Introduction to topological aspects in condensed matter physics

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Ten-fold classification of topological insulators and superconductors

1st lecture:

- Topological band theory
- Topological insulators in 1D (polyacetylene)
- Topological insulators in 2D (IQHE, QSHE)

2nd lecture:

- Topological insulators w/ TRS in 2D & 3D (Z_2 invariant)
- BdG theory for superconductors
- Topological superconductors in 1D and 2D
- Majorana bound states

3rd lecture:

- Topological superconductors in 2D and 3D w/ TRS
- Periodic table of topological insulators and superconductors

4th lecture:

- Topological crystalline insulators
- Gapless topological materials

Books and review articles

Review articles:

- M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. **82**, 3045 (2010)
- X.L. Qi and S.C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)
- S. Ryu, A. P. Schnyder, A. Furusaki, A. Ludwig, New J. Phys. **12**, 065010 (2010)
- C. Beenakker, Annual Review of Cond. Mat. Phys. **4**, 113 (2013)
- J. Alicea, Rep. Prog. Phys. **75**, 076501 (2012)
- Y. Ando, J. Phys. Soc. Jpn. **82**, 102001 (2013)

Books:

- Shun-Qing Shen, “Topological insulators”, Springer Series in Solid-State Sciences, Volume **174** (2012)
- B. Andrei Bernevig, "Topological Insulators and Topological Superconductors”, Princeton University Press (2013)
- Mikio Nakahara, "Geometry, Topology and Physics", Taylor & Francis (2003)
- A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, J. Zwanziger, “The geometric phase in quantum systems”, Springer (2003)
- M. Franz and L. Molenkamp, “Topological Insulators”, Contemporary Concepts of Condensed Matter Science, Elsevier (2013)

1st lecture: Topological band theory

1. Introduction
   - What is topology?
   - Topological band theory

2. Topological insulators in 1D
   - Berry phase
   - Simple example: Two-level system
   - Polyacetylene (Su-Schrieffer-Heeger model)
   - Domain wall states

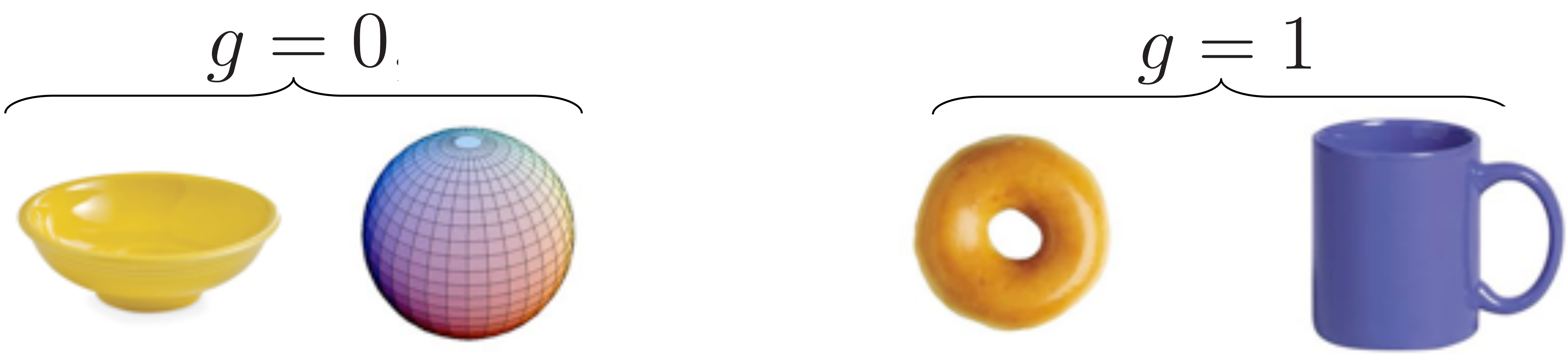
3. Topological insulators in 2D
   - Integer quantum Hall effect
   - Bulk boundary correspondence
   - Chern insulator on square lattice

What is topology?

The study of geometric properties that are insensitive to smooth deformations

For example, consider two-dimensional surfaces in three-dimensional space

Closed surface is characterized by its genus g = # holes



- ▶ g is an integer topological invariant

Gauss-Bonnet Theorem

Genus can be expressed in terms of an integral of the Gauss curvature over the surface

$$\int_S \kappa \, dA = 4\pi(1 - \underbrace{g}_{\text{topological invariant}})$$

In condensed matter physics:

Topology of insulating materials, topology of band structures

Band theory of solids and topology

Bloch's theorem: consider electron wavefunction in periodic crystal potential

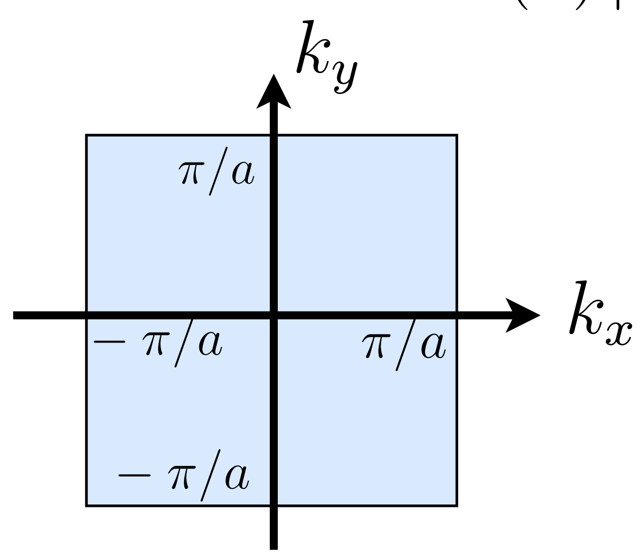
crystal momentum

Electron wavefunction in crystal $|\psi_n\rangle = e^{i\boldsymbol{k}\boldsymbol{r}}\,|u_n(\boldsymbol{k})\rangle$

Bloch wavefunction
has periodicity of potential

Bloch Hamiltonian $H(\boldsymbol{k}) = e^{-i\boldsymbol{k}\boldsymbol{r}} H e^{+i\boldsymbol{k}\boldsymbol{r}}$ $\quad H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$

$\boldsymbol{k} \in$ Brillouin Zone



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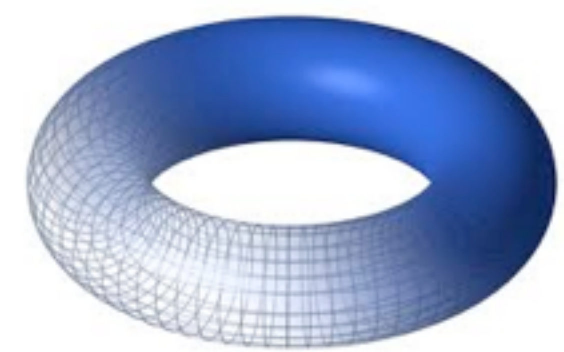
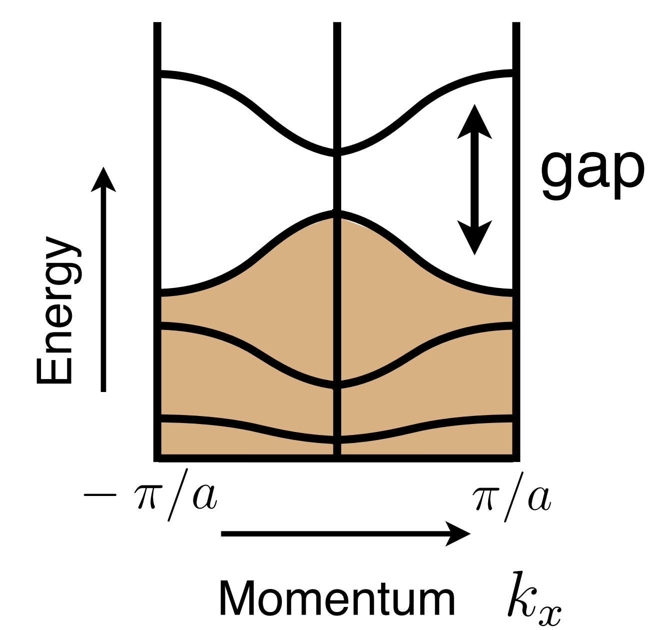


Band structure defines a mapping:

Brillouin zone $\longmapsto$ $H(\boldsymbol{k})$ Hamiltonians
with energy gap

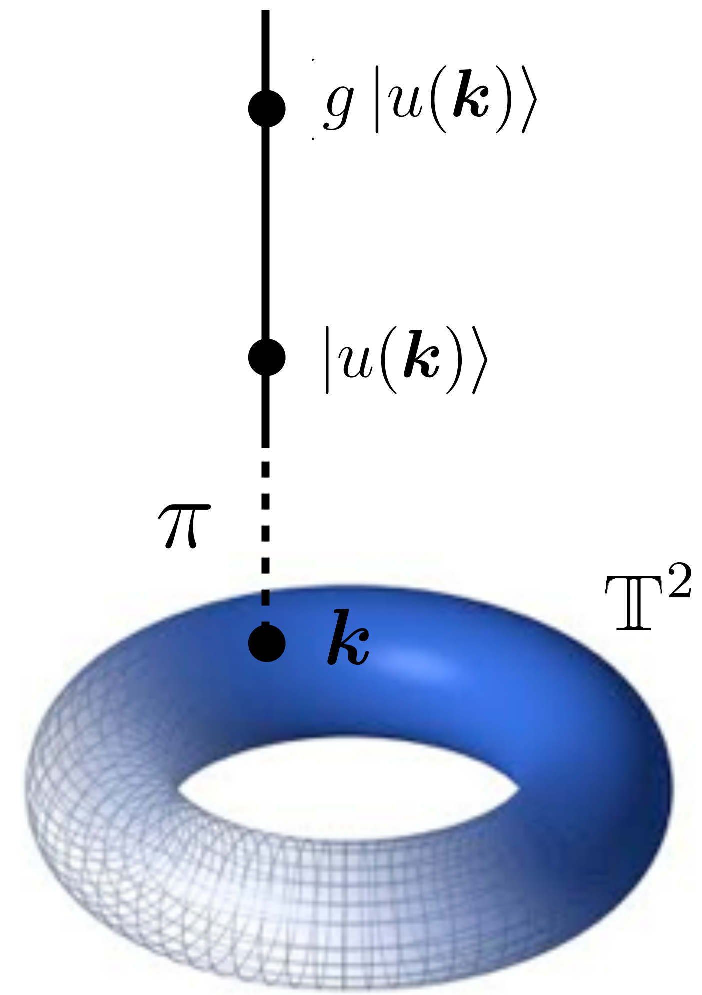


Topological equivalence:

Band structures are equivalent if they can be continuously deformed into one another without closing the energy gap

Band theory and topology

Berry phase:



Phase ambiguity of wavefucntion $|u(\boldsymbol{k})\rangle \to e^{i\phi_{\boldsymbol{k}}}\,|u(\boldsymbol{k})\rangle$

U(1) fiber bundle: to each $\boldsymbol{k}$ attach fiber $\left\{ g\,|u(\boldsymbol{k})\rangle \;\middle|\; g \in U(1) \right\}$

define Berry connection: (like EM vector potential)

$$\mathcal{A} \;=\; \langle u_{\boldsymbol{k}}| - i\nabla_k\, |u_{\boldsymbol{k}}\rangle$$

under gauge transformation:

$$|u(\boldsymbol{k})\rangle \to e^{i\phi_{\boldsymbol{k}}}\,|u(\boldsymbol{k})\rangle \quad \Longrightarrow \quad \mathcal{A} \to \mathcal{A} + \nabla_{\boldsymbol{k}}\phi_{\boldsymbol{k}}$$

Berry phase: (gauge invariant quantity)

change in phase on a closed loop

$$\gamma_C = \oint_C \mathcal{A}\cdot d\boldsymbol{k}$$

Berry curvature tensor: (gauge independent)

$$\mathcal{F}_{\mu\nu}(\mathbf{k}) = \frac{\partial}{\partial k_\mu}\mathcal{A}_\nu(\boldsymbol{k}) - \frac{\partial}{\partial k_\nu}\mathcal{A}_\mu(\boldsymbol{k})$$

For 3D: $\boldsymbol{\mathcal{F}} = \nabla_{\boldsymbol{k}} \times \mathcal{A}$ $\qquad \mathcal{F}_{\mu\nu} = \epsilon_{\mu\nu\xi}\boldsymbol{\mathcal{F}}_\xi$ $\qquad$ Stokes: $\gamma_C = \int_S \boldsymbol{\mathcal{F}}\cdot d\boldsymbol{k}$

Topological invariants of band structures:

Topological property of insulating material
given by Chern number (or winding number):

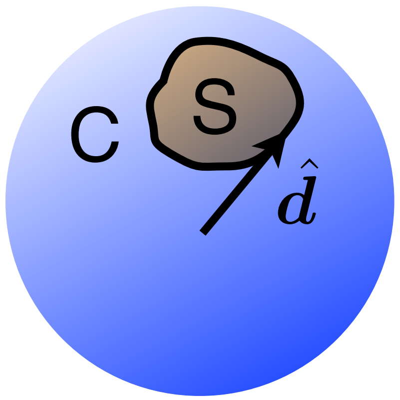
$$n = \frac{i}{2\pi}\sum_{\substack{\text{filled}\\ \text{states}}} \int \mathcal{F} d^2k$$

Berry phase for two-level system

Two-level Hamiltonian: $H(\boldsymbol{k}) = \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma} = \begin{pmatrix} d_z & d_x - i d_y \\ d_x + i d_y & -d_z \end{pmatrix}$

param. by spherical coord.: $\boldsymbol{d}(\boldsymbol{k}) = |\boldsymbol{d}|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$

two eigenvectors with energies $E_\pm = \pm|\boldsymbol{d}|$ (north pole gauge)



$$|u^-_{\boldsymbol{k}}\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{pmatrix} \qquad |u^+_{\boldsymbol{k}}\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi} \\ \sin(\theta/2) \end{pmatrix}$$

$$2\gamma_C = \substack{\text{solid angle} \\ \text{swept out by } \hat{\boldsymbol{d}}(\boldsymbol{k})}$$

Berry vector potential: (gauge dependent)

$$A_\theta = i\langle u^-_{\boldsymbol{k}}|\partial_\theta|u^-_{\boldsymbol{k}}\rangle = 0 \qquad A_\phi = i\langle u^-_{\boldsymbol{k}}|\partial_\phi|u^-_{\boldsymbol{k}}\rangle = \sin^2(\theta/2)$$

Berry curvature: (gauge independent) $\mathcal{F}_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{\sin\theta}{2}$

If $\boldsymbol{d}(\boldsymbol{k})$ depends on parameters $\boldsymbol{k}$: $\mathcal{F}_{k_i,k_j} = \frac{\sin\theta}{2}\frac{\partial(\theta,\phi)}{\partial(k_i,k_j)}$ Jacobian matrix

Simple example: $\boldsymbol{d}(\boldsymbol{k}) = \boldsymbol{k}$

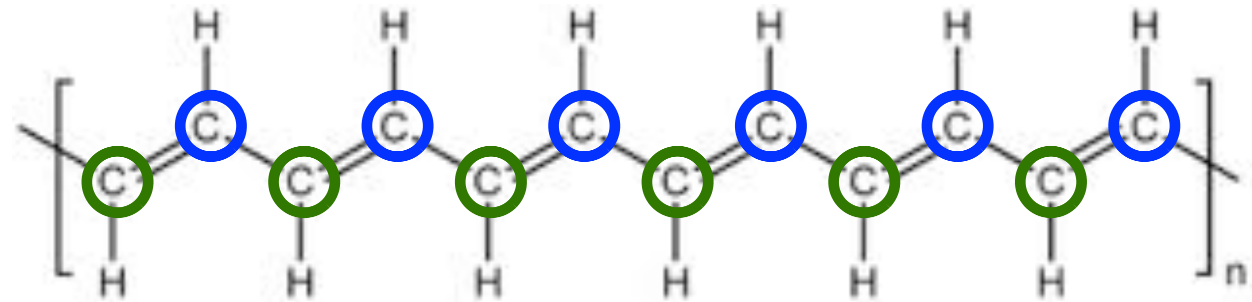
$$\boldsymbol{\mathcal{F}} = \frac{1}{2}\frac{\hat{\boldsymbol{k}}}{k^2}$$ (monopole field)

$$\gamma_C = \int_S \mathcal{F}_{\theta\phi}\, d\theta d\phi = \frac{1}{2}\left(\substack{\text{solid angle} \\ \text{swept out by } \hat{\boldsymbol{d}}(\boldsymbol{k})}\right)$$

Polyacetylene (Su-Schrieffer-Heeger model)

[Su, Schreiffer, Heeger 79]

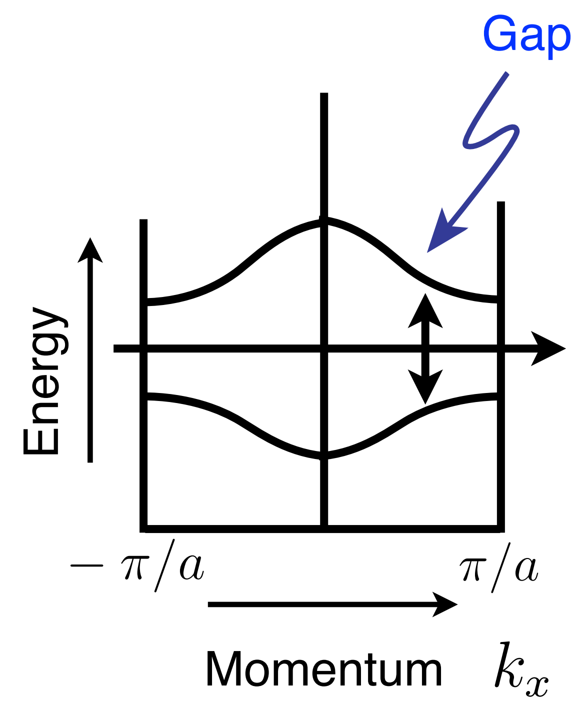
Su-Schrieffer-Heeger model
describes polyacetylene $[\mathrm{C_2H_2}]_n$



Hamiltonian:

$$\mathcal{H} = \sum_i \left[(t+\delta t) c^\dagger_{Ai} c_{Bi} + (t-\delta t) c^\dagger_{Ai+1} c_{Bi} + \mathrm{h.c.} \right]$$

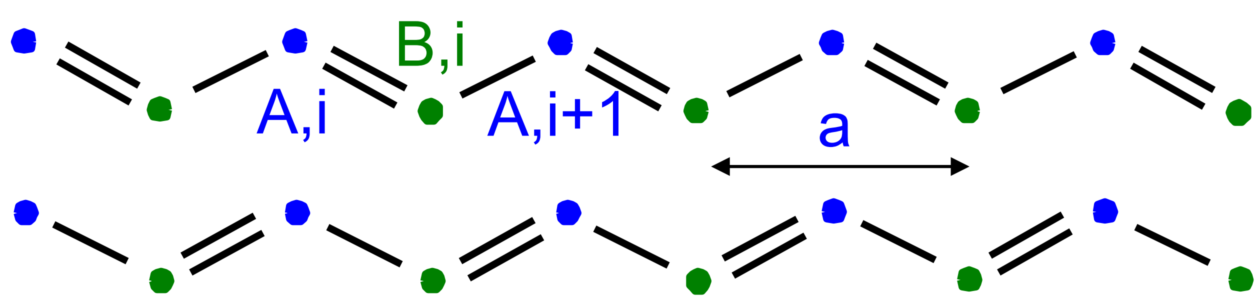
phonons lead to Peierls instability $\longrightarrow$ finite δt



two degenerate ground states:

$\delta t > 0$

$\delta t < 0$



in momentum space: $\mathcal{H}(k) = \boldsymbol{d}(k) \cdot \boldsymbol{\sigma} = \begin{pmatrix} 0 & h(k) \\ h^\dagger(k) & 0 \end{pmatrix}$

$$d_x(k) = (t+\delta t) + (t-\delta t)\cos k \qquad d_y(k) = (t-\delta t)\sin k \qquad d_z(k) = 0$$

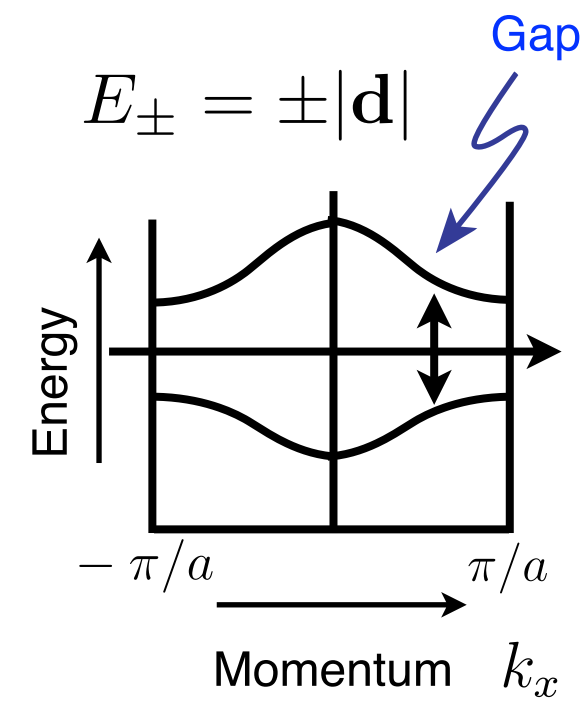
Sublattice symmetry: $\sigma_z \mathcal{H}(k) + \mathcal{H}(k)\sigma_z = 0 \longrightarrow d_z = 0$ (energy spectrum is symmetric)

Energy spectrum: $E_\pm = \pm|\mathbf{d}| = \pm\sqrt{2}\sqrt{t^2 + (\delta t)^2 + [t^2 - (\delta t)^2]\cos k}$

Polyacetylene (Su-Schrieffer-Heeger model)

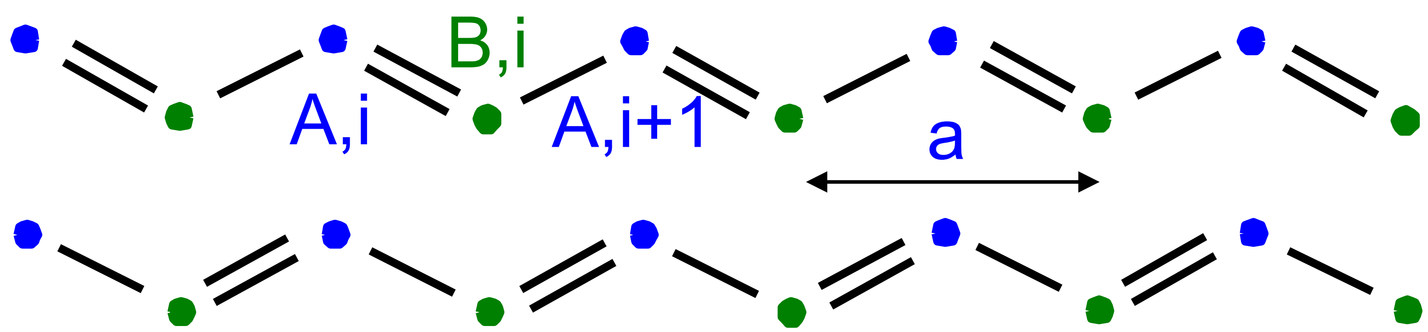
Su-Schrieffer-Heeger model describes polyacetylene $[\mathrm{C_2H_2}]_n$

$$E_{\pm} = \pm|\mathbf{d}|$$



$\delta t > 0$

$\delta t < 0$



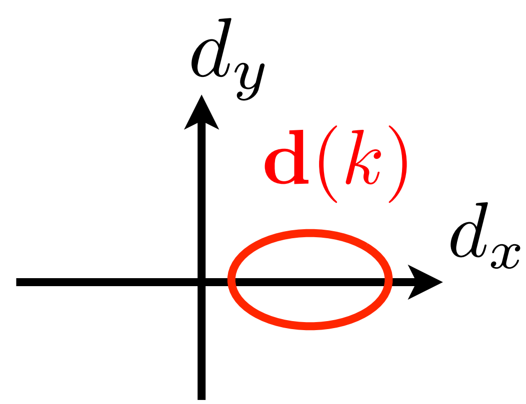
$$\mathcal{H}(k) = \boldsymbol{d}(k)\cdot\boldsymbol{\sigma} = \begin{pmatrix} 0 & h(k) \\ h^{\dagger}(k) & 0 \end{pmatrix}$$

$$d_x(k) = (t+\delta t) + (t-\delta t)\cos k$$

$$d_y(k) = (t-\delta t)\sin k \qquad d_z(k) = 0$$

Winding no: $\nu_1 = \frac{i}{2\pi}\int dk\,\left[q^{-1}\partial_k q\right]$

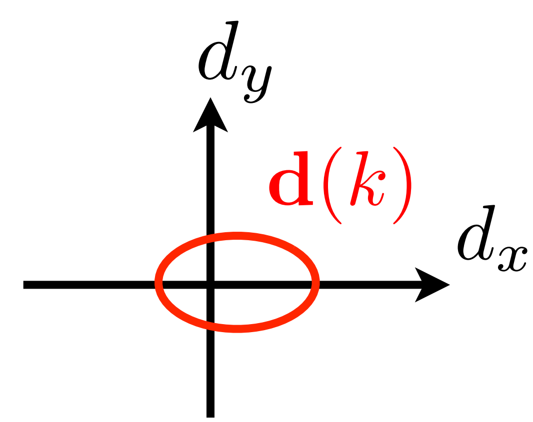
$$q(k) = \frac{h(k)}{|\mathbf{d}(k)|} \qquad q(k) : S^1 \longrightarrow S^1 \qquad \pi_1(S^1) = \mathbb{Z}$$



$\delta t > 0:$

Berry phase 0

$\nu_1 = 0$



$\delta t < 0:$

Berry phase π

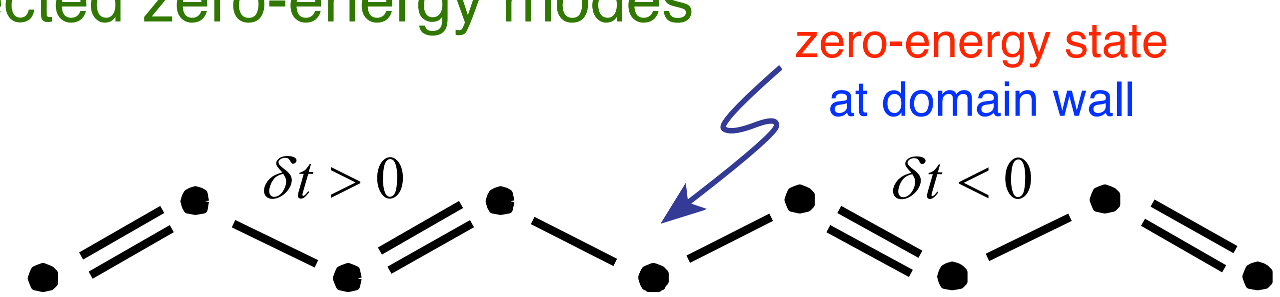
$\nu_1 = 1$

Provided $d_z = 0$ (required by sublattice symmetry) states with $\delta t > 0$ and $\delta t < 0$ are topologically distinct

Domain Wall States in Polyacetylene

Domain wall between different topological states has topologically protected zero-energy modes

[Su, Schreiffer, Heeger 79]
[Jackiw, Rebbi]



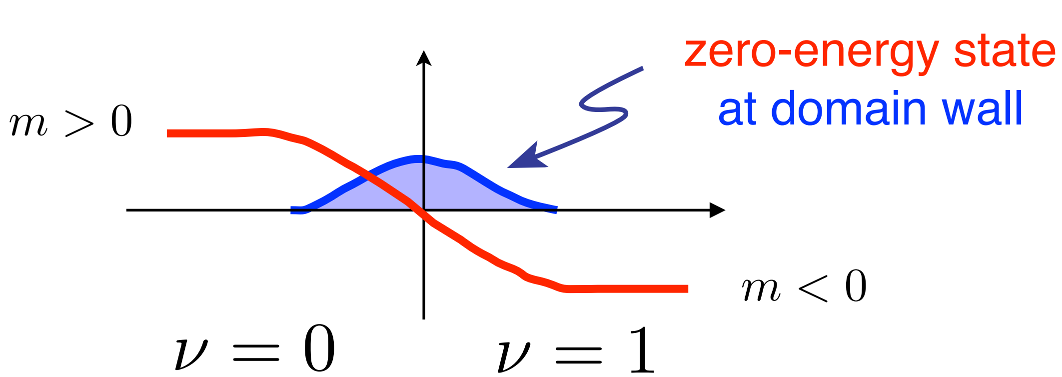
Effective low-energy continuum theory: (expand around $k_0 = \pi$) $k \to -i\partial_x$

$$H(x) = -i\sigma_y \partial_x + m(x)\sigma_x \qquad m(x) = 2\delta t$$

Dirac Hamiltonian with a mass: $E(q) = \pm\sqrt{q^2 + m^2}$

Sublattice symmetry ("chiral symmetry"): $\{\sigma_z, H\} = 0 \longrightarrow \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$

Consider domain wall:



Ansatz for boundstate: $\psi_0 = \chi e^{-\int_0^x m(x')dx'}$

$$H\psi_0 = 0 \Rightarrow \chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Bulk-boundary correspondence: $\Delta\nu = |\nu_{\rm R} - \nu_{\rm L}| = \#\,\text{zero modes}$ (topological invariant characterizing domain wall)

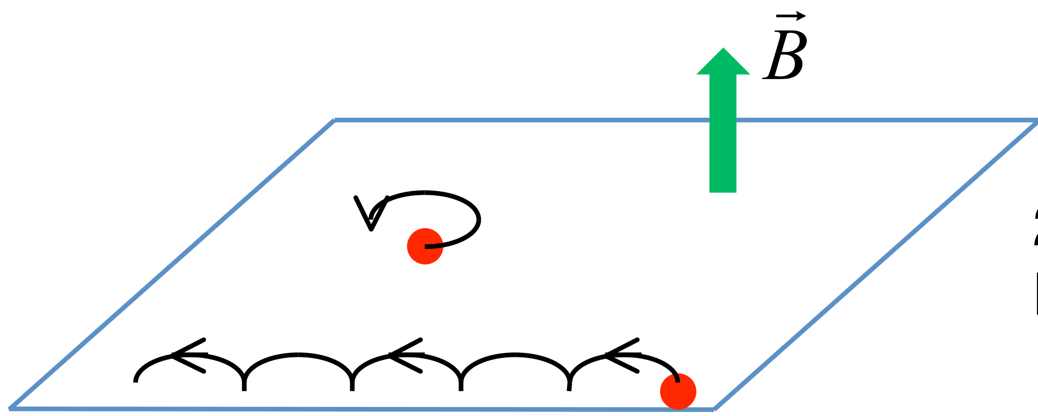
The Integer Quantum Hall State

Integer Quantum Hall State:

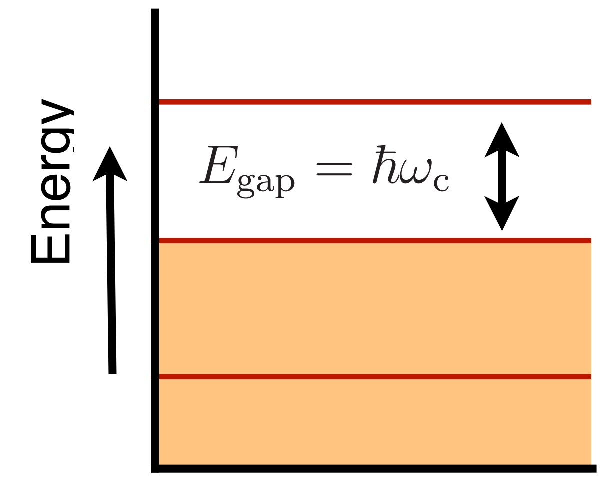
[von Klitzing '80]

First example of 2D topological material

- 2D electron gas in large magnetic field, at low T

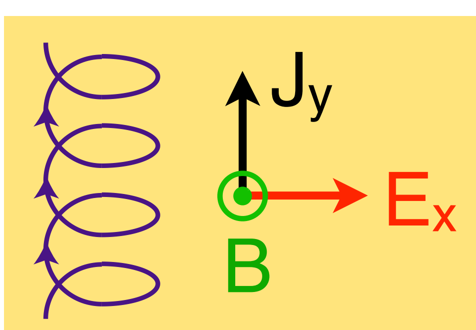


2D cyclotron motion
Landau levels

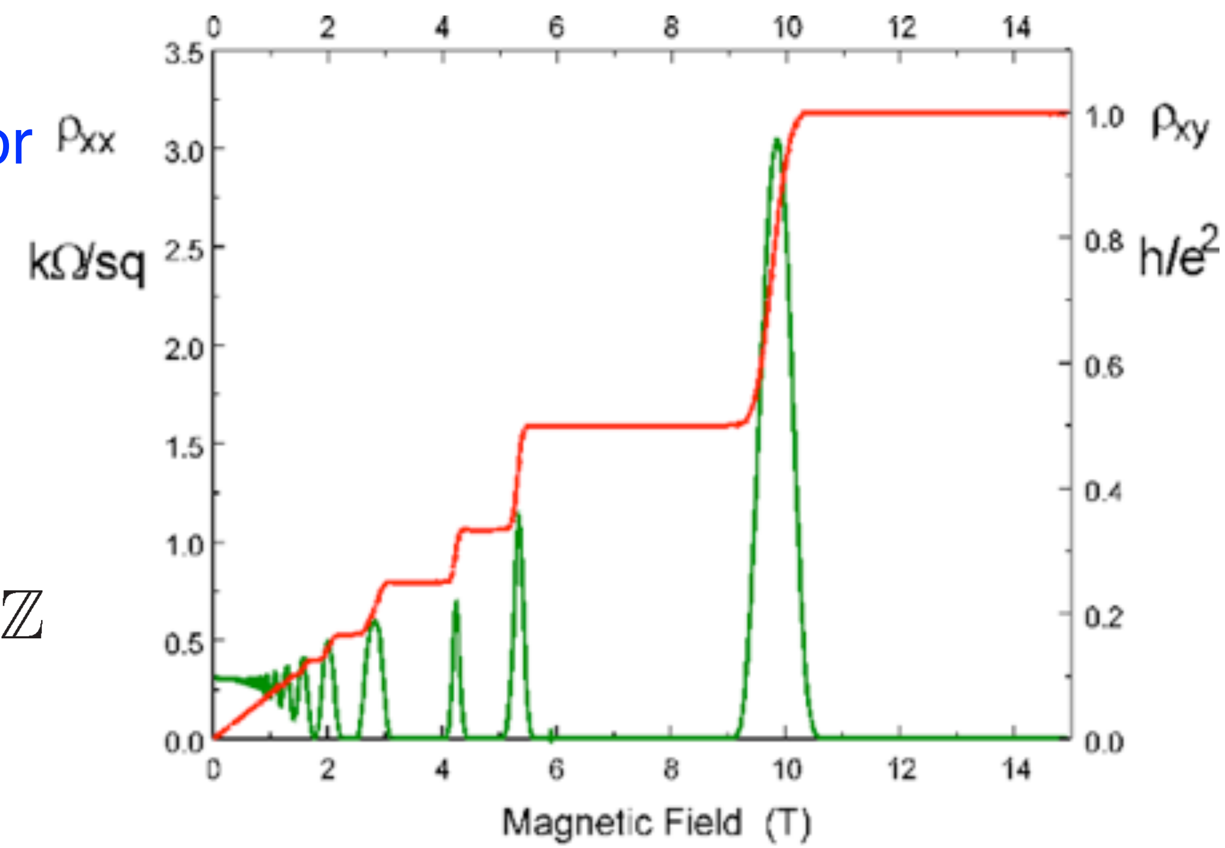


- There is an energy gap, but it is not an insulator

▶ Quantized Hall conductivity: $J_y = \sigma_{xy} E_x$



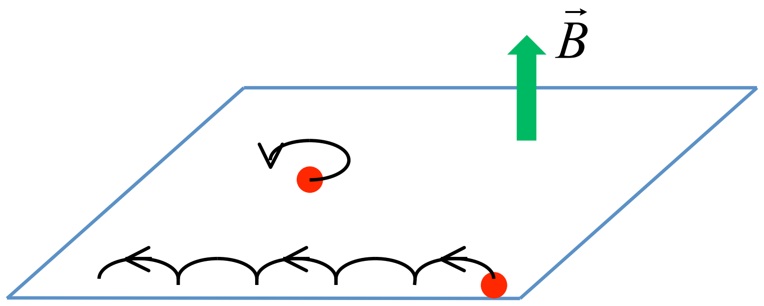
$$\sigma_{xy} = n\frac{e^2}{h} \qquad n \in \mathbb{Z}$$



- Plateaus in resistivity $\rho_{xy} = \frac{1}{n}\frac{h}{e^2}$

The Integer Quantum Hall State

What causes the precise quantization in IQHE?



Explanation One: Edge state transport

IQHE has an energy gap in the bulk:

— charge cannot flow in bulk; only along 1D channels at edges (chiral edge states)

— chiral edge state cannot be localized by disorder (no backscattering)

— edge states are perfect charge conductor!

Explanation Two: Topological band theory

Distinction between the integer quantum Hall state and a conventional insulator is a topological property of the band structure ***[Thouless et al, 84]***

$\mathcal{H}(\mathbf{k})$: Brillouin zone $\longmapsto$ Hamiltonians with energy gap

Classified by Chern number: $n = \frac{i}{2\pi} \sum_{\substack{\text{filled} \\ \text{states}}} \int \mathcal{F} d^2k$ (= topological invariant) $n \in \mathbb{Z}$

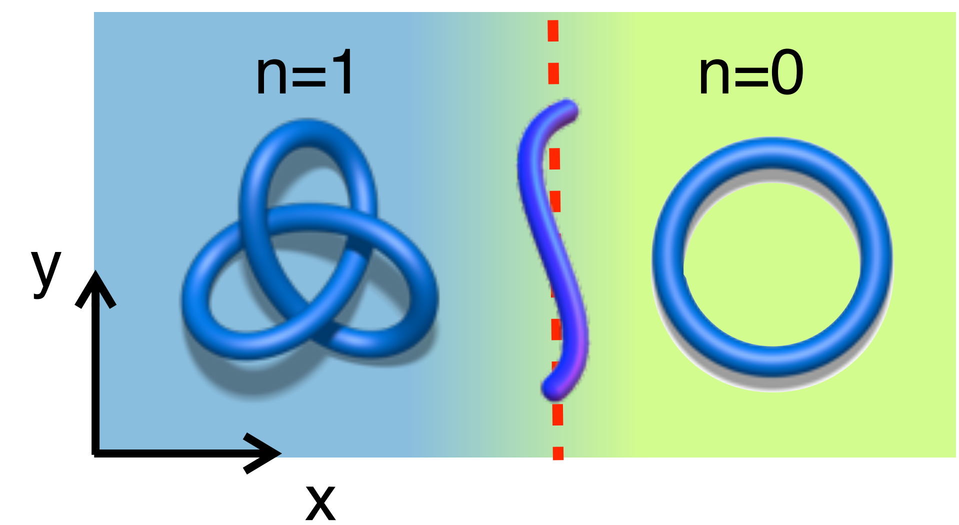
Kubo formula: $\boxed{\sigma_{xy} = \frac{e^2}{h} \frac{i}{2\pi} \sum_{\substack{\text{filled} \\ \text{states}}} \int \mathcal{F} d^2k}$

⟹ does not change under smooth deformations, as long as bulk energy gap is not closed

Bulk-boundary correspondence

topological invariant $n = \frac{i}{2\pi} \sum_{\substack{\text{filled} \\ \text{states}}} \int \mathcal{F} d^2k \qquad n \in \mathbb{Z}$

Zero-energy state at interface



Bulk-boundary correspondence:

Zero-energy states must exist at the interface between two different topological phases

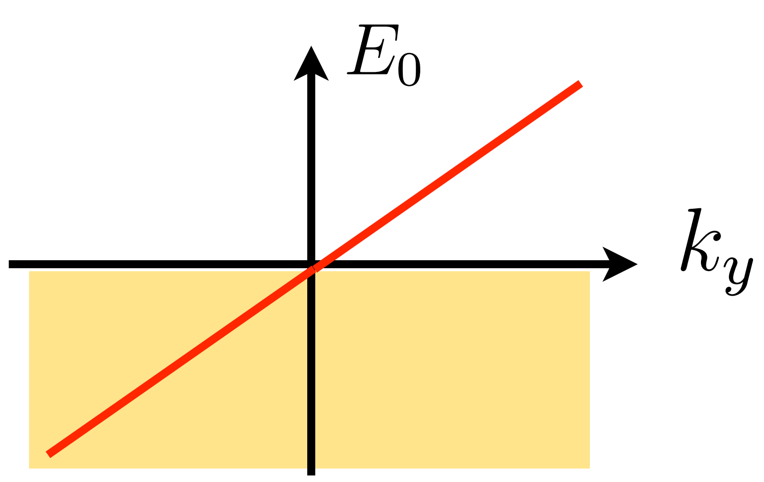
Follows from the quantization of the topological invariant.

$$\boxed{\Delta n = |n_{\mathrm{L}} - n_{\mathrm{R}}| \quad = \text{number or edge modes}}$$

Stable gapless edge states:

- robust to smooth deformations (respect symmetries of the system)
- insensitive to disorder, impossible to localize
- cannot exist in a purely 1D system (Fermion doubling theorem)

IQHE: chiral Dirac Fermion



Chern insulator on square lattice

Chern insulator = “integer quantum Hall state on a lattice”

[Bernevig, Hughes, Zhang]

(two orbital model: s and p.
Inter-orbital coupling
+ intra-orbital dispersion)

(similar to Haldane honeycomb model **[D. Haldane PRL ’88]**)

Chern insulator on square lattice: $\mathcal{H}_{\rm CI} = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma} + \epsilon_0(\mathbf{k}) \sigma_0$ (breaks time-reversal symmetry)

$$d_x(\mathbf{k}) = \sin k_x \qquad d_y(\mathbf{k}) = \sin k_y \qquad d_z(\mathbf{k}) = (2 + M - \cos k_x - \cos k_y)$$

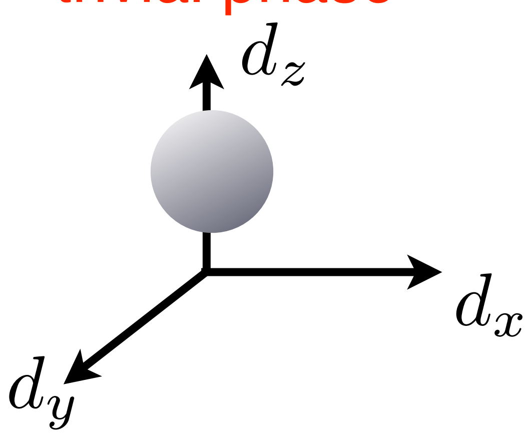
$$E_{\pm} = \pm |\mathbf{d}(\mathbf{k})|$$

Spectrum flattening: $\hat{\mathbf{d}}(\mathbf{k}) = \dfrac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|}$

trivial phase

$M > 0$ and $M < -4$

$n = 0$

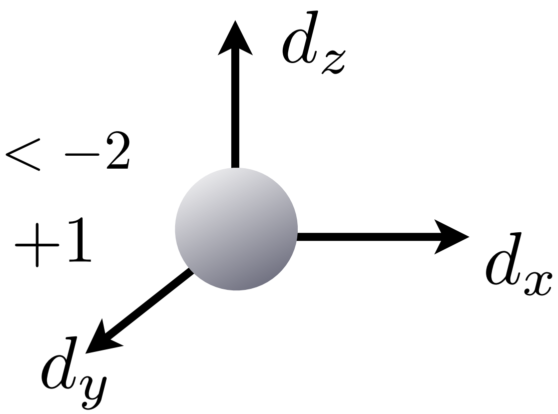


no edge state

non-trivial phase

$-4 < M < -2$

$n = +1$

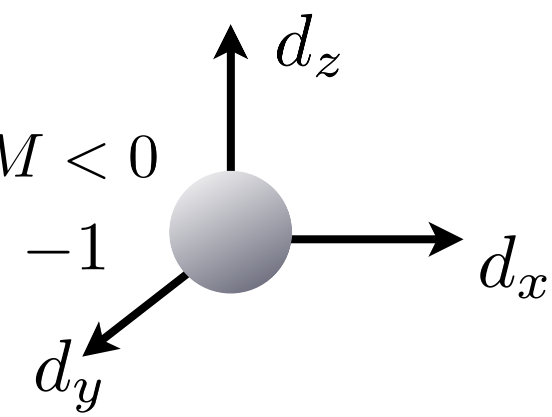


chiral edge state

non-trivial phase

$-2 < M < 0$

$n = -1$



chiral edge state

Chern number: (winding no) $n = \dfrac{1}{8\pi} \displaystyle\int_{\rm BZ} d^2\mathbf{k}\, \epsilon^{\mu\nu} \hat{\mathbf{d}} \cdot \left[\partial_{k_\mu} \hat{\mathbf{d}} \times \partial_{k_\nu} \hat{\mathbf{d}} \right]$ quantized Hall effect $\sigma_{xy} = \dfrac{e^2}{h} n$

Mapping $\hat{\mathbf{d}}(\mathbf{k})$: Brillouin zone $\longmapsto \hat{\mathbf{d}}(\mathbf{k}) \in S^2$ “$\pi_2(S^2) = \mathbb{Z}$”

Chern insulator on square lattice

Chern insulator on square lattice: $\mathcal{H}_{\text{CI}} = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma} + \epsilon_0(\mathbf{k})\sigma_0$

$$d_x(\mathbf{k}) = \sin k_x \qquad d_y(\mathbf{k}) = \sin k_y \qquad d_z(\mathbf{k}) = (2 + M - \cos k_x - \cos k_y)$$

Effective low-energy continuum theory for M=0: (expand around $\mathbf{k} = 0$; σ_0 term can be neglected)

$$H_{\text{CI}} = k_x\sigma_x + k_y\sigma_y + M\sigma_z$$

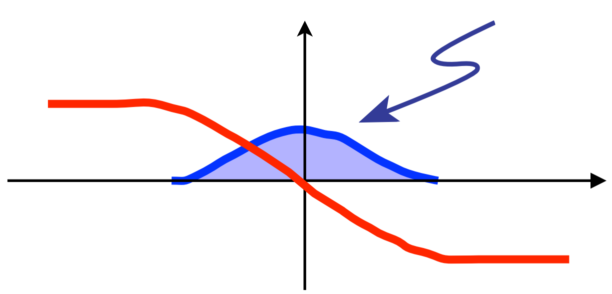
two eigenfunctions with energies: $E_\pm = \pm\lambda = \pm\sqrt{\mathbf{k}^2 + M^2}$

$$|u_{\mathbf{k}}^+\rangle = \frac{1}{\sqrt{2\lambda(\lambda - M)}} \begin{pmatrix} k_x - ik_y \\ \lambda - M \end{pmatrix} \qquad |u_{\mathbf{k}}^-\rangle = \frac{1}{\sqrt{2\lambda(\lambda + M)}} \begin{pmatrix} -k_x + ik_y \\ \lambda + M \end{pmatrix}$$

Berry curvature: $F_{xy} = \partial_{k_x} A_{k_y} - \partial_{k_y} A_{k_x} = +\dfrac{M}{2\lambda^3}$

gives nonzero Chern number
(= Hall conductance σ_{xy})

$$n = \frac{1}{2\pi}\int d^2k\, F_{xy} = \frac{1}{2}\text{sgn}(M)$$



NB: Chern number must be integer for integrals over compact manifolds.
Proper regularization of Dirac Hamiltonian will lead to $n \in \mathbb{Z}$

Chiral edge state at boundary between two Chern insulators with different n

$$\psi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ik_y y} e^{-\int_0^x M(x')dx'}$$