Introduction to topological aspects in condensed matter physics

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2nd lecture

- 1. Topological insulators w/ TRS in 2D & 3D
 - Z₂ invariant for 2D & 3D topological insulators
 - Experimental detection of 2D& 3D topological insulators
- 2. Topological superconductors in 1D
 - BdG theory for superconductors
 - Topological superconductors in 1D: Kitaev model
 - Majorana edge states
 - InSb nanowire-heterostructure
- 3. Topological superconductors in 2D (w/o TRS)
 - Topological superconductors in 2D: chiral p-wave SC
 - Majorana edge and vortex-bound state
 - Sr₂RuO₄

Band theory of solids and topology

Bloch Hamiltonian H(

 (\mathbf{k}) crystal momentum

Bloch wavefunction $H(\mathbf{k}) |u_n(\mathbf{k})\rangle = E_n(\mathbf{k}) |u_n(\mathbf{k})\rangle$

Hamiltonians

with energy gap

satisfying certain

symmetry operations

Symmetry protected topological phases:

Study topology of the following mapping:

Brillouin zone \longmapsto $H(\mathbf{k})$

Topological equivalence:

Band structures are equivalent if they can be continuously deformed into one another without closing the energy gap and without breaking the symmetries of the system.

Symmetries to consider:

- time-reversal symmetry (anti-unitary)
- particle-hole symmetry (anti-unitary)
- sublattice symmetry and other crystallographic symmetries

Note: Unitary symmetries $[H(\mathbf{k}), U_S] = 0$ (e.g. spin-rotation symmetry) can be removed by block-diagonalizing $H(\mathbf{k})$



Momentum

 π/a

 k_r

 $-\pi/a$

Time-reversal symmetry & Kramers theorem

Presence of time-reversal symmetry gives rise to new topological invariants [Kane-Mele, PRL 05]

$$\Theta: \quad t \to -t, \quad \mathbf{k} \to -\mathbf{k}, \quad \hat{S}^{\mu} \to -\hat{S}^{\mu}$$

Time-reversal symmetry implemented by anti-unitary operator:

$$\Theta = U_{\rm T} \mathcal{K} = e^{i\pi \hat{S}^y/\hbar} \mathcal{K} \checkmark \qquad \text{complex conjugation operator} \qquad \Theta \psi = e^{i\pi \hat{S}^y/\hbar} \psi^*$$

For quadratic Hamiltonians in momentum space:

$$\Theta \mathcal{H}(\mathbf{k})\Theta^{-1} = +\mathcal{H}(-\mathbf{k})$$

For spin-
$$\frac{1}{2}$$
 particles: $\Theta^2 = -1$ $U_{\rm T} = -U_{\rm T}^T$ $\Theta = i\sigma_y \mathcal{K}$ $\Theta \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix} = \begin{pmatrix} \psi_{\downarrow}^* \\ -\psi_{\uparrow}^* \end{pmatrix}$

Kramers theorem (for spin-1/2 particles): $\Theta^2 = -1 \Rightarrow \langle \psi | \Theta \psi \rangle = -\langle \psi | \Theta \psi \rangle = 0$

- \Rightarrow all eigenstates are at least two-fold degenerate
- \Rightarrow for Bloch functions in k-space:

 $|u(\mathbf{k})\rangle$ and $|u(-\mathbf{k})\rangle$ have same energy; degeneracy at TRI momenta

Consequences for edge states:

- states at time-reversal invariant momenta are degenerate
- crossing of edge states is protected
- absence of backscattering from non-magnetic impurities



Time-reversal-invariant topological insulator

2D topological insulator:

[Bernevig, Hughes, Zhang 2006]

(also known as Quantum Spin Hall insulator)

[Kane-Mele, PRL 05]

2D Bloch Hamiltonians in the presence of time-reversal symmetry:



Bulk energy gap but gapless edge: Spin filtered edge states

- protected by time-reversal symmetry
- half an ordinary 1D electron gas
- is realized in certain band insulators with strong spin-orbit coupling

TRI topological insulator: HgTe quantum wells



TRI topological insulator: HgTe quantum wells



Helical edge states are unique 1D electron conductor

- spin and momentum are locked
- no elastic backscattering from non-magnetic impurities
- perfect spin conductor!

2D topological insulator: Edge Z₂ invariant

[Kane Mele 05]

Time-reversal invariant insulators with $\Theta^2 = -1$ are classified by a **Z**₂ topological invariant (ν = 0,1)

$$\Theta \mathcal{H}(\mathbf{k})\Theta^{-1} = +\mathcal{H}(-\mathbf{k})$$

This can be understood via the bulk-boundary correspondence:

 \Rightarrow consider edge states in half of the edge Brillouin zone (other half is related by TRS)





even / odd number of Kramers pairs of edge states

2D topological insulator: First bulk Z₂ invariant

Bulk Z₂ invariant as an obstruction to define a "TR-smooth gauge": [Fu and Kane] - $|u_n^{(1)}(\mathbf{k})\rangle$ and $|u_n^{(2)}(\mathbf{k})\rangle$ denote gauge choices in the two EBZs - TR-smooth gauge: $|u_n^{(1)}(-\mathbf{k})\rangle = \Theta |u_n^{(2)}(\mathbf{k})\rangle$ $\left| t_{mn}(\mathbf{k}) = \left\langle u_m^{-}(\mathbf{k}) \right| \Theta \left| u_n^{-}(\mathbf{k}) \right\rangle$ \Rightarrow consider anti-symmetric "t-*matrix":* antisymmetry property: $t^{\mathrm{T}}(\mathbf{k}) = -t(\mathbf{k})$ $(\Pr\left[\omega(\Lambda_a)\right])^2$ e.g.: $\operatorname{Pf}\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z$ $= \det \left[\omega(\Lambda_a) \right]$ \Rightarrow Pfaffian can be defined: $Pf[t(\mathbf{k})]$ Topological index counts the number or zeroes of $Pf[t(\mathbf{k})]$ in EBZ: Λ_3 Λ_1 Λ_2 $I = \frac{1}{2\pi i} \int_{\partial(\text{EBZ})} d\mathbf{k} \cdot \nabla \log \left(\Pr\left[\langle u_m^-(\mathbf{k}) | \Theta | u_n^-(\mathbf{k}) \right] \right) \mod 2$ EBZ

[Kane Mele 05]

It follows from **bulk-boundary correspondence**: edge Z₂ invariant = bulk Z₂ invariant

2D topological insulator: Second bulk Z₂ invariant

Bulk Z₂ invariant as an obstruction to define a "TR-smooth gauge":

- $|u_n^{(1)}(\mathbf{k})\rangle$ and $|u_n^{(2)}(\mathbf{k})\rangle$ denote gauge choices in the two EBZs - TR-smooth gauge: $|u_n^{(1)}(-\mathbf{k})\rangle = \Theta |u_n^{(2)}(\mathbf{k})\rangle$
- \Rightarrow consider unitary *sewing matrix:*

$$\omega_{mn}(\mathbf{k}) = \langle u_m^-(-\mathbf{k}) | \Theta | u_n^-(\mathbf{k}) \rangle$$

antisymmetry property: $\omega^T(\mathbf{k}) = -\omega(-\mathbf{k})$

Bulk Z₂ invariant (\mathcal{V} = 0,1):

at TRI momenta: $\Lambda_a = -\Lambda_a \Rightarrow \omega^T(\Lambda_a) = -\omega(\Lambda_a)$ is antisymmetric



$$(-1)^{\nu} = \prod_{a=1}^{4} \frac{\operatorname{Pf} \left[\omega(\Lambda_a)\right]}{\sqrt{\det \left[\omega(\Lambda_a)\right]}} = \pm 1$$

(gauge invariant, but smooth gauge needed)

 $(\Pr[\omega(\Lambda_a)])^2$

 $= \det \left[\omega(\Lambda_a) \right]$

It follows from **bulk-boundary correspondence**: edge Z_2 invariant = bulk Z_2 invariant

[Kane Mele 05] [Fu and Kane]



2D topological insulator: Bulk Z₂ invariants

Three equivalent definitions for bulk Z₂ topological invariant:

(A) in terms of sewing matrix:

$$(-1)^{\nu} = \prod_{a=1}^{4} \frac{\Pr\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}} = \pm 1$$

(gauge invariant, but smooth gauge needed)

sewing matrix: $\omega_{mn}(\mathbf{k}) = \langle u_m^-(-\mathbf{k}) | \Theta | u_n^-(\mathbf{k}) \rangle$

(is unitary, and antisymmetric at TRI momenta)

(B) count number of zeroes of $Pf\left[\langle u_m^-(\mathbf{k})|\Theta|u_n^-(\mathbf{k})
ight]$ in EBZ

$$I = \frac{1}{2\pi i} \int_{\partial(\text{EBZ})} d\mathbf{k} \cdot \nabla \log \left(\Pr\left[\langle u_m^-(\mathbf{k}) | \Theta | u_n^-(\mathbf{k}) \right] \right) \mod 2$$
(antisymmetric at all momenta)

(antisymmetric at all mome but not unitary)

(C) in terms of Berry connection:

$$\nu = \frac{1}{2\pi} \left[\oint_{\partial(EBZ)} d\mathbf{k} \cdot \mathcal{A} - \int_{EBZ} d^2 \mathbf{k} \,\mathcal{F} \right] \mod 2$$



3D topological insulator: Surface Z₂ invariant



[after Hasan & Kane, RMP 2010]



Conduction band Energy OR Ef Valence band $k = \widetilde{\Lambda}_1$ $k = \widetilde{\Lambda}_2$



surface Brillouin zone

• Surface Z₂ invariant:

 $\nu = 1$: Strong topological insulator

- Fermi surface encloses odd number of TRI momenta
- independent of surface orientation
- protected by time-reversal symmetry
- $\nu = 0$: Weak topological insulator
- Fermi surface encloses even number of TRI momenta
- depends on surface orientation (quasi-2D topological insulator)
- protected by time-reversal *and* translation symmetry



3D topological insulator: Bulk Z₂ invariant

• Bulk Z₂ invariant:

[Kane-Mele, Moore-Balents, Roy, Fu-Kane-Mele (06-07)] 8 TRI momenta in bulk BZ

— Strong Z₂ invariant

$$(-1)^{\nu} = \prod_{a=1}^{8} \frac{\Pr\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}} = \pm 1$$

- Weak Z₂ invariant

$$(-1)^{\nu_i} = \prod_{a=1}^{4} \frac{\operatorname{Pf}\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}} \Big|_{k_i=0}$$



 k_{z}

 k_{u}

Bulk-boundary correspondence: edge Z₂ invariant = bulk Z₂ invariant

 k_y





Weak topological insulator





Experimental detection of 3D topological insulators

• observed in certain band insulators with strong spin-orbit coupling BiSb alloy, Bi₂Se₃, Bi₂Te₃, TIBiTe₂, TISbSe₂, etc

stable surface states cross a gap, that is opened up by spin-orbit coupling

•
$$\operatorname{Bi}_{1-x} \operatorname{Sb}_x$$
 :

[Fu, Kane, PRL 2007]

[Hsieh, Hasan et al, Nature 2008]

momentum resolved photoemission (ARPES)



five surface state bands cross E_{F} between TRI momenta $\,\Gamma\,$ and $\,M\,$

$$\Rightarrow$$
 strong topological insulator

Experimental detection of 3D topological insulators

0.3

02

0.1

-0.1

-0.2

spin resolved and momentum resolved photoemission (ARPES)



simple surface state structure, similar to graphene

Unique properties of helical surface states:

• spin and momentum are locked

• Bi_2 Se₃ :

- half of an ordinary 2DEG, "1/4 of graphene"
- robust to disorder, impossible to localize



0.2

0.1

0.3



Topological Superconductors





Bogoliubov-de Gennes theory for superconductors

Superconductor = Cooper pairs (boson) + Bogoliubov quasiparticles (fermions)



Topological superconductors

Bogoliubov-de Gennes Hamiltonian

$$H_{\rm BdG} = \begin{pmatrix} h_0 & \Delta \\ \\ \Delta^{\dagger} & -h_0^T \end{pmatrix}$$

1

\



gap in spectrum \longrightarrow can define top. invariant

$$n = \frac{i}{2\pi} \int_{\text{states}} \mathcal{F} \, d\mathbf{k}$$
with E<0

BdG band structures are equivalent if they can be continuously deformed into one another without closing the energy gap and without breaking the symmetries of the SC.

Symmetries to consider: Particle-hole symmetry, time-reversal, etc.

Bulk-boundary correspondence + particle-hole redundancy:

$$\Xi \psi_{+\boldsymbol{k},+\boldsymbol{E}} = \tau_x \psi_{-\boldsymbol{k},-\boldsymbol{E}}^*$$

• Majorana edge state at zero energy



1D topological superconductor: Majorana chain

One-dimensional spinless p-wave superconductor: Majorana chain

Hamiltonian:

$$\mathcal{H} = \sum_{j} \left[t(c_{j}^{\dagger}c_{j+1} + c_{j+1}^{\dagger}c_{j} - \mu c_{j}^{\dagger}c_{j} + \Delta(c_{j+1}^{\dagger}c_{j}^{\dagger} + c_{j}c_{j+1}) \right]$$

ce:
$$\mathcal{H} = \frac{1}{2} \sum_{k} \left(c_{k}^{\dagger} \quad c_{-k} \right) \mathcal{H}_{BdG}(k) \begin{pmatrix} c_{k} \\ c_{-k}^{\dagger} \end{pmatrix}$$

in momentum space:

 $\mathcal{U}_{\mathbf{D}}$, $\alpha(k) = \mathbf{d}(k)$

$$d_x(k) = \Delta \sin k \qquad d_y(k) = 0$$

$$d_x(k) = \Delta \sin k \qquad a_y(k)$$
$$d_z(k) = 2t \cos k - \mu$$

Particle-hole symmetry:

$$\tau_x \mathcal{H}^*_{\mathrm{BdG}}(k) \tau_x = -\mathcal{H}_{\mathrm{BdG}}(-k)$$

Time-reversal symmetry:

$$\tau_z \mathcal{H}^*_{\mathrm{BdG}}(k) \tau_z = +\mathcal{H}_{\mathrm{BdG}}(-k)$$

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



t

 $|\mu|>2t$:

trivial superconductor



topological superconductor

1D topological superconductor: Majorana chain

To reveal zero-energy edge states, consider different viewpoint: Majorana representation

Majorana fermion: Particle = Antiparticle

$$c_{j} = \frac{1}{2} \left(\gamma_{1j} + i \gamma_{2j} \right) \qquad c_{j}^{\dagger} = \frac{1}{2} \left(\gamma_{1j} - i \gamma_{2j} \right)$$

Commutation relations: $\{\gamma_{lj}, \gamma_{l'j'}\} = 2\delta_{ll'}\delta_{jj'}$ $(\gamma_{lj})^2 = 1$

 \implies Majorana chain for spinless fermions

$$H = \frac{i}{2} \sum_{j} \left[-\mu \gamma_{1j} \gamma_{2j} + (\Delta - t) \gamma_{2j} \gamma_{1j+1} + (\Delta + t) \gamma_{1j} \gamma_{2j+1} \right]$$

for $\Delta = -t$: nearest neighbor Majorana chain



[Kitaev 2000]

Experimental detection of 1D spinless topological SC

1D spinless chiral p-wave superconductor is likely (?) realized in InSb-nanowire-heterostructures

magnetic field B



Condition for topological phase:

$$B \propto E_{\text{Zeeman}} > \sqrt{\Delta^2 - \mu^2}$$

[Sau, Lutchyn, Tewari, das Sarma, et al 2009] [Oreg, von Oppen, et al 2010]

[after Alicea, Rep. Prog. Phys. 2012]



as a function of magnetic field B

[Mourik, Kouwenhoven et al, Science 2012]

Two-dimensional spinless chiral p-wave SC

Lattice BdG model: [Read & Green 00]



Majorana fermions in chiral p-wave superconductor

> Bulk-boundary correspondence: n = # Majorana edge modes

Majorana edge states are perfect heat conductor

Quantized thermal Hall conductance

$$\frac{\kappa_{xy}}{T} = \frac{\pi k_B^2}{48h} \int_{\mathrm{BZ}} d^2 \mathbf{k} \, \epsilon^{\mu\nu} \hat{\mathbf{m}} \cdot \left[\partial_{k_{\mu}} \hat{\mathbf{m}} \times \partial_{k_{\nu}} \hat{\mathbf{m}} \right]$$

- Majorana zero mode at a vortex:
 - vortex: small hole with edge states
 - Majorana zero mode for $\Phi = p \frac{h}{2e}$ with p odd (periodic vs. anti-periodic BC)





Majorana state





[[]Caroli, de Gennes, Matricon '64]

 q_m

Majorana fermions for topological quantum computing

occupied

[Kitaev 2003]

Degenerate states associated with Majorana zero modes at vortices define a topologically protected quantum memory

Two Majorana fermions define a single two level system:



- two degenerate states (occupied / empty) \Rightarrow 1 qubit
- 2N separated Majoranas corresponds to N qubits
- -information stored non-locally \implies immune to local perturbations / decoherence
- Majorana vortex bound states obey non-Abelian statistics

$$\begin{array}{c} \gamma_2 \rightarrow \gamma_1 \\ \gamma_1 \rightarrow -\gamma_2 \end{array}$$



Experimental detection of spinful chiral p-wave SC

The transition-metal-oxide Sr₂RuO₄ is likely (?) a *spinful* chiral p-wave superconductor with Chern number n=2 (per layer)

- Ru t_{2g}-orbitals (4d⁴-electrons) hybridized with O p-oribitals form quasi-two-dimensional Fermi surfaces
- transition temperature $T_C = 1.5K$
- strong anisotropies in spin dependent responses (NMR and Knight shift)
- signatures of edge states in tunneling conductance



PRL 2000]





tunneling conductance

[Maeno et al. JPSJ 81, 011009]

[Kashiwaya et al. PRL 2011]