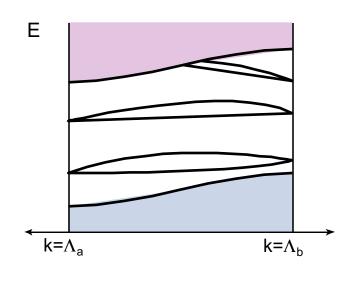
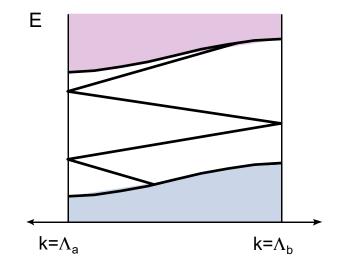
# Symmetry, Topology and Phases of Matter











# **Topological Phases of Matter**

### Many examples of topological band phenomena

States adiabatically connected to independent electrons:

- Quantum Hall (Chern) insulators
- Topological insulators
- Weak topological insulators
- Topological crystalline insulators
- Topological (Fermi, Weyl and Dirac) semimetals .....

Topological superconductivity (BCS mean field theory)

- Majorana bound states
- Quantum information

Classical analogues: topological wave phenomena

- photonic bands
- phononic bands
- isostatic lattices

Many real materials and experiments

### Beyond Band Theory: Strongly correlated states

State with intrinsic topological order (ie fractional quantum Hall effect)

- fractional quantum numbers
- topological ground state degeneracy
- quantum information
- Symmetry protected topological states
- Surface topological order ......

Much recent conceptual progress, but theory is still far from the real electrons

# **Topological Band Theory**

### Topological Band Theory I:

Introduction

Topologically protected gapless states (without symmetry)

### Topological Band Theory II:

Time Reversal symmetry

Crystal symmetry

Topological superconductivity

10 fold way

#### **Topological Mechanics**

#### General References:

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"Colloquium: Topological Insulators"
```

M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).

"Topological Band Theory and the Z<sub>2</sub> Invariant,"

C. L. Kane in "Topological insulators"

edited by M. Franz and L. Molenkamp, Elsevier, 2013.

# Topology and Band Theory I

#### I. Introduction

- Insulating state, topology and band theory

### II. Band Topology in One Dimension

- Berry phase and electric polarization
- Su Schrieffer Heeger model
- Domain walls, Jackiw Rebbi problem
- Thouless charge cump

#### III. Band Topology in Two Dimensions

- Integer quantum Hall effect
- TKNN invariant
- Edge states, chiral Dirac fermions

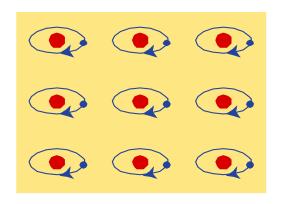
#### IV. Generalizations

- Higher dimensions
- Topological defects
- Weyl semimetal

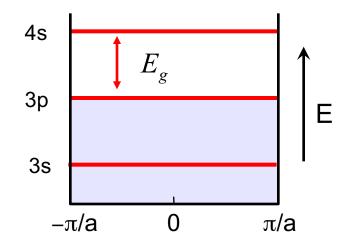
## Insulator vs Quantum Hall state

### The Insulating State

atomic insulator

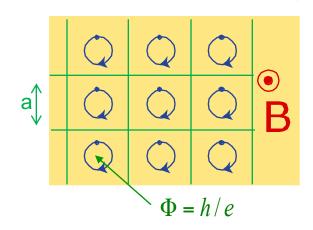


atomic energy levels

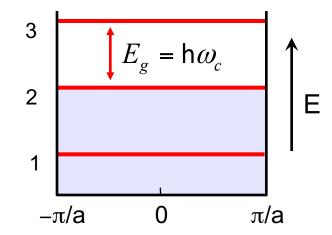


### The Integer Quantum Hall State

2D Cyclotron Motion,  $\sigma_{xy} = e^2/h$ 



Landau levels



What's the difference? Distinguished by Topological Invariant

# Topology

The study of geometrical properties that are insensitive to smooth deformations

Example: 2D surfaces in 3D

A closed surface is characterized by its genus, g = # holes



g is an integer topological invariant that can be expressed in terms of the gaussian curvature  $\kappa$  that characterizes the local radii of curvature

$$K = \frac{1}{r_1 r_2} \qquad \left( \kappa = \frac{1}{r^2} > 0 \right) \qquad \left( \kappa = 0 \right)$$

Gauss Bonnet Theorem :  $\int_{S} \kappa dA = 4\pi (1-g)$ 

A good math book: Nakahara, 'Geometry, Topology and Physics'

# Band Theory of Solids

### Bloch Theorem:

Lattice translation symmetry 
$$T(\mathbf{R})|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}|\psi\rangle$$
  $|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u(\mathbf{k})\rangle$ 

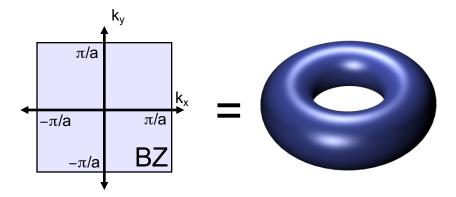
$$|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u(\mathbf{k})|$$

**Bloch Hamiltonian** 

$$H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}}$$
  $H(\mathbf{k})|u_n(\mathbf{k})\rangle = E_n(\mathbf{k})|u_n(\mathbf{k})\rangle$ 

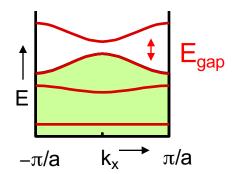
k∈ Brillouin Zone = Torus,  $T^d$ 



### Band Structure:

A mapping  $\mathbf{k}$  a  $H(\mathbf{k})$ 

(or equivalently to  $E_n(\mathbf{k})$  and  $|u_n(\mathbf{k})\rangle$ )

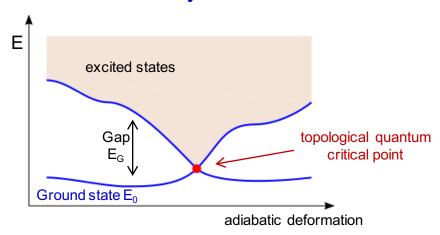


# **Topology and Quantum Phases**

#### Topological Equivalence: Principle of Adiabatic Continuity

Quantum phases with an energy gap are topologically equivalent if they can be smoothly deformed into one another without closing the gap.

Topologically distinct phases are separated by quantum phase transition.



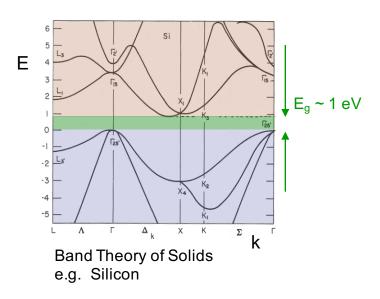
#### **Topological Band Theory**

Describe states that are adiabatically connected to non interacting fermions

Classify single particle Bloch band structures

 $H(\mathbf{k})$ : Brillouin zone (torus) a

Bloch Hamiltonans with energy gap



# **Berry Phase**

Phase ambiguity of quantum mechanical wave function

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

Berry connection : like a vector potential  $\mathbf{A} = -i \langle u(\mathbf{k}) | \nabla_{\mathbf{k}} | u(\mathbf{k}) \rangle$ 

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla_{\mathbf{k}} \phi(\mathbf{k})$$

Berry phase : change in phase on a closed loop C  $\gamma_C = \int_C \mathbf{A} \cdot d\mathbf{k}$ 

Berry curvature: 
$$\mathbf{F} = \nabla_{\mathbf{k}} \times \mathbf{A}$$
  $\gamma_C = \int_S \mathbf{F} d^2 k$ 

Famous example: eigenstates of 2 level Hamiltonian

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \overset{\mathbf{r}}{\sigma} = \begin{pmatrix} d_z & d_x - id_y \\ d_x + id_y & -d_z \end{pmatrix}$$

$$H(\mathbf{k}) |u(\mathbf{k})\rangle = + |\mathbf{d}(\mathbf{k})| |u(\mathbf{k})\rangle$$

$$\gamma_C = \frac{1}{2} \left( \text{Solid Angle swept out by } \mathbf{\hat{d}}(\mathbf{k}) \right)$$

### Topology in one dimension: Berry phase and electric polarization

see, e.g. Resta, RMP 66, 899 (1994)

### Classical electric polarization:

$$P = \frac{\text{dipole moment}}{\text{length}} -Q \longrightarrow +C$$

Bound charge density  $\rho_{bound} = \nabla \cdot P$ 

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

### Proposition: The quantum polarization is a Berry phase

$$P = \frac{e}{2\pi} \int_{BZ} A(k) dk$$

$$BZ = 1D \text{ Brillouin Zone} = S^{1} \int_{-\pi/a}^{\pi/a} e^{-\pi/a}$$

### Circumstantial evidence #1:

The polarization and the Berry phase share the same ambiguity:

They are both only defined modulo an integer.

• The end charge is not completely determined by the bulk polarization P because integer charges can be added or removed from the ends:

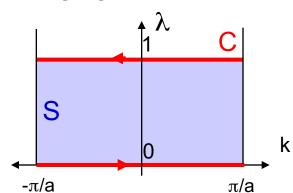
$$Q_{\text{end}} = P \mod e$$

• The Berry phase is gauge invariant under continuous gauge transformations, but is **not** gauge invariant under "large" gauge transformations.

$$P \rightarrow P + en$$
 when  $|u(k)\rangle \rightarrow e^{i\phi(k)}|u(k)\rangle$  with  $\phi(\pi/a) - \phi(-\pi/a) = 2\pi n$ 

Changes in P, due to adiabatic variation are well defined and gauge invariant

$$\begin{aligned} \left| u(k) \right\rangle &\rightarrow \left| u(k,\lambda(t)) \right\rangle \\ \Delta P &= P_{\lambda=1} - P_{\lambda=0} = \frac{e}{2\pi} \int_{C} \mathbf{A} dk = \frac{e}{2\pi} \int_{S} \mathbf{F} dk d\lambda \\ \text{gauge invariant Berry curvature} \end{aligned}$$



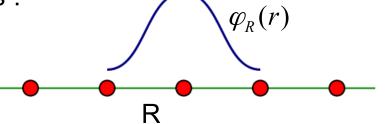
# Circumstantial evidence #2: $r: i \nabla_k$

"
$$P = e \int_{BZ} \frac{dk}{2\pi} \langle u(k) | r | u(k) \rangle = \frac{ie}{2\pi} \int_{BZ} \langle u(k) | \nabla_k | u(k) \rangle$$
"

### A more rigorous argument:

Construct Localized Wannier Orbitals:

$$\left|\varphi(R)\right\rangle = \int_{BZ} \frac{dk}{2\pi} e^{-ik(R-r)} \left|u(k)\right\rangle$$



Wannier states are gauge dependent, but for a sufficiently smooth gauge, they are localized states associated with a Bravais Lattice point R

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

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

# Su Schrieffer Heeger Model

 $d_z(k) = 0$ 

model for polyacetylene simplest "two band" model

 $\delta t$ <0: Berry phase  $\pi$ 

P = e/2

$$H = \sum_{i} (t + \delta t) c_{Ai}^{\dagger} c_{Bi} + (t - \delta t) c_{Ai+1}^{\dagger} c_{Bi} + h.c.$$

$$\delta t > 0$$

$$A_{,i} = A_{,i+1}$$

$$\delta t < 0$$

$$A_{,i+1} = A_{,i+1}$$

$$A_{,i+1} = A_{,$$

Provided symmetry requires  $d_z(k)=0$ , the states with  $\delta t>0$  and  $\delta t<0$  are distinguished by an integer winding number. Without extra symmetry, all 1D band structures are topologically equivalent.

# Symmetries of the SSH model

"Chiral" Symmetry: 
$$\{H(k), \sigma_z\} = 0$$
 (or  $\sigma_z H(k) \sigma_z = -H(k)$ )

- Artificial symmetry of polyacetylene. Consequence of bipartite lattice with only A-B hopping:  $c_{iA} \rightarrow c_{iA} c_{iB} \rightarrow -c_{iB}$
- Requires  $d_z(k)=0$ : integer winding number
- Leads to particle-hole symmetric spectrum:

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

# Reflection Symmetry: $H(-k) = \sigma_x H(k) \sigma_x$

- Real symmetry of polyacetylene.
- Allows  $d_z(k)\neq 0$ , but constrains  $d_x(-k)=d_x(k)$ ,  $d_{v,z}(-k)=-d_{v,z}(k)$
- No p-h symmetry, but polarization is quantized: Z<sub>2</sub> invariant

$$P = 0$$
 or  $e/2$  mod  $e$ 

### **Domain Wall States**

An interface between different topological states has topologically protected midgap states



### Low energy continuum theory:

For small  $\delta t$  focus on low energy states with  $k \sim \pi/a$ 

$$k \to \frac{\pi}{a} + q$$
 ;  $q \to -i\partial_x$ 

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

$$V_F = ta$$
 ;  $m = 2\delta t$ 

Massive 1+1 D Dirac Hamiltonian  $E(q) = \pm \sqrt{(v_F q)^2 + m^2}$ 

$$E(q) = \pm \sqrt{(\mathsf{V}_F q)^2 + m^2}$$

"Chiral" Symmetry: 
$$\{\sigma_z, H\} = 0 \rightarrow \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$$
 Any eigenstate at +E has a partner at -E

Zero mode: topologically protected eigenstate at E=0

(Jackiw and Rebbi 76, Su Schrieffer, Heeger 79)

Domain wall bound state 
$$\psi_0$$

$$E_{gap}=2|\mathbf{m}| \qquad \psi_0(x)=e^{\int_0^x m(x')dx'/\mathbf{v}_F} \begin{pmatrix} 1\\0 \end{pmatrix}$$

# **Thouless Charge Pump**

The integer charge pumped across a 1D insulator in one period of an adiabatic cycle is a topological invariant that characterizes the cycle.

$$H(k, t + T) = H(k, t)$$

$$t = T$$

$$\Delta P = \frac{e}{2\pi} \left( \int \Delta(k, T) dk - \int \Delta(k, 0) dk \right) = ne$$

$$n = \frac{1}{2\pi} \int_{T^2} \mathbf{F} dk dt$$

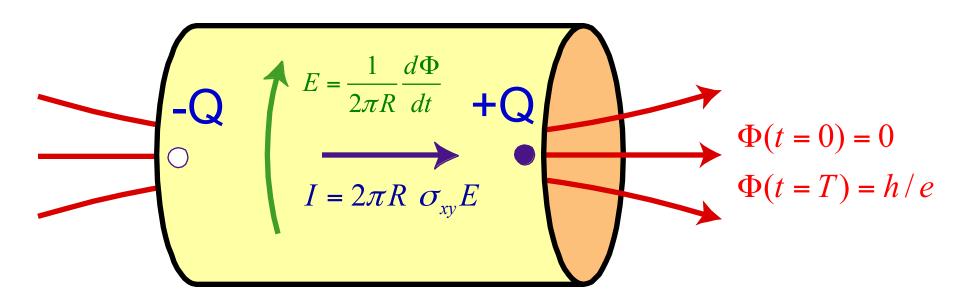
The integral of the Berry curvature defines the first Chern number, n, an integer topological invariant characterizing the occupied Bloch states,  $|u(k,t)\rangle$ 

In the 2 band model, the Chern number is related to the solid angle swept out by  $\hat{\mathbf{d}}(k,t)$ , which must wrap around the sphere an integer n times.

$$n = \frac{1}{4\pi} \int_{T^2} dk dt \ \hat{\mathbf{d}} \cdot (\partial_k \hat{\mathbf{d}} \times \partial_t \hat{\mathbf{d}})$$

### Integer Quantum Hall Effect: Laughlin Argument

Adiabatically thread a quantum of magnetic flux through cylinder.



$$\Delta Q = \int_{0}^{T} \sigma_{xy} \frac{d\Phi}{dt} dt = \sigma_{xy} \frac{h}{e}$$

Just like a Thouless pump :  $H(T) = U^{\dagger}H(0)U$ 

$$\Delta Q = ne \rightarrow \sigma_{xy} = n \frac{e^2}{h}$$

### **TKNN Invariant**

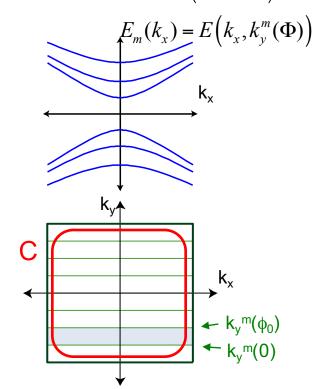
Thouless, Kohmoto, Nightingale and den Nijs 82

View cylinder as 1D system with subbands labeled by  $k_y^m(\Phi) = \frac{1}{R} \left( m + \frac{\Phi}{\phi_0} \right)$ 

$$\Delta Q = \sum_{m} \frac{e}{2\pi} \int_{0}^{\phi_{0}} d\Phi \int dk_{x} \mathbf{F}(k_{x}, k_{y}^{m}(\Phi)) = ne$$

TKNN number = Chern number  $\sigma_{xy} = n \frac{e^2}{h}$ 

$$n = \frac{1}{2\pi} \int_{BZ} d^2k \mathbf{F}(\mathbf{k}) = \frac{1}{2\pi} \int_{C} \mathbf{A} \cdot d\mathbf{k}$$



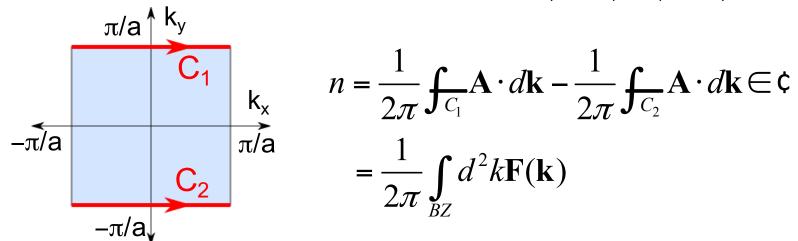
Distinguishes topologically distinct 2D band structures. Analogous to Gauss-Bonnet thm.

Alternative calculation: compute  $\sigma_{xy}$  via Kubo formula

# **TKNN Invariant**

Thouless, Kohmoto, Nightingale and den Nijs 82

For a 2D band structure, define  $\mathbf{A}(\mathbf{k}) = -i \langle u(\mathbf{k}) | \nabla_{\mathbf{k}} | u(\mathbf{k}) \rangle$ 



Physical meaning: Hall conductivity  $\sigma_{xy} = n \frac{e^2}{h}$ 

Laughlin Argument: Thread magnetic flux  $\phi_0$  = h/e through a 1D cylinder Polarization changes by  $\sigma_{xy}$   $\phi_0$ 

