Topological Physics in Band Insulators IV

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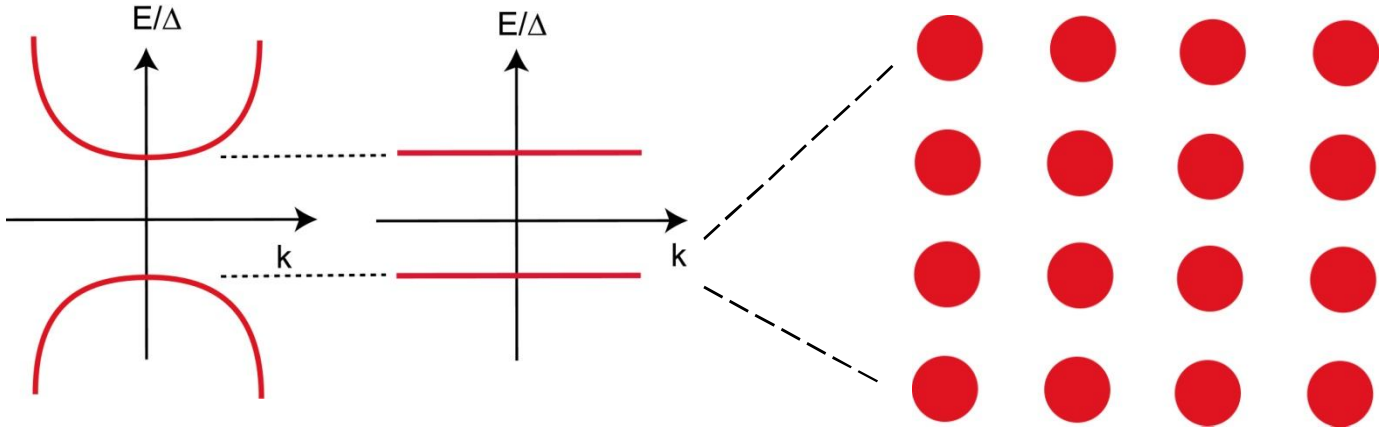
Wannier representation and band projectors

Modern view: Gapped electronic states are equivalent

Kohn (1964): insulator is exponentially insensitivity to boundary conditions



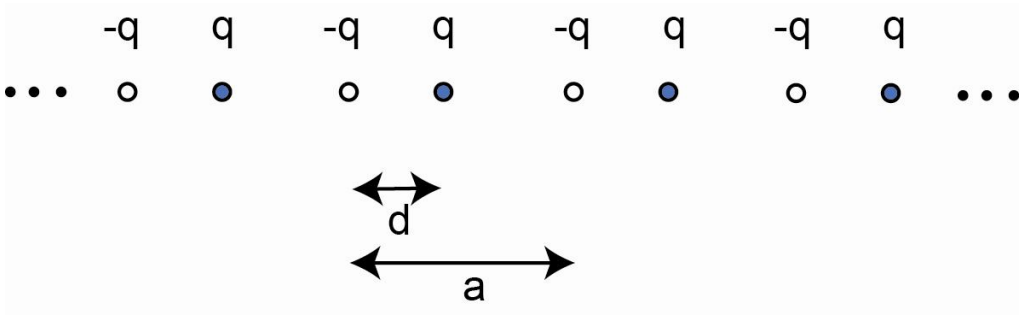
weak coupling strong coupling "nearsighted", local

Postmodern: Gapped electronic states are distinguished by topological invariants

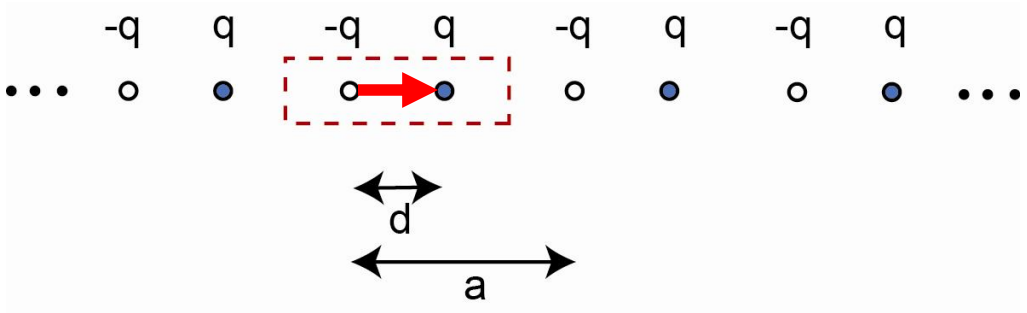
Introduction:

Exercise: consider three problems (of increasing complexity) and their solutions

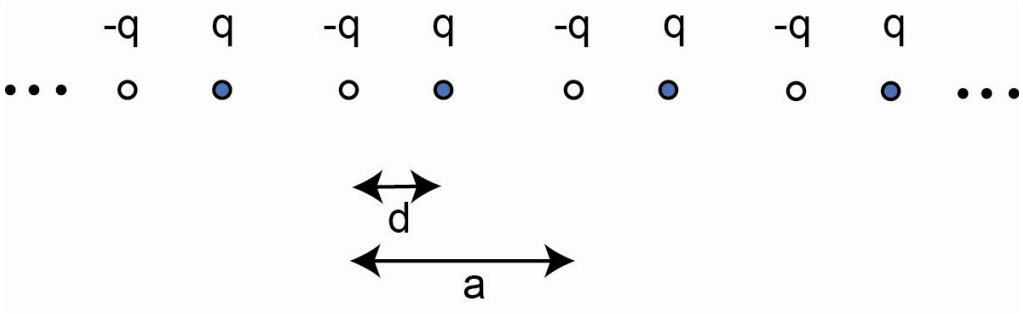
P1. Polarization (dipole density) of a one dimensional classical lattice



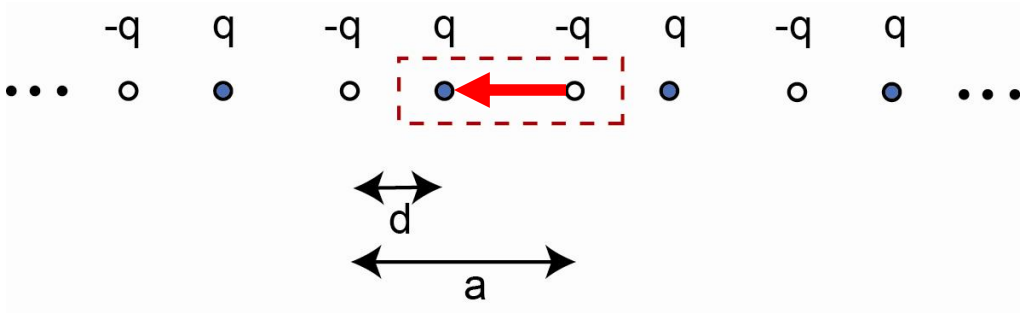
$$\frac{P}{L} = \frac{1}{Na}\sum_{i=1}^{N} q_i x_i = \frac{1}{a}\sum_{i\in\{1\}} q_i x_i = q\frac{d}{a}$$



P1. Polarization (dipole density) of a one dimensional classical lattice

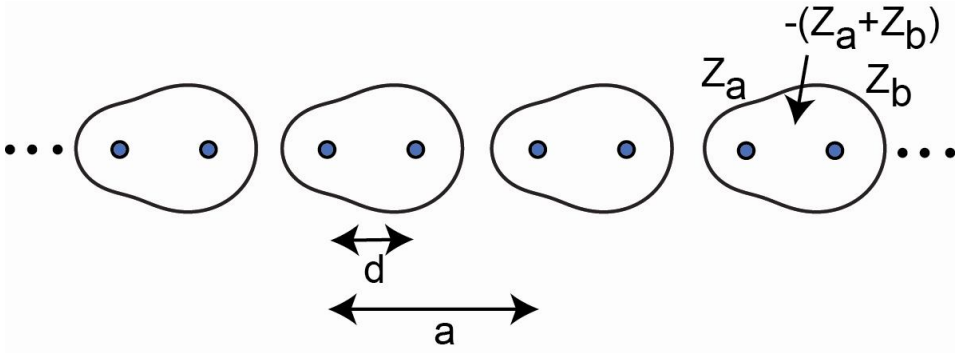


$$\frac{P_{tot}}{L} = \frac{1}{Na}\sum_{i=1}^{N} q_i x_i = \frac{1}{a}\sum_{i\in\{1\}} q_i x_i = q\left(\frac{d}{a} - 1\right)$$



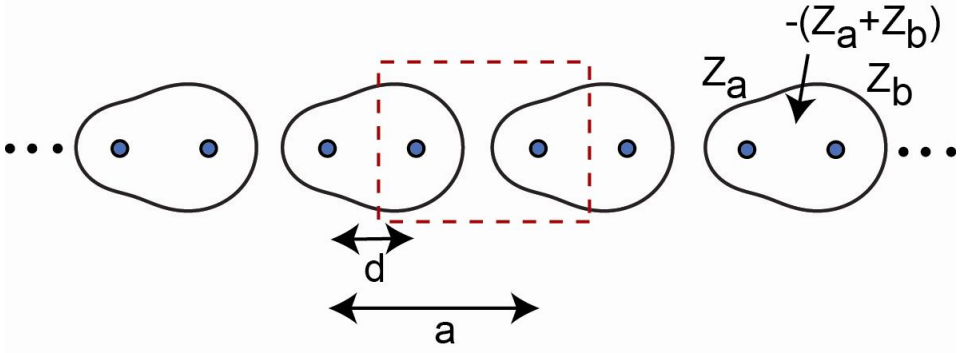
P is only defined modulo a **unit of polarization** (q in 1D)

P2. Polarization (dipole density) of a one dimensional quantum lattice



$$\frac{P}{L} = \frac{1}{a}\left(\sum_{i \in \{1\}} eZ_i x_i + e\int_a n(x)\, dx \right)$$

P2. Polarization (dipole density) of a one dimensional quantum lattice



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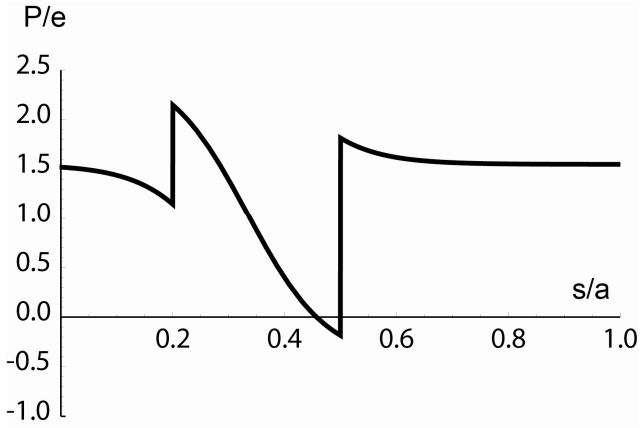


P depends on the choice of unit cell: with **discrete jumps** when classical cores cross boundary, and **continuous variation** due to quantum n(x)

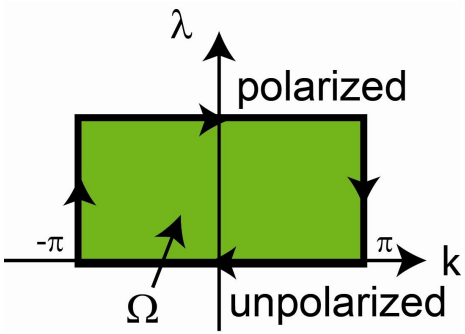
Is quantum P undefinable as a bulk quantity?

Quantum theory of polarization

Consider adiabatic evolution from an unpolarized state

$$P(\lambda(T) = Z_a - Z_b) - P(\lambda = 0) = \int_0^T \langle J \rangle \, dt$$

$$= \int_0^{\lambda(T)} \frac{\partial P}{\partial \lambda} \, d\lambda = \frac{e}{2\pi} \sum_n \int_0^{\lambda} d\lambda \int_{-\pi}^{\pi} dk \; \Omega_{\lambda,k}$$



with Berry curvature

$$\Omega_{\lambda,k} = i\left(\langle \partial_\lambda u_n(k) \,|\, \partial_k u_n(k) \rangle - \langle \partial_k u_n(k) \,|\, \partial_\lambda u_n(k) \rangle\right)$$

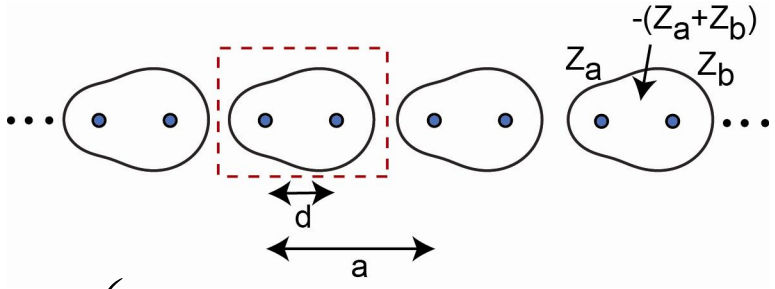
Stokes: loop integral of connection on (λ,k) circuit

$$P(\lambda(T) = Z_a - Z_b) - P(\lambda = 0) = \frac{ie}{2\pi} \sum_n \int_{-\pi}^{\pi} dk \; \langle u_n(k) \,|\, \partial_k u_n(k) \rangle \Big|_0^{\lambda} = \frac{e\gamma}{2\pi}$$

Bulk P is defined up to its quantum (e) even for a smoothly distributed n(x). **This information is not in n(x) but in γ (i.e. in Ψ(x))** (King-Smith & Vanderbilt, Resta)

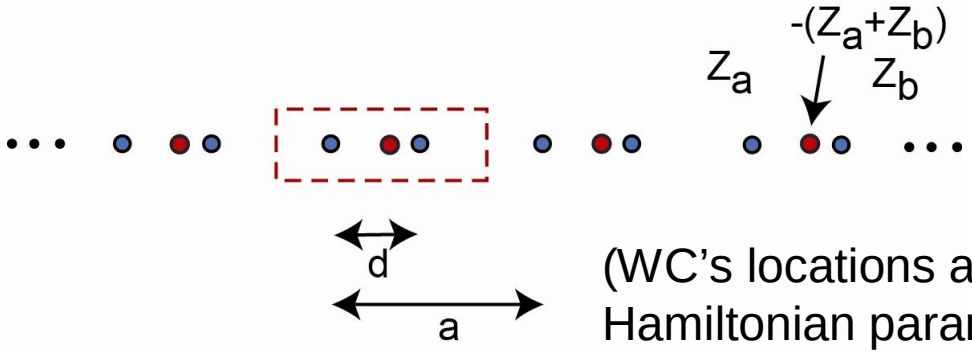
Interpretation: Wannier-charge-centers are discrete

Ground state average over n(x) contains the first moments of the charge densities in its Wannier functions.



continuous

$$\frac{P}{L} = \frac{1}{a}\left(\sum_{i\in\{1\}} eZ_i x_i + e\sum_n \int x \left| w_n(x) \right|^2 dx \right)$$



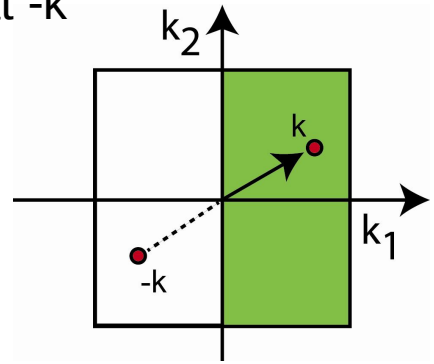
discrete

(WC's locations are functions of Hamiltonian parameters)

P3. Determine the Z_2 index of a generic* time-reversal-invariant band insulator

Z_2 index counts the number (mod 2) of band inversions from the filled manifold of a T-invariant insulator.

Calculate the overlap of the cell-periodic Bloch function u(-k) with its time reversed partner at -k



$$w_{mn}(\vec{k}) = \left\langle u_m(-\vec{k}) \,|\, \Theta \,|\, u_n(\vec{k}) \right\rangle$$

Count the complex zeroes of Pf [w] within **one half** of Brillouin zone (difficulty: the overlap is k-nonlocal)

*time reversal & lattice translations only

Some possible solutions:

1. Parity test: for crystal with inversion symmetry

$$(-1)^{\nu} = \prod_{a=1}^{N} \delta_a \qquad \delta_a = \prod_{m} \xi_{2m} \qquad \text{(parity eigenvalues, } \pm 1\text{)}$$

Requires an inversion symmetric space group (nongeneric)

2. Adiabatic continuity. Apply parity test to reference inversion-symmetric structure and check for no gap closure under a slow deformation to P-breaking structure of interest.

3. Gap closure: Compare the level ordering in band insulator computed without and with spin orbit coupling. Band inversion requires a gap closure and (may) denote transition to topological phase, verified by surface spectrum.

4. **Transformation to Wannier representation**.

Wannier functions: definitions

$$\left[H, T_{\vec{R}}\right] = 0 \;\Rightarrow\; \psi_{n,k}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_n(\vec{k};\vec{r}) \qquad h(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}} H e^{i\vec{k}\cdot\vec{r}}$$

Wave packet is constructed from a BZ integral

$$w_n(\vec{r}) = \frac{V}{(2\pi)^d} \int_\Omega d\mathrm{k}\, \psi_{n,\vec{k}} = \frac{V}{(2\pi)^d} \int_\Omega d\mathrm{k}\, e^{i\vec{k}\cdot\vec{r}} u_n(\vec{k};\vec{r})$$

And its discrete lattice translates:

$$w_n(\vec{r}-\vec{R}) = \frac{V}{(2\pi)^d} \int_\Omega d\mathrm{k}\, e^{i\vec{k}\cdot\left(\vec{r}-\vec{R}\right)} u_n(\vec{k};\vec{r})$$

$$\left\langle m, \vec{R} \,|\, n, \vec{R}' \right\rangle = \delta_{m,n}\delta_{\vec{R},\vec{R}'} \qquad \psi_{n,\vec{k}} = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} w_n(\vec{r}-\vec{R})$$

This is a reconstruction of ψ from a lattice sum

Wannier functions: nonuniqueness

1. U(1) gauge freedom

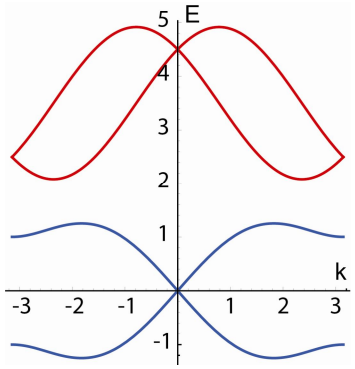
$$w_n(\vec{r}) = \frac{V}{(2\pi)^d} \int_{\Omega} d\mathrm{k}\, e^{i\vec{k}\cdot\vec{r}} u_n(\vec{k};\vec{r})$$

superposition from eigenfunctions of disconnected sectors, h(k)

$$\tilde{u}_n(\vec{k};\vec{r}) = e^{i\phi(k)} u_n(\vec{k};\vec{r})$$

exponentially localized wf's require a smooth $\phi(\vec{k}) = \phi(\vec{k} + \vec{G})$

2. U(N) freedom



index switching at a band crossing generates power law tails in its single band Wannier functions.

removable by specification of a k-differentiable (i.e. smooth) composite manifold: $\tilde{u}_m(\vec{k};\vec{r}) = U_{mn}(\vec{k}) u_n(\vec{k};\vec{r})$

Maximally localized wf's

Degree of localization is measured by the spread functional Ω

$$\Omega = \sum_{n \in \text{occ}} \left[\left\langle r^2 \right\rangle_n - \left\langle \vec{r} \right\rangle_n \bullet \left\langle \vec{r} \right\rangle_n \right]$$

Task: Minimize Ω with respect to U(k) to obtain the **smoothest possible** k-dependence of its quasi-Bloch states and the **optimum localization** of its Wannier representation.

Physics contained in a projected subspace

$$\hat{P} = \sum_{\mathbf{k}, n \in \text{occ}} \left| \psi_{nk} \right\rangle \left\langle \psi_{nk} \right| = \sum_{\mathbf{R}, n \in \text{occ}} \left| n, R \right\rangle \left\langle n, R \right|$$

$$\hat{Q} = \hat{I} - \hat{P}$$

These band projectors are invariant under choice of U(k)

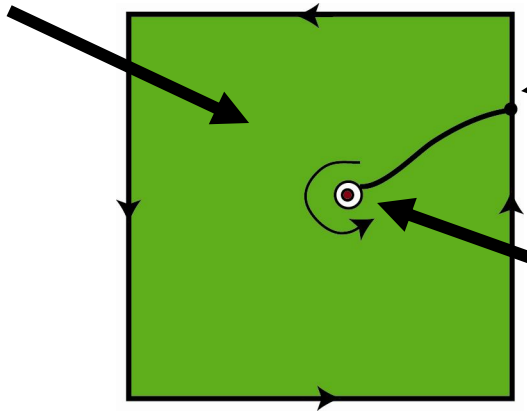
Topological obstruction

A smooth periodic gauge is impossible for a band insulator with a nonzero Chern number (i.e. one with a nonzero Hall conductance).

Chern insulators are not Wannier-representable*

$$\frac{i}{2\pi}\oint d\mathbf{k}\cdot\langle u_k|\nabla_k u_k\rangle = \begin{cases} 0 \text{ when } \psi_{n,k} = \psi_{n,k+G} \\ C \neq 0 \text{ in Chern insulator} \end{cases}$$

smooth $\langle u_k|\nabla_k u_k\rangle$



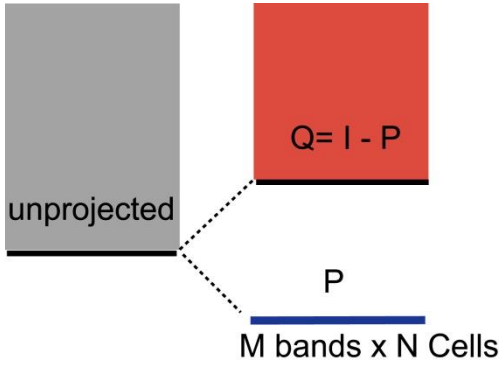
$\langle u_k|\nabla_k u_k\rangle$ jumps here

vortex

It is perhaps not surprising that the existence of a representation of the magnetic subband In terms of propertly localized states precludes the existence of a Hall current. - Thouless (1984)

Alternative route to WF's: Band Projection

$$\hat{P} = \sum_{\mathbf{k},n\in\mathrm{OCC}} |\psi_{nk}\rangle\langle\psi_{nk}| = \sum_{\mathbf{R},n\in\mathrm{OCC}} |n,R\rangle\langle n,R|$$



Projected "M-band" problem

Choose M (localized) trial functions $\{\tau_\alpha\}$ with N lattice translates

Ground state projected image: $\{\tilde{\tau}_\alpha\} = \{\hat{P}\tau_\alpha\}$

With symmetric orthogonalization:

$w_m = S_{m,n}^{-1/2}\tilde{\tau}_n$; $\quad S_{m,n} = \langle\tilde{\tau}_m \,|\, \tilde{\tau}_n\rangle$ (M×M for each k)

Comments

The k-space construction and the projection method are **complementary**

K-space: find smoothest possible quasi Bloch states $\{v_{nk}\}$
whose superposition produces most localized wavepackets (minimize Ω)

Projection: choose M localized trial functions $\{\tau_\alpha\}$ whose valence band projections are minimally inflated by the projector

Note: while projectors of the form $\hat{P} = \sum_{\mathbf{k},n\in\text{occ}} |\psi_{nk}\rangle\langle\psi_{nk}| = \sum_{\mathbf{R},n\in\text{occ}} |n,R\rangle\langle n,R|$
are invariant under U(N).

the charge "centers" of individual wf's $\bar{x}_{\alpha,n} = \langle \vec{R},n \,|\, \hat{X}_\alpha \,|\, \vec{R},n \rangle$
are not (clearly gauge dependent)

but the "sum of charge centers" $\sum_n^M \bar{x}_{\alpha,n}$ are gauge invariant modulo $\vec{R}$

Special considerations for topological insulators

1. TI's are time-reversal invariant (Chern number = 0) thus the topological obstruction to the construction of exponentially localized wf's is formally absent.

2. In S_z-conserving models (e.g. Haldane[2]) the ground state has disconnected sectors each of which **contains** a topological obstruction

3. k-space criterion (Pfaffian) for TI requires that we work in a globally smooth gauge.

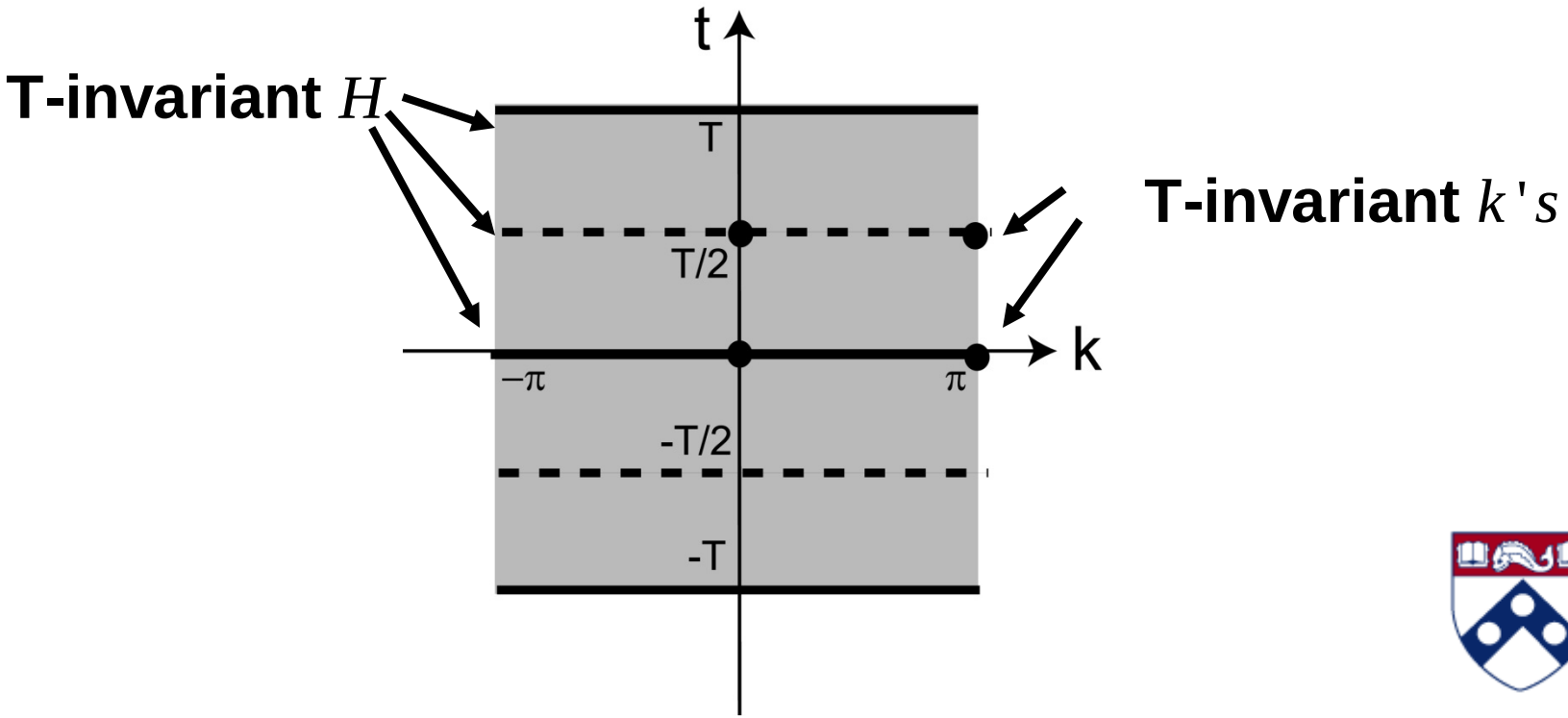
natural vs. smooth gauge

Time Reversal Polarization

simple model: parametric pump for one dimensional lattice

$$H[t+T] = H[t]$$

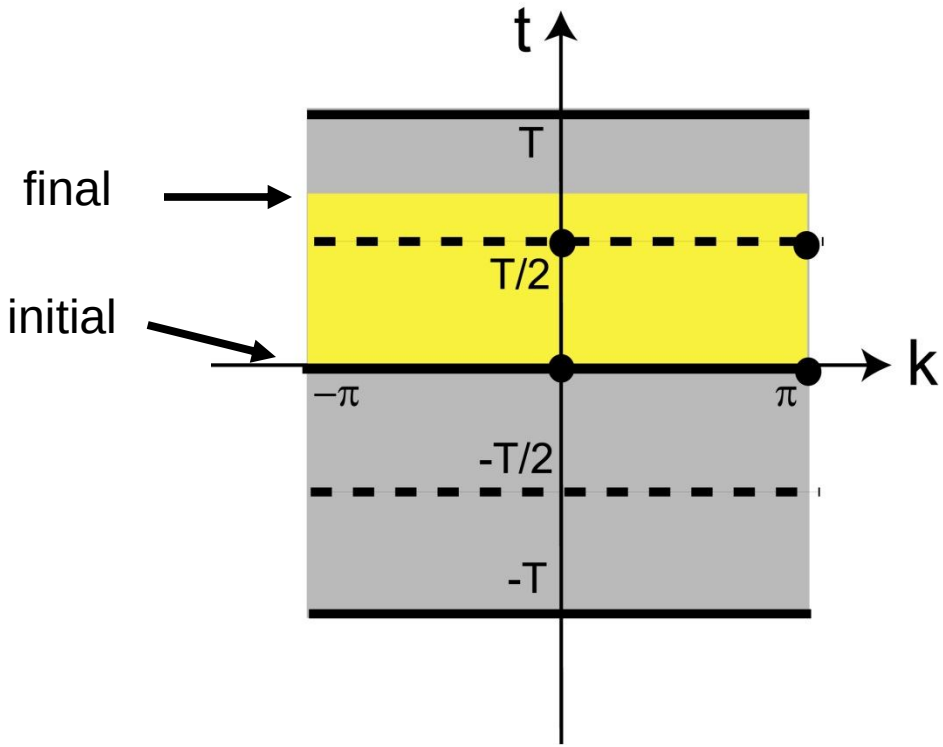
$$H[-t] = \Theta H[t]\Theta^{-1}; \qquad \Theta = i\sigma_y K$$



Time Reversal Polarization

simplest model: parametric pump for one dimensional lattice

$$P_\rho(t) - P_\rho(0) = \frac{1}{2\pi}\int_A dt\, dk\, \mathbf{F}_{t,k} = \frac{1}{2\pi}\left(\int_t dk\, \mathbf{A} - \int_0 dk\, \mathbf{A}\right)$$

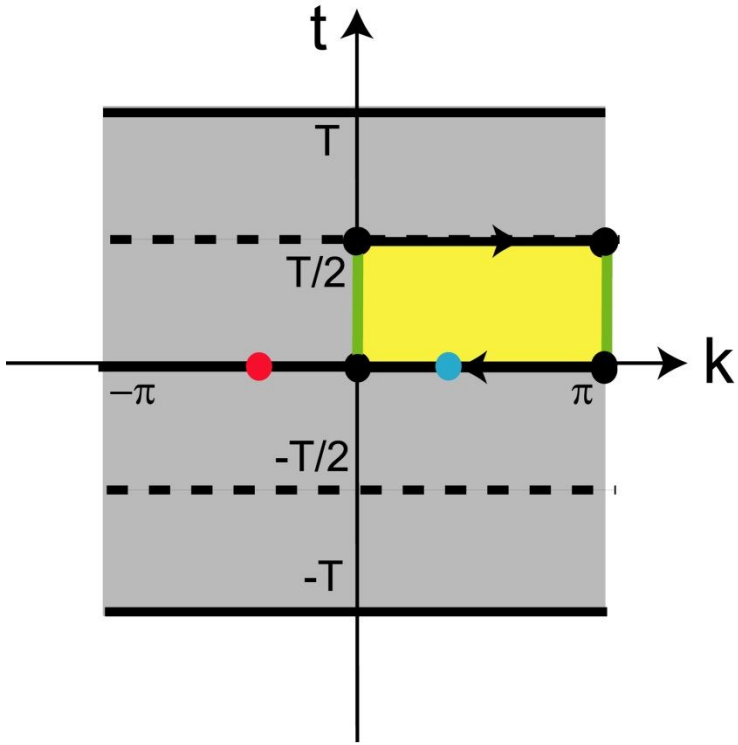


Time Reversal Polarization

For termination at T/2 the loop integral can be reduced to a **half zone** in a (locally smooth) gauge that explicitly respects T-symmetry at t=0,T/2

$$u^{I}_{-k,m} = -e^{i\chi_{k,m}}\Theta\, u^{II}_{k,m}$$

$$u^{II}_{-k,m} = e^{i\chi_{-k,m}}\Theta\, u^{I}_{k,m}$$



Time Reversal Polarization

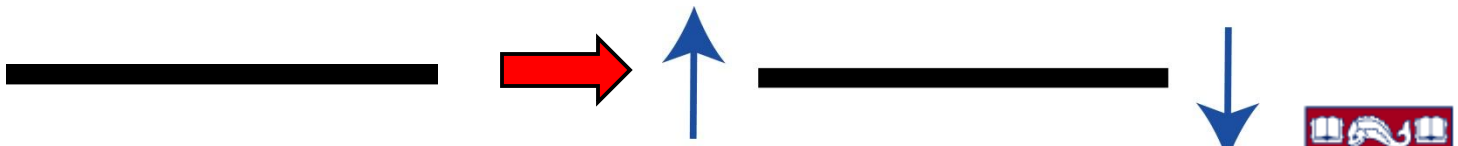
$$\mathbf{A}(k) = i\left\langle u_{nk} \mid \partial_k u_{nk} \right\rangle = \mathbf{A}^{I}(k) + \mathbf{A}^{II}(k)$$

$$\Delta P_{\rho} = \Delta P_{I} + \Delta P_{II}$$

$$\Delta P_{\Theta} = \Delta P_{I} - \Delta P_{II}$$

ΔP_{ρ} is the ordinary charge polarization (and vanishes if $C = 0$).

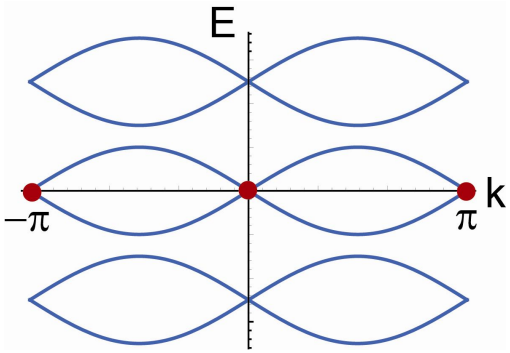
ΔP_{Θ} for a half period measures the bulk flow of time reversed partners to the boundaries (integer mod 2)



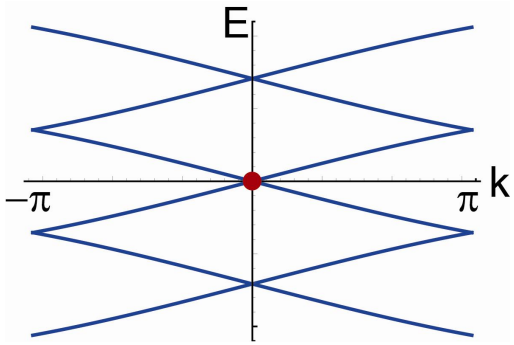
TI Surface States

Parametric pump $(k,t) \Rightarrow$ Band topology (k_1, k_2)

ΔP_Θ integrated over a half zone distinguishes the binding/liberation of its Kramers partners



vs



ordinary

topological

Wannier states for Z_2 insulators

Impossible for TI using the TRG. If the gauge
is smooth over the full zone then Z_2=0 (ordinary insulator) so that Z_2=1
(topological insulator) can occur only if the time reversal
gauge contains an unremovable singularity.

Nonetheless TI's are gapped states with Chern number =0, i.e.
in an **unobstructed gapped state**, thus Wannier representable.

TOPOLOGICAL INSULATOR IS WANNIER-REPRESENTABLE
THOUGH NOT IN THE TIME REVERSAL SYMMETRIC GAUGE.

WF's by band projection

$$\hat{P} = \sum_{\mathbf{k},n\in\mathrm{OCC}} |\psi_{nk}\rangle\langle\psi_{nk}| = \sum_{\mathbf{R},n\in\mathrm{OCC}} |n,R\rangle\langle n,R|$$

The projection recipe is algorithmic

Choose M (localized) trial functions $\{\tau_\alpha\}$ with N lattice translates

Ground state projected image: $\{\tilde{\tau}_\alpha\} = \{\hat{P}\tau_\alpha\}$

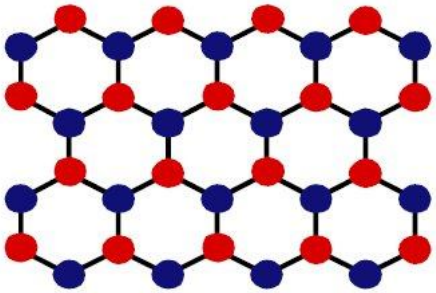
With symmetric orthogonalization:

$w_m = S_{m,n}^{-1/2}\tilde{\tau}_n$; $S_{m,n} = \langle\tilde{\tau}_m | \tilde{\tau}_n\rangle$ (M×M for each k)

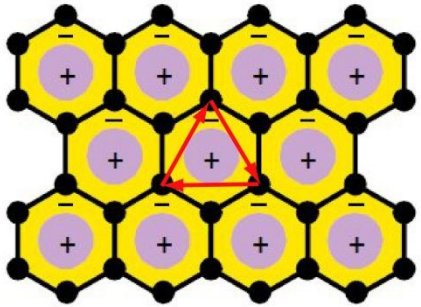
The obstruction appears here

Example 1: Haldane Model

Spinless tight binding model on honeycomb lattice
with two distinct gapped phases

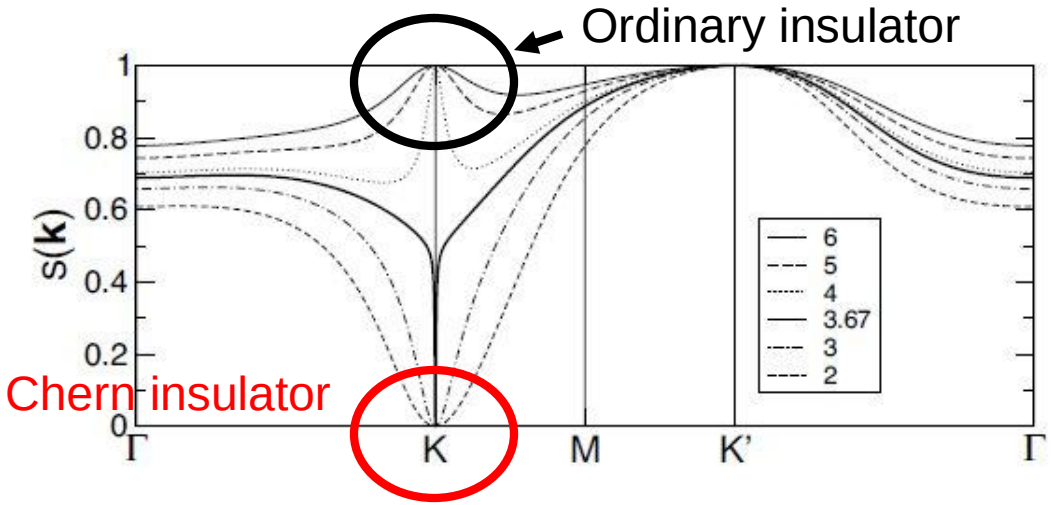


Ordinary insulator: breaks P



Chern insulator: breaks T

Fourier spectrum of its overlap matrix eigenvalues

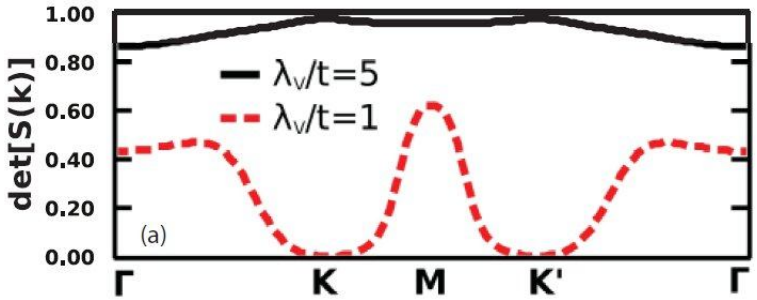


Ref: Thonhauser and
Vanderbilt (2006)

Example 2: Spin-full graphene

Ordinary insulator: sublattice potential breaks P

Z_2 odd insulator: spin-orbit term gaps the K point



Trial states:

Kramers pair $\left|A,\uparrow_z\right\rangle, \left|A,\downarrow_z\right\rangle$

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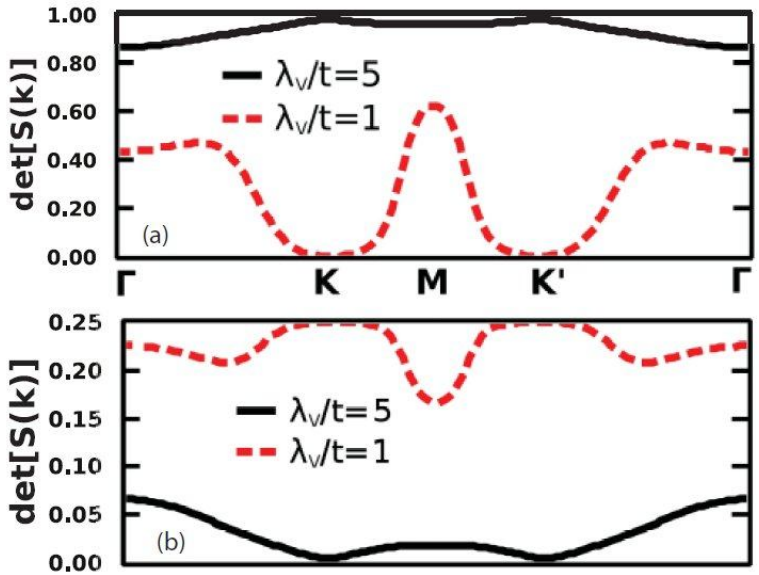


Trial states:
Kramers pair $\left|A,\uparrow_z\right\rangle, \left|A,\downarrow_z\right\rangle$

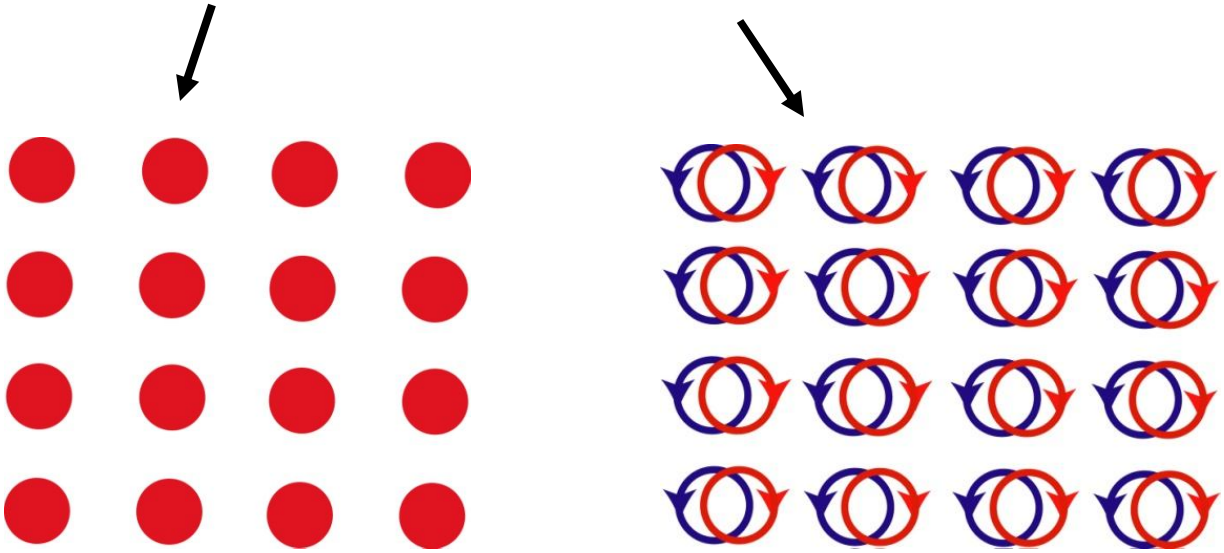
Trial states:
TR-polarized pair $\left|A,\uparrow_x\right\rangle, \left|B,\downarrow_x\right\rangle$

Soluyanov and Vanderbilt (2011)

Breaking Kramers symmetry in real space avoids the the Z_2 obstruction.

Schematically

Ordinary insulators and topological insulators are both **nearsighted gapped phases** with Wannier representations as **Kramers partners** (ordinary) or as **time-reversal polarized partners** (topological)



Local Diagnostics for Topological Order

In an M-band Chern insulator

$$C = -\frac{1}{\pi}\,\mathrm{Im}\sum_{n=1}^{M}\int_{BZ} d\mathrm{k}\left\langle \frac{\partial u_{n\mathrm{k}}}{\partial k_x}\middle|\frac{\partial u_{n\mathrm{k}}}{\partial k_y}\right\rangle$$

after some algebra

$$C = \frac{4\pi}{A}\,\mathrm{Im}\,\mathrm{Tr}\{Px\,Py\};$$

$P =$ Ground state projector

C=0 for finite system with open boundary conditions (trivial topology)

P is a short ranged operator (insulator is nearsighted)

$\tilde{X}(\mathrm{r},\mathrm{r}') \equiv \int d\,\mathrm{r}''\,P(\mathrm{r},\mathrm{r}'')x''P(\mathrm{r}'',\mathrm{r}')$ (Note: projected translations: $\left[\tilde{X},\tilde{Y}\right] \neq 0$)

"Chern number density": replace global trace by a local trace

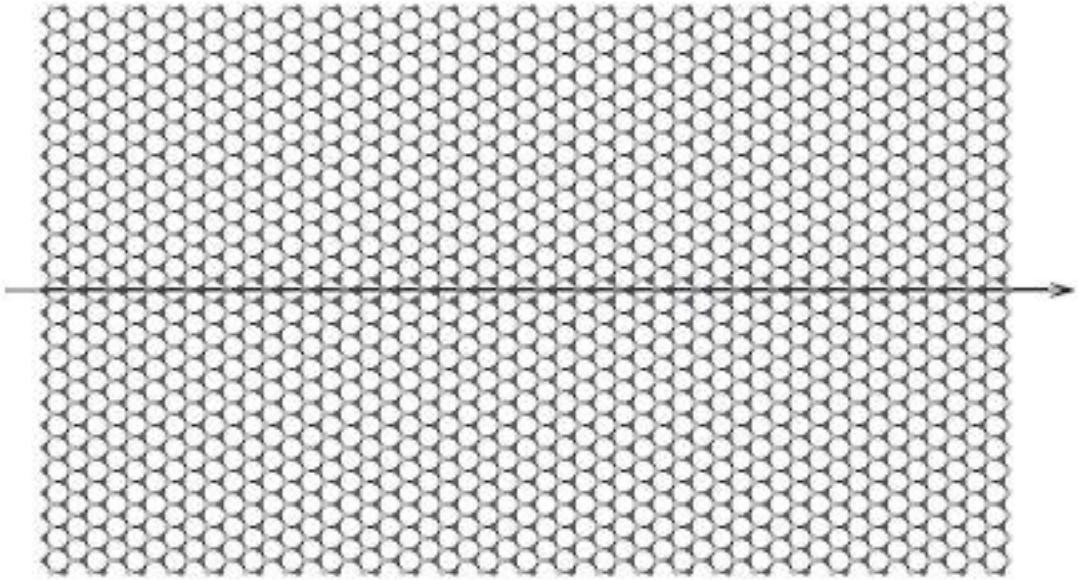
$$\mathrm{C} = \frac{4\pi}{A_c}\,\mathrm{Im}\,\mathrm{Tr}_c\{Px\,Py\} = -2\pi i\int d\,\mathrm{r}'\left[\tilde{X}(\mathrm{r},\mathrm{r}')\tilde{Y}(\mathrm{r}',\mathrm{r}) - \tilde{Y}(\mathrm{r},\mathrm{r}')\tilde{X}(\mathrm{r}',\mathrm{r})\right]$$

Bianco and Resta (2011)

Local Diagnostics for Topological Order

$\int d\,\mathrm{r}\; \mathrm{C}(\mathrm{r}) = 0$ with $\mathrm{C}(\mathrm{r}) \neq 0$

Chern density is a local marker for topological order

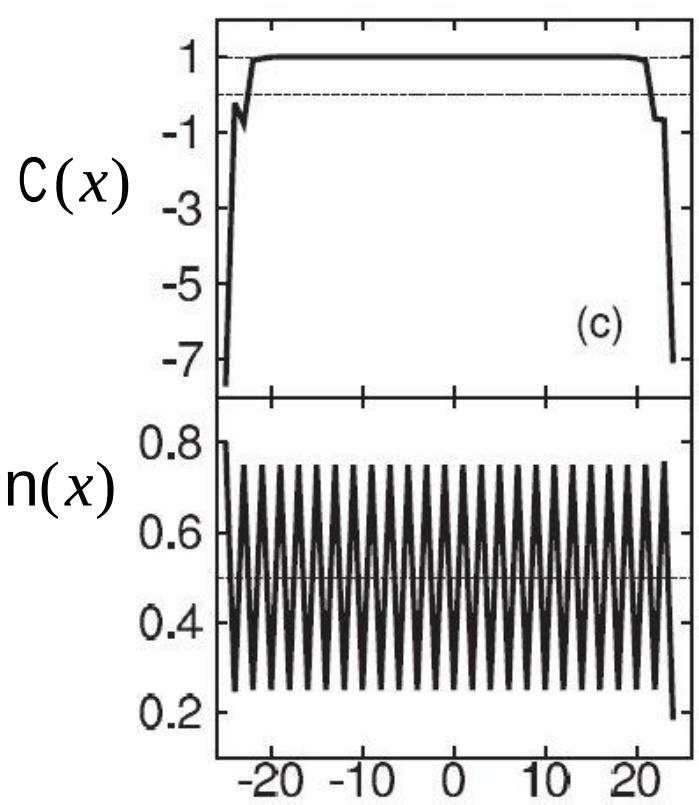


Bianco and Resta (2011)

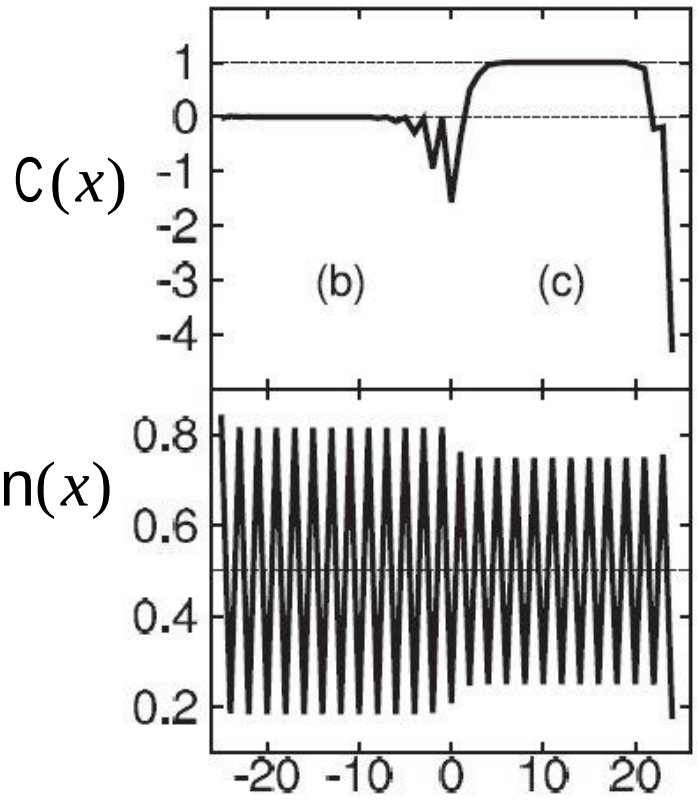
Local Diagnostics for Topological Order

$$\int d\,\mathrm{r}\; C(\mathrm{r}) = 0 \text{ with } C(\mathrm{r}) \neq 0$$

Chern density is a local marker for topological order



Chern ribbon



Normal/Chern interface

Bianco and Resta (2011)

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