial} \end{cases}$$

Define

$$\boxed{C = \frac{1}{2\pi}\int_0^{2\pi} d\theta \int_0^{2\pi/a} dk\, F_{k\theta}} = -\frac{\Delta\phi^{(\text{cycle})}}{2\pi}$$

Chern number

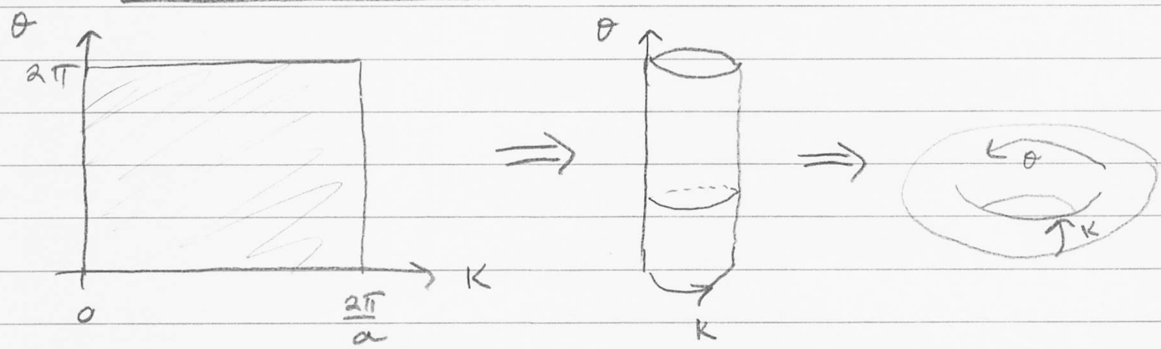
$$C = \begin{cases} 0 & \text{trivial cycle} \\ +1 & \text{nontrivial cycle} \end{cases}$$

$$\Delta P_{\text{bulk}}^{(\text{cycle})} = -e\,\frac{\Delta\phi^{(\text{cycle})}}{2\pi} = P_{\text{bulk}}(\theta=2\pi) - P_{\text{bulk}}(\theta=0)$$

$$= +e\,C$$

Same state $\Rightarrow$ P_{bulk} must be same up to $e \times$ (integer) [Eq. (15)]

$\Rightarrow$ $\boxed{C \text{ is an integer}}$



closed manifold (2-torus T^2)

Chern theorem

$$\boxed{\oint F\, dS = 2\pi \times C} \qquad C = \text{integer}$$

Any closed manifold and vector field defined on it

Comments

① $F_{k\theta}$ gauge-inv. $\Rightarrow$ C uniquely defined

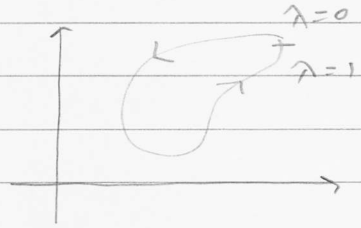
$$|\tilde{u}\rangle = e^{-i\beta(k,\theta)}|u\rangle$$

$$\Rightarrow \langle\partial_k \tilde{u}|\partial_\theta \tilde{u}\rangle = \langle\partial_k u|\partial_\theta u\rangle + (\partial_k\beta)(\partial_\theta\beta)$$

$$+ (\partial_k\beta)\, \underbrace{i\langle u|\partial_\theta u\rangle}_{A_\theta \text{ (real)}} - (\partial_\theta\beta)\, \underbrace{i\langle\partial_k u|u\rangle}_{-A_k \text{ (real)}}$$

Im(...) $\Rightarrow$ $\tilde{F}_{k\theta} = F_{k\theta}$ ✓

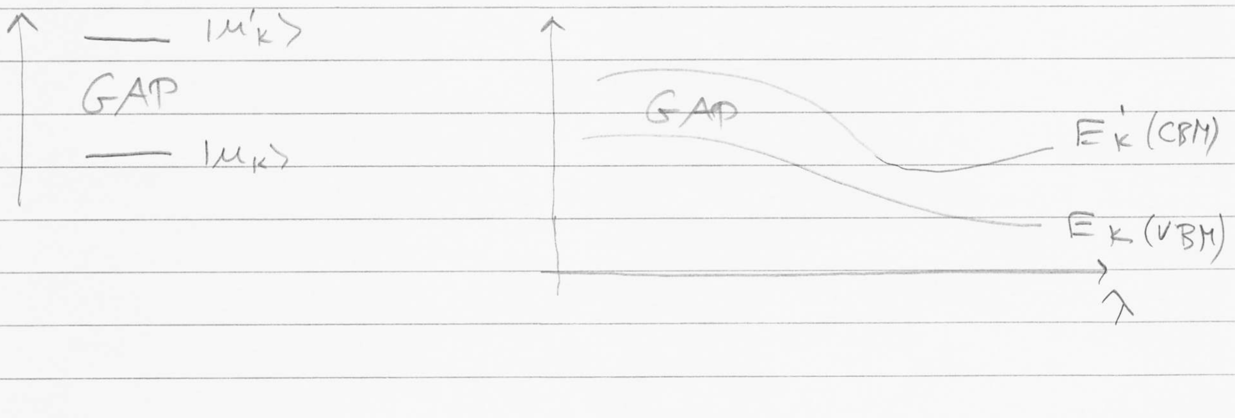
② C = what integer? Well, can't change under smooth deformation of the path



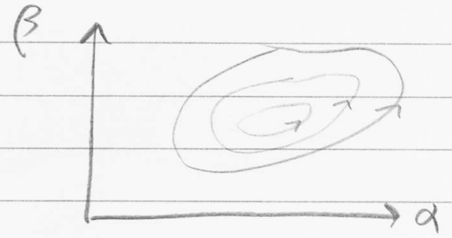
(Replace $\theta \to \lambda$ for non-circ. path)

$$C = \frac{1}{2\pi}\int_0^1 d\lambda \int_0^{2\pi/a} dk\, F_{k\lambda}$$

Smoothness condition: valence states $|u_k\rangle$ remain separated everywhere from conduction states



Can't we prove $C=0$ always by slowly contracting path?

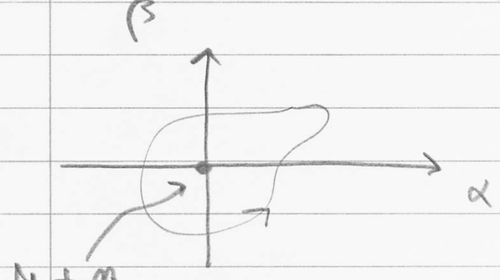


When contracted to a point, obviously $\Delta P_{bulk} = -e\,C = 0$ (system never leaves initial state!)

But integer C can't change smoothly

Thus C was always zero

Works for a cycle that does not enclose metallic pt ✓



Cannot contract path to zero!

$C \neq 0$ allowed

Discretized Berry curvature (numerics)

Note that $F_{k\lambda} = \partial_k A_\lambda - \partial_\lambda A_k$

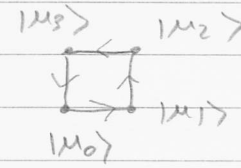
$A_k = i\langle u|\partial_k u\rangle$, $A_\lambda = i\langle u|\partial_\lambda u\rangle$

$$2\pi C = \int_0^{2\pi/a} dk \int_0^1 d\lambda\, F_{k\lambda} = \sum_{▨} \int_{▨} dk\, d\lambda\, (\partial_k A_\lambda - \partial_\lambda A_k)$$

Let $\underline{\xi} = (k, \lambda)$ $\qquad \underline{A} = i\langle u | \partial_{\underline{\xi}} u\rangle$

$$2\pi C = \sum_{\boxtimes} \underbrace{\oint_{\square} \underline{A} \cdot d\underline{\xi}}_{\phi(\square) \,=\, \text{"Plaquette Berry phase"}}$$

Discretize



$$\phi(\square) \simeq -\mathrm{Im} \ln \langle u_0|u_1\rangle\langle u_1|u_2\rangle\langle u_2|u_3\rangle\langle u_3|u_0\rangle$$

Not a Zak phase! (Doesn't go across BZ)

Purely geometrical Berry phase

same, call diag. only once

$\therefore$

$$\boxed{C = \frac{1}{2\pi} \sum_{\square} \phi(\square)}$$

plaquettes cover $[0, \frac{2\pi}{a}] \times [0, 1]$

Comments

① Guaranteed to get an integer

② C on LHS uniquely defined, but each $\phi(\square)$ on RHS only defined mod 2π! How to ensure we get the right integer?!

Strategy: Divide into many small plaquettes, such that the Berry-curv. flux through each plaquette is $|\text{flux}| \ll 2\pi$

$\rightarrow$ choose $-\pi < \phi(\square) < \pi$

$$\rightarrow C = \frac{1}{2\pi} \int_0^{2\pi} dk \int_0^1 d\lambda \, F_{k\lambda}$$

$\therefore$ Berry curvature = "Loop Berry phase per unit area"