Topological Superconductors B. Andrei Bernevig



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Topological Phases of Matter

Do not have a local order parameters, cannot be described by symmetry breaking.

Have topological order (Wen)

Are all bulk insulators - gapped ground-states; characterized by "topological" numbers

Several remarkable things occur:

Interacting topological states of matter feel the topology (genus) of the manifold:



Interacting topological states have degeneracies.

Non-interacting states of matter (band insulators and BdG superconductors) have unique ground states: topologically nontrivial insulator occurs when it cannot be adiabatically continued to (any/an) atomic limit

What is a topological insulator/superconductor?

- Bulk of material is completely gapped
- On the boundaries there are gapless, protected fermionic modes (chiral, Dirac, Majorana, chiral-Majorana) which are holographic
- Bulk state characterized by a non-zero topological invariant
- May require an auxiliary symmetry to be a stable phase (T,C,...)
- Examples: IQHE, QAHE, QSH, 3d strong topological insulator,p+ip superconductor, d+id superconductor

Topological Band Insulators Have Gapless Edge States (Mostly)

• Pick lattice. On each site - atomic orbitals

 Atomic limit = on-site energies of the s and p orbitals, but no hopping (or overlap) between orbitals on different sites



Atomic limit - if the lattice constant is very large (for ex the size of a galaxy)

Thought experiment: shrink the lattice constant to the normal Angstrom - size. Question: can we do that without closing the bulk gap (adiabatically)?

NO? Material is a topological insulator with gapless edge modes at the boundary with a trivial insulator.



States of Matter: Topological Properties

•Exceptions: Integer Quantum Hall:

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

- n related to number of edge states
- With applied magnetic field (explicit Time-Reversal breaking).
- The quantum Hall effect in the presence of a magnetic field also subtly breaks another symmetry- translational invariance.

•Topological insulators and superconductors dont break symmetries of the lattice. They can have time reversal, charge conjugation, or not.



Can We Obtain a Quantum Hall State Without Applied Field?

YES (Haldane) (still need time-reversal breaking). Simplest model is a 2 by 2 Dirac Hamiltonian.

$$\begin{pmatrix} m & v(k_x - ik_y) \\ v(k_x + ik_y) & -m \end{pmatrix}$$

For the full system, we have: For a single Dirac Fermion, we hence have: σ σ yy m > 0xQuantum Hall without 1 m < 0applied B m (Haldane 1988) Similar to Callan, Harvey, Kaplan fermions

m > 0

Almost everything in these lectures will be at the level of single-particle BdG formalism

"Topological" gapped bulk, for most purposes (but not generically true), possesses gapless edge or surface states

We will try to understand the different topological superconductors that can appear in 1,2, and 3 Dimensions

A BdG gapped superconductor can be thought of as an insulator with a C "symmetry"

The atomic "limit" of our superconductors is always the strong pairing limit

Example of BdG Formalism For S-wave Sc

Take a simple free metal:
$$H = \sum_{\mathbf{p},\sigma} c^{\dagger}_{\mathbf{p}\sigma} \left(\frac{p^2}{2m} - \mu \right) c_{\mathbf{p}\sigma} \equiv \sum_{\mathbf{p},\sigma} c^{\dagger}_{\mathbf{p}\sigma} \epsilon(p) c_{\mathbf{p}\sigma},$$

Artificially double the number of degrees of freedom: $\Psi_{\mathbf{p}} \equiv (c_{\mathbf{p}\uparrow} \ c_{\mathbf{p}\downarrow} \ c_{-\mathbf{p}\uparrow}^{\dagger} \ c_{-\mathbf{p}\downarrow}^{\dagger})^T$

The Hamiltonian in this basis: $H = \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} H_{BdG}(\mathbf{p}) \Psi_{\mathbf{p}} + \text{constant}, \quad H_{BdG}(\mathbf{p}) = \frac{1}{2} \begin{pmatrix} \epsilon(p) & 0 & 0 & 0 \\ 0 & \epsilon(p) & 0 & 0 \\ 0 & 0 & -\epsilon(-p) & 0 \\ 0 & 0 & 0 & -\epsilon(-p) \end{pmatrix}$

Has a "symmetry" (redundancy): $H_{BdG}(\mathbf{p}) = -CH_{BdG}^T(-\mathbf{p})C^{-1}$ $C = \tau^x \otimes I_{2\times 2}$

Only two out of the four bands give us independent quasiparticle energies - we created an artificial redundancy, masked as a symmetry

For the non-interacting metal above, this redundancy can be back-tracked to the original two-band free metal. This is not possible once pairing is introduced: the basis in which we diagonalize the Hamiltonian cannot be made non-redundant (the Bogoliubov operators have the text-book relations: $\gamma^{\dagger}_{+,\mathbf{p}\uparrow} = \gamma_{-,-\mathbf{p}\downarrow} \quad \gamma^{\dagger}_{+,\mathbf{p}\downarrow} = \gamma_{-,-\mathbf{p}\uparrow}$

Example of BdG Formalism For S-wave Sc

Introduce a simple pairing term: $H_{\Delta} = \Delta c_{\mathbf{p}\uparrow}^{\dagger} c_{-\mathbf{p}\downarrow}^{\dagger} + \Delta^* c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow}$

This splits the electron and hole-bands of the redundant metal in the previous slide:



Charge Conjugation "symmetry" still holds:

$$H_{\text{BdG}}(\mathbf{p}) = -CH_{\text{BdG}}^{T}(-\mathbf{p})C^{-1} \qquad C = \tau^{x} \otimes I_{2\times 2}$$

(easy trick to see the symmetry: in a tensor product look at what commutes and anticommutes in each space: tau_x anticommutes with tau_z and tau_y giving the - sign for the kinetic term and the Re(Delta) - the tau_y sigma_y transpose is itself. tau_x commutes with Im(Delta) term, but the - sign there comes from the transpose of sigma_y.)

There is an important difference between a superconductor and an insulator, even at BdG level: the excitations of the former are combinations of particle and hole states

Possible Charge Conjugation and Time-Reversal Symmetries

Transformations of the field operators (time reversal also acts as complex conjugation):

$$\mathcal{T}\psi_A \mathcal{T}^{-1} = \sum_B (U_T)_{A,B} \psi_B \qquad \qquad \mathcal{C}\psi_A \mathcal{C}^{-1} = \sum_B (U_C^*)_{A,B} \psi_B^{\dagger}$$

Anti-unitary "symmetries" (conditions on first quantized Hamiltonians):

$$\mathcal{T}: \quad U_T^{\dagger} \ \mathcal{H}^* \ U_T = +\mathcal{H} \qquad \qquad \mathcal{C}: \quad U_C^{\dagger} \ \mathcal{H}^* \ U_C = -\mathcal{H}$$

The square of the time-reversal of charge conjugation commutes with Hamiltonian:

$$(U_T^*U_T)^{\dagger} \mathcal{H}(U_T^*U_T) = \mathcal{H} \qquad (U_C^*U_C)^{\dagger} \mathcal{H}(U_C^*U_C) = \mathcal{H}$$

The square of TR and CC are proportional to identity matrix, and because unitary:

$$U_T^* U_T = \pm I_N \qquad \qquad U_C^* U_C = \pm I_N$$

So the two possibilities are spinless and spinful TR and CC:

$$\mathcal{T}^2 = \pm 1 \qquad \qquad T = e^{-i\pi S_y} K \qquad \qquad \mathcal{C}^2 = \pm 1$$

The 10-fold way

In terms of TR and CC there are 10 possibilities (in any dimension):

$\exp(\mathrm{i} t \mathcal{H})$

Cartan label	Т	С	S	Hamiltonian	d = 1	d = 2	d = 3
A (unitary)	0	0	0	U(N)	-	\mathbb{Z}	-
AI (orthogonal)	+1	0	0	U(N)/O(N)	-	-	-
AII (symplectic)	-1	0	0	U(2N)/Sp(2N)	-	\mathbb{Z}_2	\mathbb{Z}_2
AIII (ch. unit.)	0	0	1	$U(N+M)/U(N) \times U(M)$	\mathbb{Z}	-	\mathbb{Z}
BDI (ch. orth.)	+1	+1	1	$O(N+M)/O(N) \times O(M)$	\mathbb{Z}	-	-
CII (ch. sympl.)	-1	-1	1	$\operatorname{Sp}(N+M)/\operatorname{Sp}(N) \times \operatorname{Sp}(M)$	\mathbb{Z}	-	\mathbb{Z}_2
D (BdG)	0	+1	0	SO(2N)	\mathbb{Z}_2	\mathbb{Z}	-
C (BdG)	0	-1	0	$\operatorname{Sp}(2N)$	-	\mathbb{Z}	-
DIII (BdG)	-1	+1	1	SO(2N)/U(N)	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
CI (BdG)	+1	-1	1	$\operatorname{Sp}(2N)/\operatorname{U}(N)$	-	-	\mathbb{Z}

Why are there (some of) different classes in different dimensions 1,2,3? (we could go to higher dimensions but...)

Avenues Towards Topological Insulator

How to get topological superconductivity:

Method I: Take a system with a simple bandstructure and add momentum dependent pairing. Examples: spinless and spinful p+ip superconductors, He-3B, chiral d-wave in 2d

Method II: Take a system with a rich bandstructure and add s-wave, or extended s-wave pairing Examples: surface of 3d topological insulator with typical s-wave, QAHE with s-wave, non-centrosymmetric superconductors with extended s-wave (more about this later...), possibly many more.

Zero-Dimensional Topological Classification

Although historically the p+ip superconductor (class D or C) in 2-d came as the first example of a topological superconductor, a simpler class exists: class D in 1-d

	Cartan label	Т	С	S	Hamiltonian	d = 1	d = 2	d = 3	
	A (unitary)	0	0	0	U(N)	-	\mathbb{Z}	-	
	AI (orthogonal)	+1	0	0	U(N)/O(N)	-	-	-	
	AII (symplectic)	-1	0	0	U(2N)/Sp(2N)	-	\mathbb{Z}_2	\mathbb{Z}_2	
	AIII (ch. unit.)	0	0	1	$U(N+M)/U(N) \times U(M)$	\mathbb{Z}	-	\mathbb{Z}	
	BDI (ch. orth.)	+1	+1	1	$O(N+M)/O(N) \times O(M)$	\mathbb{Z}	-	-	
_	CII (ch. sympl.)	-1	-1	1	$\operatorname{Sp}(N+M)/\operatorname{Sp}(N) \times \operatorname{Sp}(M)$	\mathbb{Z}	-	\mathbb{Z}_2	
(D (BdG)	0	+1	0	SO(2N)	\mathbb{Z}_2	\mathbb{Z}	-	
	C (BdG)	0	-1	0	$\operatorname{Sp}(2N)$	-	\mathbb{Z}	-	
	DIII (BdG)	-1	+1	1	SO(2N)/U(N)	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	
	CI (BdG)	+1	-1	1	$\operatorname{Sp}(2N)/\operatorname{U}(N)$	-	-	\mathbb{Z}	

Simplest Example: class D in 0-d, charge conjugation squares to +1 (as before)

A Single Site problem (positive chemical potential), in a magnetic field (no TR), with an onsite superconducting gap.

$$\mathbf{B} \quad H = -\mu c_{\sigma}^{\dagger} c_{\sigma} + B c_{\sigma}^{\dagger} \sigma_{\sigma,\sigma'}^{z} c_{\sigma'} + \Delta_{0} (c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} + c_{\downarrow} c_{\uparrow})$$

For very small pairing gap (almost negligible), ask what happens to the MANY-BODY ground-state as we keep chemical potential fixed and vary magnetic field from zero to large.

For ZERO gap, particle number is still a good quantum number:





 $B > \mu$

one spin

occupied

For finite (small) superconducting gap, particle number is not a good quantum number BUT mod 2 it is! Fermion parity is still different between these two states, and gives a Z2 index of superconductors in zero dimensions

Majorana Formalism

There is a proper way of implementing the charge conjugation redundancy (and obtaining indices) through the use of Majorana fermions. We now analyze the problem in the previous slide through this prism.

Since the Charge conjugation is a reality condition, it seems a good idea to split each complex fermions (irrespective of any quantum numbers like spin, orbital, etc) into two real (Majorana) fermions:

$$c_{\sigma}^{\dagger} = \frac{1}{2}(a_{1\sigma} - ia_{2\sigma}) \qquad c_{\sigma} = \frac{1}{2}(a_{1\sigma} + ia_{2\sigma})$$
$$a_{n\sigma}^{\dagger} = a_{n\sigma}, \quad \{a_{n\sigma}, a_{m\sigma'}\} = 2\delta_{nm}\delta_{\sigma,\sigma'} \qquad a_{n\sigma}^2 = 1$$

Re-write the one-site in magnetic field Hamiltonian in this Majorana basis:

$$H = \frac{i}{2}((B - \mu)a_{1\uparrow}a_{2\uparrow} - (B + \mu)a_{1\downarrow}a_{2\downarrow} + \Delta_0(a_{1\downarrow}a_{2\uparrow} + a_{2\downarrow}a_{1\uparrow}) = \frac{i}{4}\sum_{l,m=1}^2 a_{lo}A_{l\sigma;m\sigma}a_{m\sigma'}$$

In the Majorana basis, the first quantized Hamiltonian is an ANTI-SYMMETRIC REAL matrix:
$$\begin{pmatrix} 0 & 0 & B - \mu & -\Delta_0 \\ 0 & 0 & \Delta_0 & -B - \mu \\ -B + \mu & -\Delta_0 & 0 & 0 \\ \Delta_0 & B + \mu & 0 & 0 \end{pmatrix}$$

Majorana Formalism and First Topological Index

The energy levels are determined by the eigenvalues of the antisymmetric matrix.

$$E_1 = \frac{1}{4}(-B - \sqrt{\mu^2 + \Delta_0^2}), \quad E_2 = \frac{1}{4}(B - \sqrt{\mu^2 + \Delta_0^2}), \quad E_3 = \frac{1}{4}(-B + \sqrt{\mu^2 + \Delta_0^2}), \quad E_4 = \frac{1}{4}(B + \sqrt{\mu^2 + \Delta_0^2})$$

If the determinant is ever zero, we have a phase transition! Notice for small gap, the phase transition occurs when the B field becomes comparable to the chemical potential

Going through a phase transition two levels cross, the determinant of the matrix doesnt change sign (goes to zero then goes back to same sign).

However, if we could take the square root of the determinant, that would change sign, because it would track the energy of one level, which goes thru zero for a superconductor

Matrix is antisymmetric: we do have the square root: PFAFFIAN - $(-B^2 + \mu^2 + \Delta_0^2)$

Change in sign of pfaffian means going through a phase transition between even fermion parity $|B| < \sqrt{\mu^2 + \Delta_0^2}$ and odd fermion parity $|B| > \sqrt{\mu^2 + \Delta_0^2}$

We have now learned the Majorana formalism, the pfaffian index, its relation to phase transitions and its capability to classify the different phases of a superconductor

Kitaev P-Wave Wire

The 0-d model good for concepts. 1-d model much more interesting!

Simple model of spinless chain of electrons. Spinless, so we must have p-wave pairing

E

(p)
$$\sqrt{(2t \cos p \ \mu)^2 \ 4 \,\Delta^2 \sin^2 p}$$

 $\Psi_p \qquad (c_p \quad c^{\dagger}_{-p})^T$

2 Fermi points
 Pairing A sin p changes sign between the two Fermi points
 Energy 0
 (2μ) (2μ)

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

$$= \frac{1}{p} = H_{BdG} = \frac{1}{2} \sum_{p} \Psi_{p}^{\dagger} \left(\frac{-2t \cos p - \mu - 2i \Delta \sin p}{-2i \Delta \sin p - 2t \cos p - \mu} \right) \Psi_{p}$$

P-wave in 1-d is gapped, unlike in 2-d where we need p+ip to get a gapped spectrum. This is related to Wigner von Neumann classification of crossings by co-dimension.

There is a transition at p=0, Pi and $\mu_c = \frac{1}{2}2t$

Trivial state, kinetic term doesnt "wind". Pre-paring insulator

Non-trivial state, kinetic term "winds" between p=0, Pi. Pre-paring metal

Majorana Formalism and Phases of Kitaev P-Wave Wire

The model in Majorana form is much more revealing. Split each on-site complex fermion into 2 real Majoranas



$$H_{\text{BdG}} = \frac{1}{2} \sum_{j} \left(-\mu a_{2j-1} a_{2j} + (t+|\Delta|) a_{2j} a_{2j+1} + (-t+|\Delta|) a_{2j-1} a_{2j+2} \right)$$

We can easily understand the phases by looking at the following limiting cases:

"Strong pairing" case, kinetic energy term doesnt wind (in the previous slide), trivial state because the Majoranas are bound on-site (basically each site is occupied with a complex fermion, or an original site bound state of two real majoranas)

"Weak pairing" case, kinetic energy term does wind (in the previous slide), non-trivial state: Majoranas are dimerized offsite. If we now cut the chain in between the complex fermion sites we see clearly the appearance of ZERO energy end Majorana states. NON-LOCAL zero mode Hilbert space!



These two limiting cases are not generic, as the gap protects against adiabatic deformations!

Kitaev P-Wave Wire and Majorana End Modes

Away from the limiting cases of the previous slide, the Majorana modes at the two ends of the chain will start talking, but splitting is exponentially suppressed by hopping across the chain over the bulk gap.

The real majorana ZERO mode at one end and the one at the other end form a non-local complex fermion hilbert space.

Majorana zero modes exist with open boundary conditions in the nontrivial phase, and will only disappear once the BULK of the system has gone trivial through a phase transition

Edges are the mirror of an otherwise featureless topological bulk



There is a bulk index that tells us whether the system is topological or not. This index is a Z2 quantity. The existence of a Z2 quantity can also be understood from edges. Two edges = trivial = local edge hilbert space.



Kitaev P-Wave Wire and Bulk Indices

Bulk topological indices should be computed only with periodic boundary conditions. The index is again the pfaffian index of the real space first quantized Hamiltonian!

With translational invariance, easier job:

$$- \qquad \overline{\sqrt{}} \sum_{n=1}^{\infty} \sum$$

Because of the q ->-q symmetry (charge conjugation) only q=0, Pi are relevant as they do not come in pairs. The contribution of the other points to the pfaffian of the real space matrix is positive, as they come in pairs.



Kitaev P-Wave Wire, Bulk Index and Fermion Parity

Another equivalent classification is that for even number of sites, the topologically nontrivial state has ODD fermion parity.

Only k=0, Pi momenta are important. Other momenta are contributing even fermion parity because they come in pairs $(u_{\mathbf{k}} + v_{\mathbf{k}}c^{\dagger}_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}})$



At k=0, Pi the p-wave gap Sin(k) vanishes.

Hence whether k=0, Pi is occupied or not depends on the sign of:

 $2t\cos[k] + \mu$

For $|\mu| < 2t$ we are guaranteed that one of k=0, Pi will be occupied, while the other not (remember how we spoke about the winding?)

 $sign(\mu + 2t)sign(\mu - 2t)$

$$|\Omega\rangle = \prod_{\mathbf{k}\neq\mathbf{0}}' (u_{\mathbf{k}} + v_{\mathbf{k}}c_{\mathbf{k}}^{\dagger}c_{-\mathbf{k}}^{\dagger})c_{\mathbf{0}}^{\dagger}|0\rangle$$

Realizing Majorana Zero Modes in Experiments

Unfortunately p-wave gap is not easy to realize, especially in 1D. Hence we engineer it!

Add a chain of magnetic, classical highspin atoms on the top of an S-wave superconductor (no spin-orbit coupling). Can be done by STM

Key Ingredient: spiral arrangement of magnetic moments, usual magnetic spiral is expected





$$H = \sum_{n\alpha} t_n f_{n\alpha}^{\dagger} f_{n+1\alpha} + t_n^* f_{n+1\alpha}^{\dagger} f_{n\alpha} - \mu \sum_{n\alpha} f_{n\alpha}^{\dagger} f_{n\alpha} + \sum_{n\alpha\beta} (\vec{B}_n \cdot \vec{\sigma})_{\alpha\beta} f_{n\alpha}^{\dagger} f_{n\beta} + \sum_n \Delta_0 f_{n\uparrow}^{\dagger} f_{n\downarrow}^{\dagger} + \Delta_0 f_{n\downarrow} f_{n\uparrow}^{\dagger} + \Delta_0 f_{n\downarrow} f_{n\downarrow}^{\dagger} + \Delta_0 f_{n\downarrow} f_{n\uparrow}^{\dagger} + \Delta_0 f_{n\downarrow} f_{n\downarrow}^{\dagger} + \Delta_0 f_{n\downarrow} f_{n\downarrow} f_{n\downarrow}^{\dagger} + \Delta_0 f_{n\downarrow} f_{$$

For classical large atom spin (effective spiral B), each electron spin on chain is in low energy state antiparallel to the LOCAL B.

Realizing Majorana Zero Modes in Experiments

We go to a local basis of spin parallel and antiparallel to the magnetic moment on-site:

We go to a local basis of spin parallel and antiparallel to the magnetic moment on-site:

$$\widehat{\theta}_{n}$$

$$\begin{pmatrix} f_{n\uparrow} \\ f_{n\downarrow} \end{pmatrix} = U_n \begin{pmatrix} g_{n\uparrow} \\ g_{n\downarrow} \end{pmatrix} = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta_n/2)e^{-i\phi_n} \\ \sin(\theta_n/2)e^{i\phi} & \cos(\theta_n/2) \end{pmatrix} \begin{pmatrix} g_{n\uparrow} \\ g_{n\downarrow} \end{pmatrix}$$

$$H = \sum_{n,\alpha,\beta} t_n \Omega_{n,\alpha,\beta} g_{n\alpha}^{\dagger} g_{n+1\beta} + t_n^* \Omega_{n,\beta,\alpha}^* g_{n+1\alpha}^{\dagger} g_{n\beta} + B_0 \sigma_{z\alpha\beta} g_{n\alpha}^{\dagger} g_{n\beta} - \mu \sum_{n\alpha} g_{n\alpha}^{\dagger} g_{n\alpha} + \sum_n \Delta_0 (g_{n\uparrow}^{\dagger} g_{n\downarrow}^{\dagger} + g_{n\downarrow} g_{n\uparrow})$$

$$\beta_n = \sin \frac{\theta_{n+1} - \theta_n}{2}$$
Diagonal

$$\Omega_n = U_n^{\dagger} U_{n+1} = \begin{pmatrix} \alpha_n & -\beta_n^* \\ \beta_n & \alpha_n^* \end{pmatrix}$$
If magnetic spiral, hopping amplitude dependent
on spin - effectively creating spin-orbit coupling
(remember all the proposals to create Majorana with Rashba wires, B
field and superconducting - similar Hamiltonian)

Cassical atom spin (effective B), electron spin on chain has low energy state antiparallel to the LOCAL B. We can integrate out the high spin band to obtain effective p-wave pairing



Effective p-wave in lowest band $(\Delta_0 t_n/B)\Omega_{n\downarrow\uparrow}g_{n-1\downarrow}^{\dagger}g_{n\downarrow}^{\dagger}$

Realizing Kitaev P-Wave Wire in Experiments

More "realistic" self-consistent calculations can be performed



Open boundary conditions



5

6

3

4

 B/Δ





