Boulder Summer School July 11-15, 2016

4 lectures × 1.5 hours.

Topological Insulators, Topological Band Theory

Outline:

0. Introduction: symmetry, topology and quantum phases.

I. Topological Band Theory

A. Topology in $d=1$

- berry phase, electric polarization
- SSH model
- domain wall states, Jackim Rebbi
- thouless charge pump

B. Topology in $d=2$

- Integer Quantum Hall Effect
- Chern number
- Edge States
- Graphene Model (Haldane)

C. Generalizations

- Weyl
- Higher D.
- Topological defects

II Topological Insulators in 2 dimensions

- Time Reversal Symmetry, Kramers' Theorem
- Graphene Model
- Z_2 "Helical" edge states
- Meaning of $\mathbb{Z}_2$
- Formula for $\mathbb{Z}_2$

III Topological Superconductivity

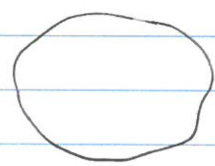
Lecture #1 7/11/16

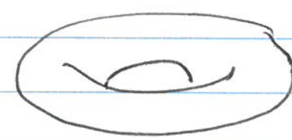
Symmetry: What changes leave a system invariant

- conceptual simplification
- conservation laws
- classify phases of matter according to broken symmetries
  - crystals (translations/rotations, reflections)
  - superconductor (gauge)

Topology: what stays the same when you deform

Classic example:





sphere: genus $g=0$ donut: $g=1$

Gauss-Bonnet Theorem

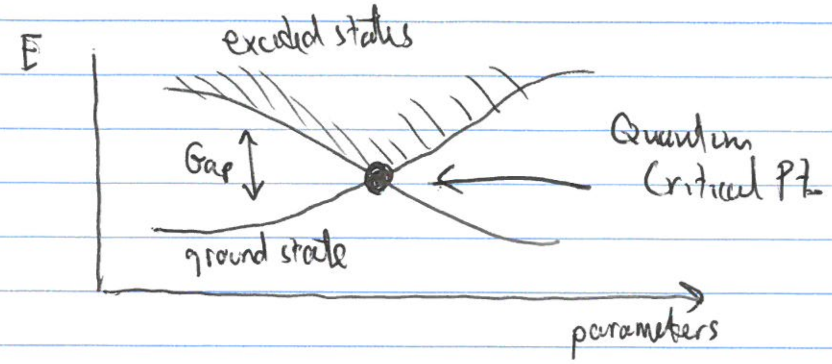
$$\int_S K\,dA = 4\pi(1-g)$$

gaussian curvature $\frac{1}{R_1R_2}$

Topological Phases of matter

Topological Equivalence $\longleftrightarrow$ Adiabatic continuity

Requires energy gap.



Goal: Classify and Characterize Topological Phases
with or without symmetries

Hard Problem: not completely solved.
- many body problem

Manageable Goal: Classify and Characterize "Single Particle Topological Phases"

- states adiabatically connected to free fermions: ground state is Slater determinant of single particle states.

- Describes interacting systems, provided interactions not "too large"

Further simplification: Crystalline matter.

$\Rightarrow$ Topological Band Theory

When band theory works it works really well.

Consequential Theory!

Topological Band Theory

Bloch Theorem: $\mathcal{H}|\psi\rangle = E|\psi\rangle \quad [\mathcal{H}, T(R)] = 0$

$$T(R)|\psi_k\rangle = e^{ik\cdot R}|\psi_k\rangle \Rightarrow |\psi\rangle = e^{ik\cdot r}|u_k\rangle$$

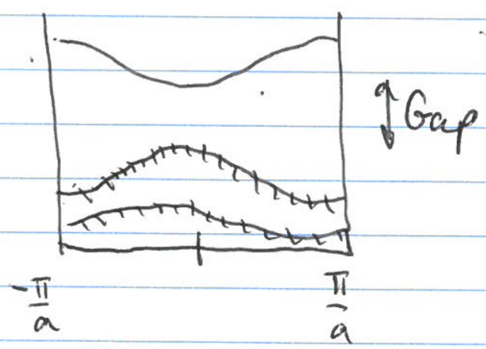
$$k \in BZ = T^d$$

defined in single unit cell, periodic

Bloch Hamiltonian

$$\mathcal{H}(k) = e^{-ik\cdot r}\mathcal{H}e^{ik\cdot r}$$: defined in single unit cell

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



"Band Structure"

Classify Gapped Band Structures $\mathcal{H}(k)$

We now have 1 body QM problem parameterized by k.

Berry Phase

Wave functions in QM have intrinsic phase ambiguity:

$$|u(k)\rangle \Rightarrow e^{i\phi(k)}|u(k)\rangle$$

Similar to electromagnetic gauge transformation, (except in momentum space rather than real space).

Berry Connection (like vector potential)

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

Under a gauge transformation

$$A \to A + \nabla_k \phi$$

Berry Phase: change in phase on closed loop C:

$$\gamma_C = \oint_C A \cdot dk = \int_S F\, d^2k$$

$$F = \vec{\nabla} \times \vec{A} = \text{"Berry Curvature"}$$

Gauge Invariant, like Magnetic Field.

Important Example: 2 level system

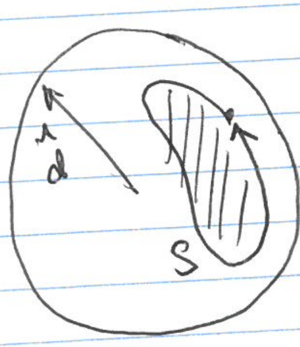
$$\mathcal{H}(k) = d_0(k)\mathbb{I} + \vec{d}(k) \cdot \vec{\sigma}$$

$$= \begin{pmatrix} d_0 + d_z & d_x - i d_y \\ d_x + i d_y & d_0 - d_z \end{pmatrix}$$

like a spin $\frac{1}{2}$ in a magnetic field.

$$\mathcal{H}(k) \left| u_\pm(k) \right\rangle = \pm \left| \vec{d}(k) \right| \left| u_\pm(k) \right\rangle$$

The state only depends on the direction $\hat{d}(k)$



$$\gamma_C = \frac{1}{2} \left(\begin{array}{c} \text{solid angle swept} \\ \text{out by } \hat{d}(k) \end{array} \right)$$

Example: rotate spin by 2π

$$\gamma_C = \pi$$

"My favorite minus sign"

Topology in One Dimension: Electric Polarization

Classical: $P = \dfrac{\text{dipole moment}}{\text{length}}$

Bound charge: $\rho_b = -\nabla \cdot P$

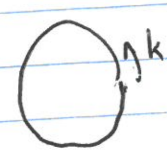
$Q_{end} = P \cdot \hat{n}$

How do you compute polarization in band theory?
Nontrivial problem.

Proposition: P is a Berry Phase

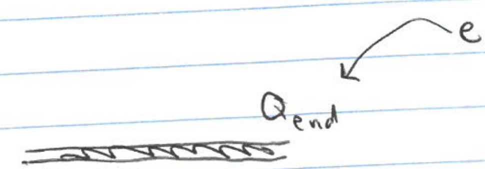
$$P = \frac{e}{2\pi} \oint_{BZ} A \cdot dk \qquad A = -i\langle u_k | \nabla_k | u_k \rangle$$

$BZ = S^1$



First argue that it makes sense. Then sketch a proof.

Intrinsic ambiguity:



- $Q_{end} = P \bmod e$

End charge only determined by bulk modulo e. Can add electron at end.

- Berry Phase under gauge transformation

$$|u_k\rangle \to e^{i\phi(k)} |u_k\rangle$$

$$\gamma = \oint A \cdot dk \to \gamma + \int_{-\pi/a}^{\pi/a} dk \cdot \nabla_k \phi(k) = \gamma + \phi(k)\Big|_{-\pi/a}^{\pi/a}$$

"Large" gauge transformation $\phi\left(\frac{\pi}{a}\right) - \phi\left(\frac{-\pi}{a}\right) = 2\pi n$.

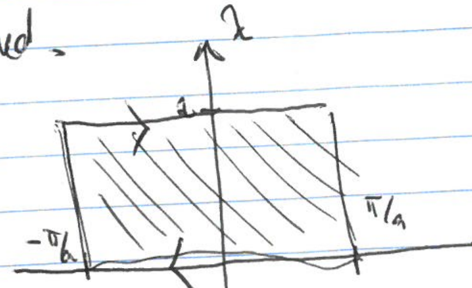
$$\gamma \to \gamma + 2\pi n$$

$$P \to P + ne$$

Possible because $BZ = S^1$ is not boundary of interior. It has a "hole" in it, can't use Stoke's Thm.

<u>Changes</u> in polarization are well defined.

$$|u(k)\rangle \Rightarrow |u(k, \lambda(t))\rangle$$



$$\Delta P = P(\lambda=1) - P(\lambda=0) = \frac{e}{2\pi}\oint A \cdot dk = \frac{e}{2\pi}\int dk\, d\lambda\, F$$

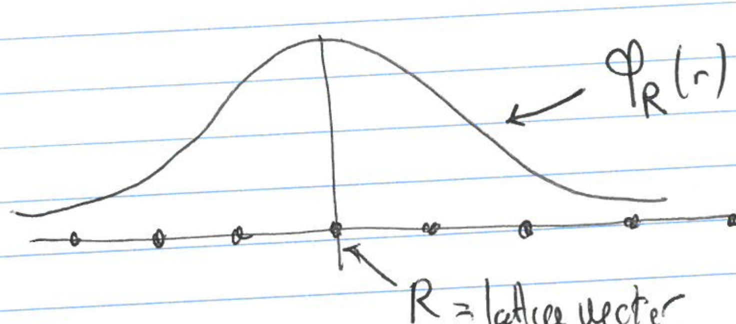
Compute $P := e\langle r \rangle$: dipole moment

$$\cancel{P \overset{?}{=} e\int \frac{dk}{2\pi} \langle u_k | r | u_k \rangle}$$: dipole moment density

But not well defined. Fix by defining localized Wannier States

Wannier States defined for each R : lattice vector

$$|\varphi(R)\rangle = \int_{BZ} \frac{dk}{2\pi}\, e^{-ik(R-\hat{r})} |u_k\rangle$$



localized for sufficiently smooth gauge

Gauge dependent, but localized.

$$P = e\langle \varphi(R) | r - R | \varphi(R) \rangle$$

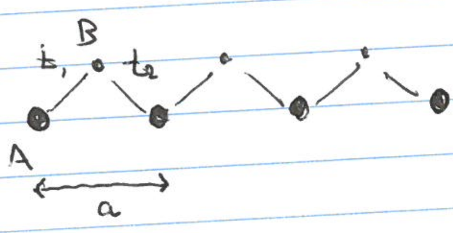
$$= \frac{ie}{2\pi} \oint_{BZ} \langle u(k) | \nabla_k | u(k) \rangle$$

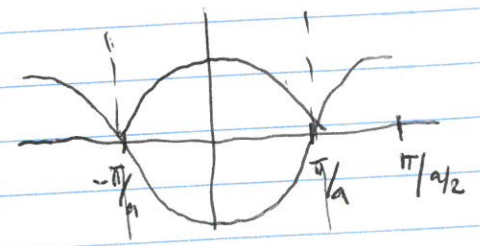
Su-Schrieffer-Heeger Model

- Model system for "polyacetalene" 1980's
- Simplest example for topological band phenomena
- 1D chain (spinless electrons)

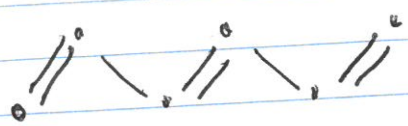
$$\mathcal{H} = \sum_i t_1 c^\dagger_{iA} c_{iB} + t_2 c^\dagger_{iB} c_{i+1\,A} + h.c.$$

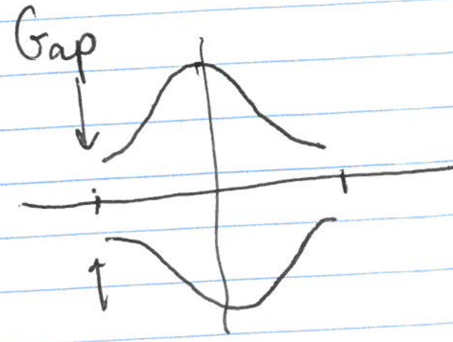
$t_1 = t_2$: 1D metal half filled band



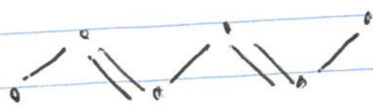


$t_1 > t_2$: "A phase"





$t_1 < t_2$: "B phase"



A and B are topologically distinct

Solve by Fourier Transform

$$\mathcal{H} = \sum_k c_{kA}^\dagger c_{kB} \left(t_1 + t_2 e^{ika} \right) = \sum_k h_{ab}(k)\, c_{ka}^\dagger c_{kb}$$

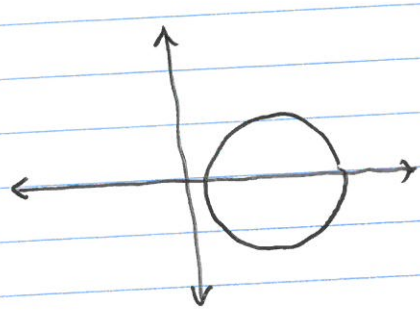
$$h(k) = \vec{d}(k) \cdot \vec{\sigma}$$

$$d_x = t_1 + t_2 \cos ka$$

$$d_y = -t_2 \sin ka$$

$$d_z = 0$$

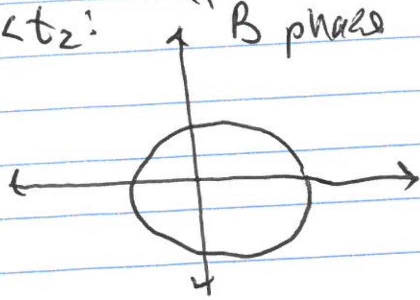
$t_1 > t_2$: "A phase"



Berry Phase 0

$P = 0$

$t_1 < t_2$: "B phase"

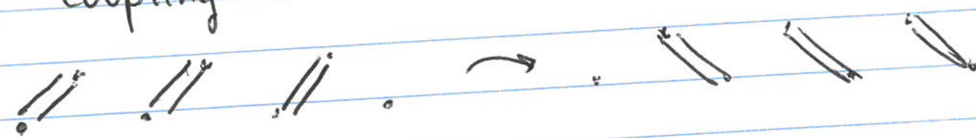


Berry Phase π

$$P = \frac{e}{2}$$

Comments:

1) Easy to understand polarization in strong coupling limit.



Move e over by 1/2.

2.) Gauge dependent. Trade off:

1. Gauge violates $A \leftrightarrow B$ sublattice symmetry

2. Gauge satisfies $\mathcal{H}(k+G) = \mathcal{H}(k)$

Can't have both.

3.) A and B are topologically distinct

provided $d_z = 0 \Rightarrow$ Quantized P

But that requires symmetry

Symmetries of SSH model

1. "Chiral Symmetry"

$$\{\mathcal{H}(k), \sigma^z\} = 0$$

- Artificial symmetry in polyacetalene. Consequence of bipartite lattice with only $A \to B$ hopping.

$$c_A \to c_A, \quad c_B \to -c_B \quad \Rightarrow \mathcal{H} \to -\mathcal{H}.$$

- Requires $d_z = 0$

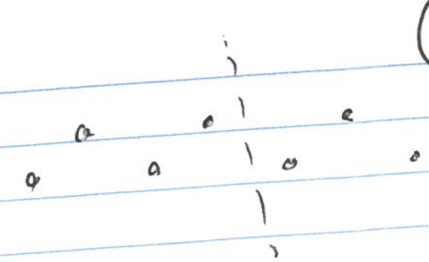
  $\Rightarrow$ Integer Topological invariant (= winding number of $d(k)$)

- Leads to particle-hole symmetric spectrum

$$\mathcal{H}\, \sigma_z |\psi_E\rangle = -\sigma_z \mathcal{H} |\psi_E\rangle = -E\, \sigma_z |\psi_E\rangle$$

$$\sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$$

2. Reflection Symmetry



$$\mathcal{H}(-k) = \sigma_x \mathcal{H}(k) \sigma_x$$

- Real symmetry of polyacetylene
- Allows $d_z(k) \neq 0$, but requires

$$d_x(-k) = d_x(k)$$

$$d_{y,z}(-k) = -d_{y,z}(k)$$

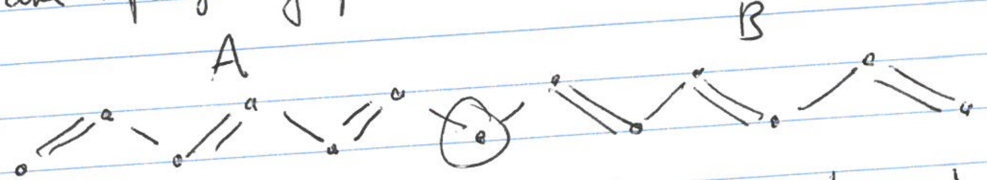
- No p-h symmetry, but polarization is quantized

$$P = -P \quad (\text{mod } e)$$

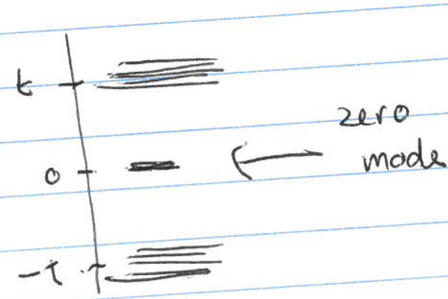
$$P = 0 \text{ or } \frac{e}{2} \Rightarrow \mathbb{Z}_2 \text{ topo. invariant.}$$

Domain Wall States

At the interface between different topological states there are topologically protected midgap states



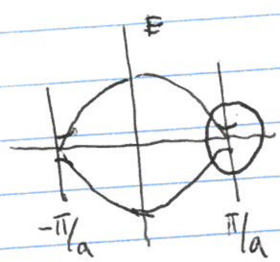
Simplest in strong coupling limit : $t_{min} = 0$, $t_{max} = t$



Chiral symmetry : zero mode persists even for $0 \leq t_{min} < t_{max}$

Instructive to consider opposite limit $t_1 - t_2 \ll t_{1,2}$

$\Longrightarrow$ Low energy continuum theory



For $k = \frac{\pi}{a} + q$:

$$d_x = t_1 - t_2$$

$$d_y = t_2 a q$$

$$v_F = t_2 a$$

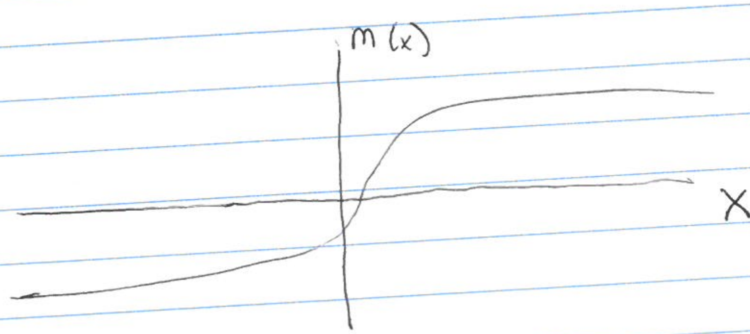
$$H = v_F q \sigma_y + m \sigma_x \qquad m = t_1 - t_2$$

$$E_{\pm}(q) = \pm\sqrt{v_F^2 q^2 + M^2}$$

Now allow spatial variation: $q \to -i\partial_x$

$$\mathcal{H} = -iv_F\sigma^y\partial_x + m(x)\sigma^x \quad : \quad \text{1+1D massive Dirac Eq.}$$

Domain Wall State (Jackiw & Rebbi)



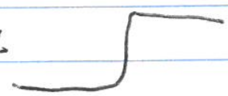
Solve for zero mode

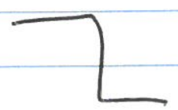
$$\frac{i}{v_F}\sigma^y\left[-iv_F\sigma^y\partial_x + m(x)\sigma^x\right]\psi = 0$$

$$\left[\partial_x + \frac{m(x)}{v_F}\sigma^z\right]\psi = 0$$

For $\sigma^z = \pm 1$ solution is

$$\psi_{\pm} = e^{\mp\int_0^x \frac{m(x')}{v_F}dx'}\,\phi_{\pm} \qquad \begin{pmatrix}1\\0\end{pmatrix} \text{ or } \begin{pmatrix}0\\1\end{pmatrix}$$

+ kink:  $\psi_+ = e^{-\int_0^{|x|} \frac{m}{v} dx'} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

- kink  $\psi_- = e^{+\int_0^{|x|} \frac{m(x')}{v} dx'} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

} normalizable states

Exact zero energy states independent of details.

Topological insulating states in 1D required symmetry (chiral or reflection). Without symmetry all 1D insulators are equivalent.

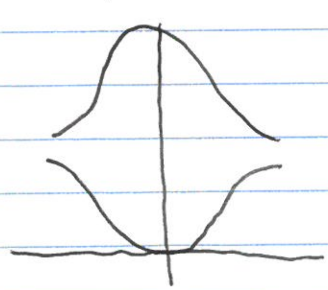
But there is a topological phenomenon in 1D:

Thouless Charge Pump

Adiabatic cycle in 1D insulator. Since P is defined mod e, the integer can change.

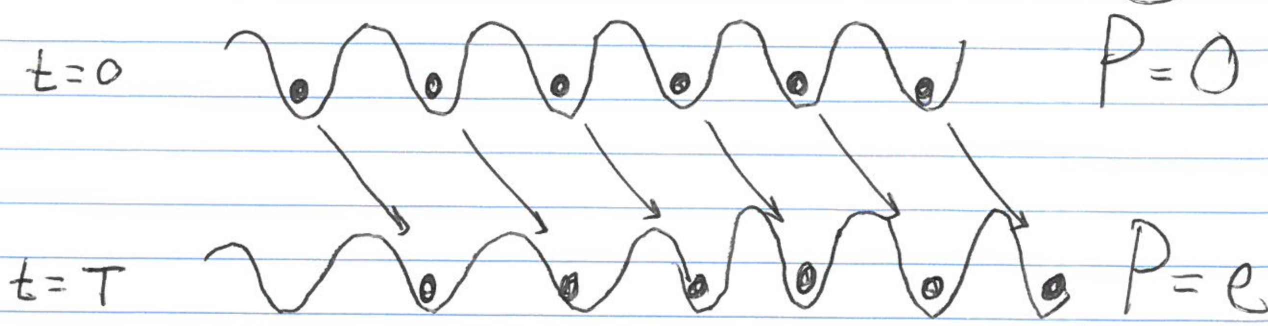
$$\mathcal{H}(k, t+T) = \mathcal{H}(k, t)$$

Example: Nearly free electron gas



$$V_G = V_0 e^{i\phi(t)}$$; phase of periodic potential

$$\phi(t) = \frac{2\pi}{T} t$$

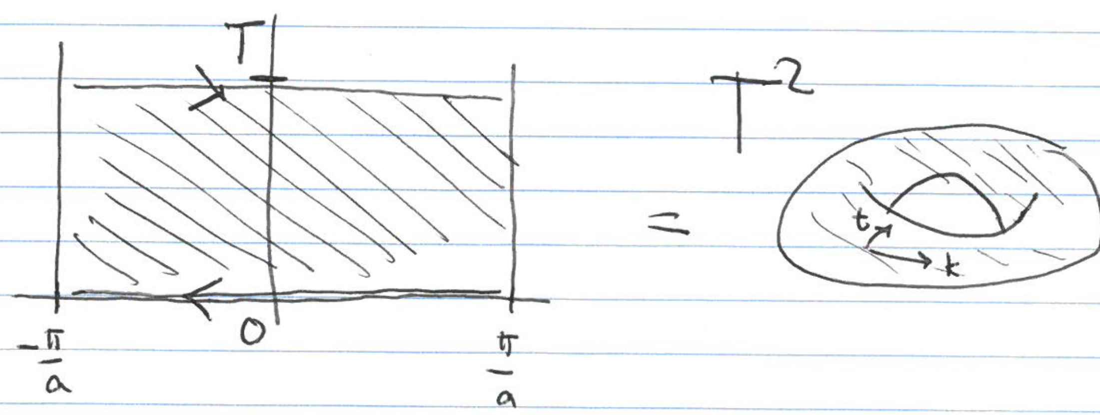


Since the system is periodic $\Delta P = n\,e$

n is an integer topological invariant characterizing the cycle.

Compute:

$$\Delta P = \frac{e}{2\pi}\left[\oint A(k,T)\,dk - \oint A(k,0)\,dk\right] = \frac{e}{2\pi}\int F\,d^2k$$



$$\cancel{n = \frac{1}{2\pi}\int_{T^2} F\,d^2k}$$

Since $\mathcal{H}(k,T)=\mathcal{H}(k,0)$,

$$|u(k,T)\rangle = e^{i\phi(k)}|u(k,0)\rangle$$

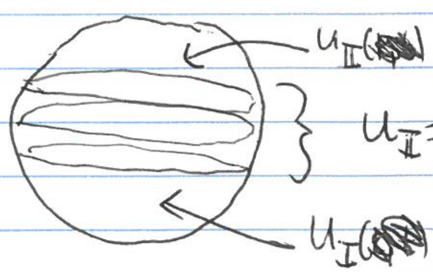
$$\oint \left(A(k,T)-A(k,0)\right)dk = \oint \nabla\phi(k) = 2\pi n$$

$$n = \frac{1}{2\pi}\int F\, d^2k \in \mathbb{Z}$$

Chern Number

- Integer topological invariant characterizing $|u(k,t)\rangle$ for $(k,t)\in T^2$ (or any closed 2D space)
- n is the obstruction to defining $|u(k,t)\rangle$ smoothly throughout T^2.

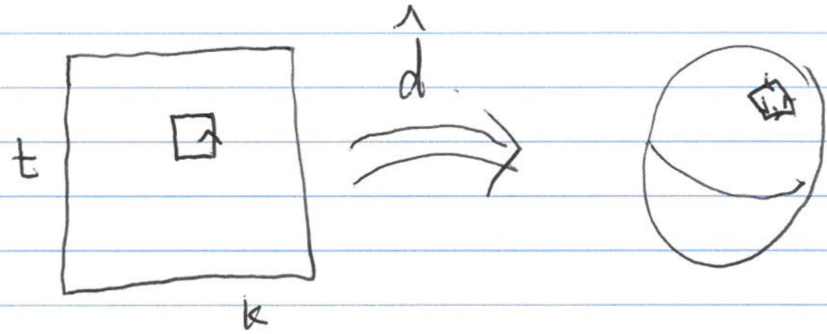
A smooth gauge can be defined on open patches, but they are related by a non trivial (large) gauge transformation



$$u_{II} = u_I e^{i\phi} \qquad \frac{1}{2\pi}\oint\nabla\phi = n$$

Two level system

$$\mathcal{H}(k,t) = \vec{d}(k,t)\cdot\vec{\sigma} + d_0(k,t)\,\mathbb{1}$$



$$F(k,t)\,dk\,dt \Longrightarrow \frac{1}{2}\text{ Solid angle}$$

$$= \frac{1}{2}\,\hat{d}\cdot\left(\partial_k\hat{d}\times\partial_t\hat{d}\right)dk\,dt$$

$$n = \frac{1}{2\pi}\int F\,dk\,dt = \frac{1}{4\pi}\times\underbrace{\int \hat{d}\cdot\left(\partial_k\hat{d}\times\partial_t\hat{d}\right)dk\,dt}_{\text{total solid angle}}$$

= Wrapping number for

$$\hat{d} : T^2 \to S^2$$

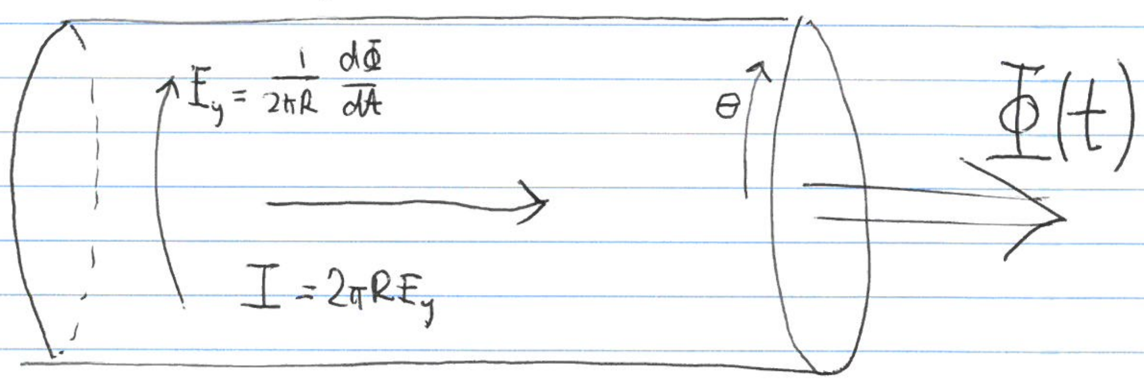
Integer Quantum Hall Effect : Laughlin Argument

2D "Insulator" $\quad \sigma_{xx} = 0 \quad \vec{J} = \sigma_{xy}\, \hat{z} \times \vec{E}$

$\sigma_{xy} \neq 0$

What values can σ_{xy} have?

Consider a cylinder



$$\Phi(t=0) = 0$$

$$\Phi(t=T) = \phi_0 = h/e \quad : \text{Magnetic flux quantum}$$

(1) A magnetic flux quantum threading a hole can be eliminated by a "large" gauge transformation

$$\psi(\vec{r}) \Rightarrow \psi(\vec{r})\, e^{i\theta(\vec{r})}$$

$$\vec{A}_{em} \Rightarrow \vec{A}_{em} + \frac{\hbar}{e} \nabla\theta$$

$$\Phi = \oint A \cdot dl \Rightarrow \Phi + \underbrace{2\pi \hbar/e}_{\phi_0}$$

Thus

$$H(T) = U^{\dagger} H(0) U$$: Similar to a thouless charge pump.

$$\Rightarrow \Delta Q = ne$$

Current :

$$I_x(t) = \sigma_{xy} E_y(t) \cdot 2\pi R$$

$$= \sigma_{xy} \frac{d\Phi}{dt}$$

$$\Delta Q = \int_0^T dt \frac{dI}{dt} = \sigma_{xy} \left(\Phi(T) - \Phi(0) \right)$$

$$= \sigma_{xy} \frac{h}{e}$$

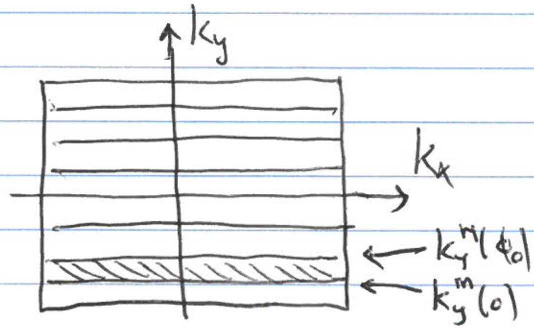
$$= ne$$

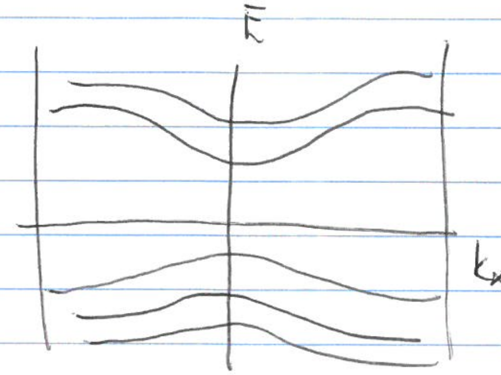
Conclude $\sigma_{xy} = n \frac{e^2}{h}$

TKNN Invariant

View cylinder as 1D systems with sub bands indexed by quantized k_y:

$$k_y^m(\Phi) = \frac{1}{R}\left(m + \frac{\Phi}{\phi_0}\right)$$





Treat as Thouless Pump

$$\Delta Q = \sum_m \frac{e}{2\pi} \int_0^{\phi_0} d\Phi \int dk_x \, F(k_x, k_y^m(\Phi))$$

$$= \frac{e}{2\pi} \int_{BZ} d^2k \, F(k_x, k_y) = ne$$

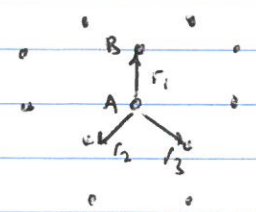
Chern number $\quad n = \frac{1}{2\pi} \int d^2k \, F \quad$ characterizes a 2D band structure $\mathcal{H}(k_x, k_y)$

Distinguishes topologically distinct 2D band structures
Analogous to Gauss Bonnet.

Alternative calculation (TKNN):

Compute σ_{xy} via Linear Response (Kubo)

Model System: Graphene



Two band model $\mathcal{H} = -t \sum_{\langle ij \rangle} c_{iA}^{\dagger} c_{jB} = \sum_k c_{ka}^{\dagger} c_{kb} h_{ab}$

$$h_{ab} = \cancel{\Sigma}\,{-t} \begin{pmatrix} 0 & \sum_j e^{ik\cdot r_j} \\ \sum_j e^{-ik\cdot r_j} & 0 \end{pmatrix} = \vec{d}(k)\cdot\vec{\sigma}$$

$$d_x = -t \sum_j \cos k\cdot r_j$$
$$d_y = -t \sum_j \sin k\cdot r_j$$
$$d_z = 0$$

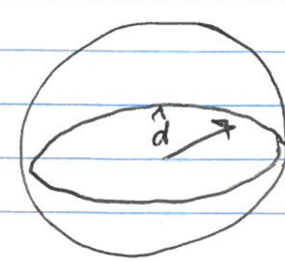
Symmetries:

1. Chiral $\{\mathcal{H}, \sigma_z\} = 0$ (artificial)

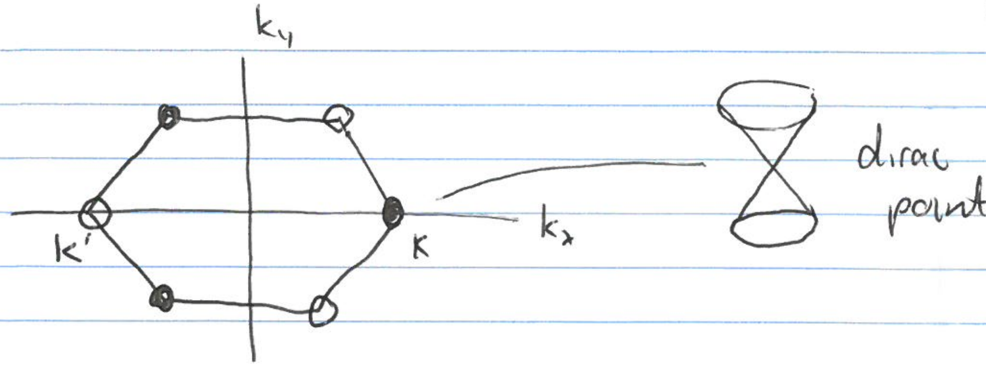
2. P : $\mathcal{H}(-k) = \sigma_x \mathcal{H}(+k) \sigma_x \Rightarrow d_z(-k) = -d_z(k)$

3. T : $\mathcal{H}(-k) = \mathcal{H}(k)^{*} \Rightarrow d_z(-k) = +d_z(k)$

$PT \Rightarrow d_z = 0 \qquad \hat{d} \in S^1$



Allows point defects in $\vec{d}(k)$.

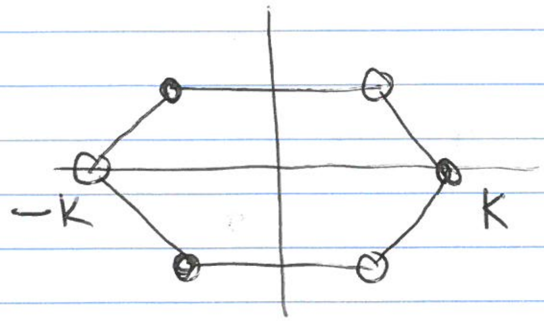


Dirac Points: $\vec{d}(k) = 0$ for $k = \pm K$

$$\mathcal{H}(K+q) = v\,\vec{\sigma}\cdot q$$ Massless Dirac Hamiltonian

Crystal symmetry fixes Dirac point at K, K'. Lowering symmetry (keeping PT) allows them to move, but they remain protected by PT. (π Berry phase)

Dirac Points are interesting, but they also provide a route to realizing interesting gapped phases when symmetry is lowered.



Dirac Points: $\vec{d}(\pm K) = 0$

$$\mathcal{H}(\pm K + q) = v_F(\pm \sigma_x q_x + \sigma_y q_y)$$ Massless Dirac Hamiltonian

Crystal symmetry fixes Dirac Point at K, K'. Lowering symmetry (keeping PT) allows them to move, but they remain protected. Berry phase = $0, \pi$.

Dirac points are interesting, but they also provide a route to interesting gapped states when symmetry is lowered.

Gapped Phases of Graphene

Break P or T

$$\mathcal{H}(\pm K + q) = v_F(\pm \sigma_x q_x + \sigma_y q_y) + m_\pm \sigma_z$$

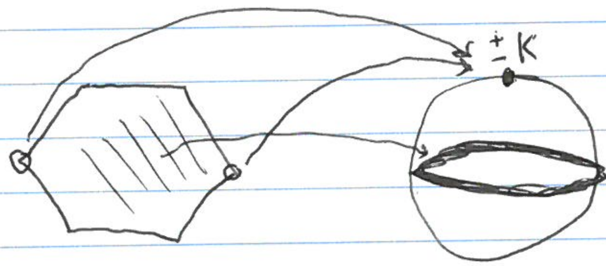
$$E(q) = \pm\sqrt{v_F^2 q^2 + m_\pm^2}$$

Chern Number:

n = Wrapping # for $\hat{d}(\vec{k})$

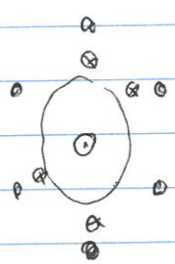
1. Break P (eg BN) keep T

$$\Delta\mathcal{H} = m\sigma_z \qquad m_+ = m_-$$



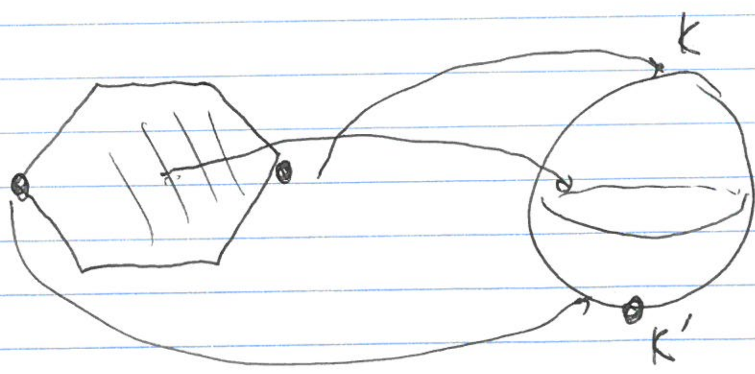
$n = 0$: Trivial Insulator

2. Break T (keep P) : Haldane '88



Periodic $B(\vec{r}) = 0$ on average.

$$m_+ = -m_-$$

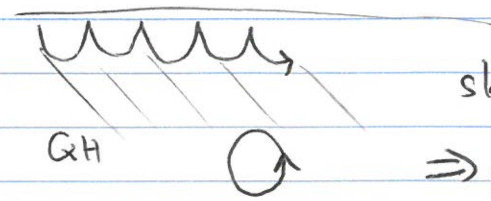


$n = 1$

Quantum Hall State

Edge States

Classical Picture

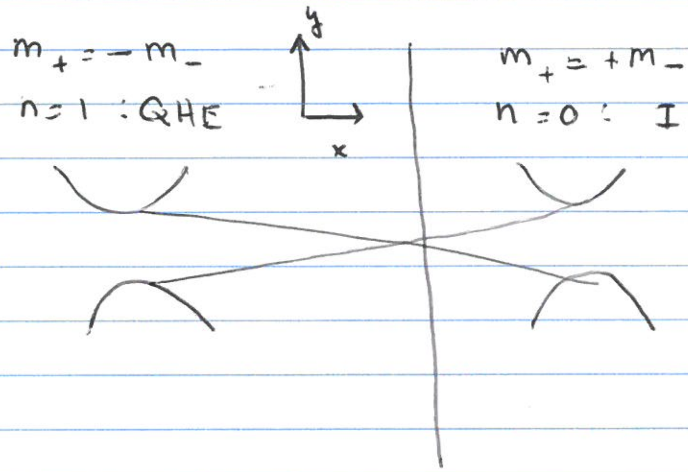


skipping orbit

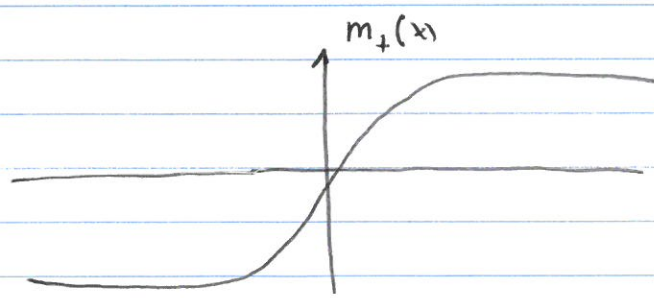
$\Rightarrow$ propagating state

"one way"

Topological boundary modes



band inversion

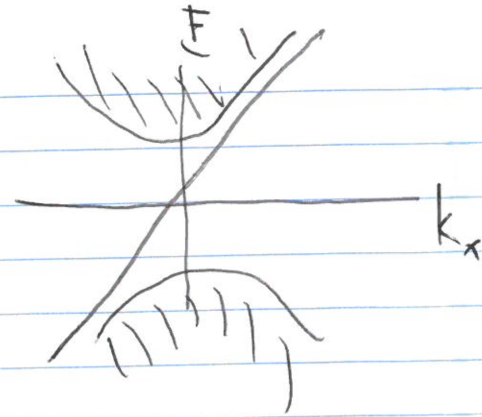


$$\mathcal{H} = v_F\left(-i\sigma_x \partial_x + k_y \sigma_y\right) + m_+(x)\,\sigma_z$$

Same as Jackiw-Rebbi for fixed k_y.

Zero mode $|\psi\rangle = e^{ik_y y}\, e^{-\int^{|x|} \frac{m_+(x)}{v}} \,|\sigma_y +\rangle$

$E|\psi\rangle = +v_F k_y |\psi\rangle$



chiral Dirac fermion

Other edge: $|\psi\rangle \propto |\sigma^y_-\rangle$

$E = -v_F k_y$

Chiral Dirac Fermion

1. One way : no choice but to go forward
2. Robust : Insensitive to disorder (nowhere to go)
   Impossible to localize
3. Impossible in purely 1D :
   Fermion doubling thm: What goes up must go down
   Evaded by spatially separating right & left movers.