

(Topological) Superconductivity with BdG

OUTLINE:

- ① Bogoliubov-de Gennes (BdG) theory
- ② Kitaev chain model & Majorana's
- ③ Engineering a TSC
- ④ Gapped TSC classes in $d=1,2,3$
- ⑤ Point and Line defects in TSC
- ⑥ Materials & signatures

→ LECTURE NOTES

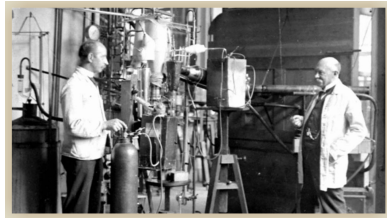
What is missing?

- Microscopic mechanism for pairing (like BCS)
 - Phenomenology
 - The order parameter(s) (beyond mean-field)
 - Exotic states
- } LATER
THIS
WEEK

Superconductivity



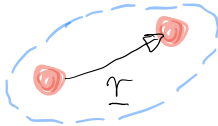
$\text{YBa}_2\text{Cu}_3\text{O}_{7+x} \rightarrow T_c = 93\text{K}$



K. ONNES,
LEIDEN [1911.]

Theory [1957.]

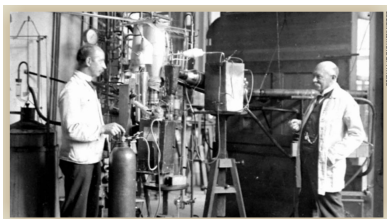
Electrons form Cooper pairs
due to effective attraction



Superconductivity



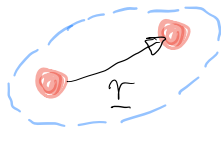
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Theory [1957]

Electrons form Cooper pairs
due to effective attraction



$$\langle C_{k\sigma}^\dagger C_{-k\sigma}^\dagger \rangle_{sc} \neq 0, \quad \begin{cases} k = \text{electron momentum} \\ \sigma = \text{electron spin} \end{cases}$$

$$\text{Relevant e-e interaction: } \sum_{\substack{k, k', \\ \sigma, \sigma', \lambda, \lambda'}} V_{kk'}^{\sigma\sigma'\lambda\lambda'} \underbrace{C_{k\sigma}^\dagger C_{-k\sigma}^\dagger} \underbrace{C_{-k'\lambda} C_{k'\lambda}}$$

Mean-field

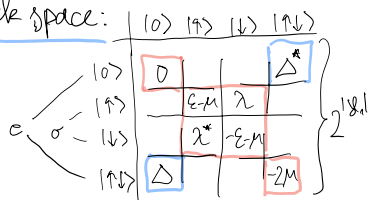
$$\text{Pairing function: } \Delta_k^{\sigma\sigma'} = \sum_{\lambda, \lambda'} V_{k, -k}^{\lambda\lambda'\sigma\sigma'} \langle C_{-k\lambda} C_{k\lambda'} \rangle$$

$$\hat{H}_{\text{pair}} = \sum_{k, \sigma, \sigma'} \left(\Delta_k^{\sigma\sigma'} C_{k\sigma}^\dagger C_{-k\sigma'}^\dagger + \text{h.c.} \right)$$

BdG or not? Single-site example

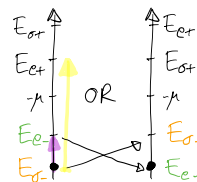
- 1-site, spinful: $\hat{H} = \varepsilon (C_{\uparrow}^{\dagger} C_{\uparrow} - C_{\downarrow}^{\dagger} C_{\downarrow}) + (\lambda C_{\uparrow}^{\dagger} C_{\downarrow} + \text{h.c.}) - \mu (n_{\uparrow} + n_{\downarrow}) + (\Delta C_{\uparrow}^{\dagger} C_{\downarrow}^{\dagger} + \text{h.c.})$

① Fock space:



$$E_{\sigma\pm} = \pm \sqrt{\varepsilon^2 + |\lambda|^2} - \mu$$

$$E_{e\pm} = \pm \sqrt{\mu^2 + |\Delta|^2} - \mu$$



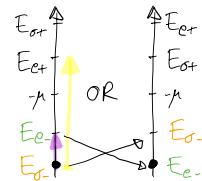
BdG or not? Single-site example

- 1-site, spinful: $\hat{H} = \varepsilon (C_{\uparrow}^{\dagger} C_{\uparrow} - C_{\downarrow}^{\dagger} C_{\downarrow}) + (\lambda C_{\uparrow}^{\dagger} C_{\downarrow} + \text{h.c.}) - \mu (n_{\uparrow} + n_{\downarrow}) + (\Delta C_{\uparrow}^{\dagger} C_{\downarrow}^{\dagger} + \text{h.c.})$

① Fock space:

$$\begin{array}{c}
 \begin{array}{c}
 |0\rangle \\
 |1\uparrow\rangle \\
 |1\downarrow\rangle \\
 |1\uparrow\downarrow\rangle
 \end{array}
 \begin{array}{c}
 \left\{ \begin{array}{c}
 \begin{array}{|c|c|c|c|}
 \hline
 0 & & & \Delta^* \\
 \hline
 \varepsilon - \mu & \lambda & & \\
 \hline
 \lambda^* & -\varepsilon - \mu & & \\
 \hline
 \Delta & & & -2\mu \\
 \hline
 \end{array}
 \end{array}
 \right\} 2 \cdot |8_n|
 \end{array}$$

$$\begin{aligned}
 E_{\sigma\pm} &= \pm \sqrt{\varepsilon^2 + |\lambda|^2} - \mu \\
 E_{e\pm} &= \pm \sqrt{\mu^2 + |\Delta|^2} - \mu
 \end{aligned}$$

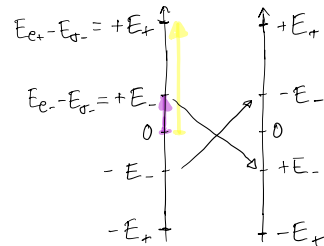


② BdG: $\hat{H} = \frac{1}{2} \hat{\Psi}^{\dagger} H_{\text{BdG}} \hat{\Psi} + \text{const}$

$$\hat{\Psi} \equiv \begin{pmatrix} C_{\uparrow} \\ C_{\downarrow} \\ C_{\uparrow}^{\dagger} \\ C_{\downarrow}^{\dagger} \end{pmatrix}$$

$$H_{\text{BdG}} = \begin{array}{c}
 \begin{array}{cc}
 C_{\uparrow} & C_{\downarrow} \\
 C_{\uparrow}^{\dagger} & C_{\downarrow}^{\dagger}
 \end{array}
 \begin{array}{|c|c|c|c|}
 \hline
 \varepsilon - \mu & \lambda & 0 & \Delta \\
 \hline
 \lambda^* & -\varepsilon - \mu & -\Delta & 0 \\
 \hline
 0 & -\Delta^* & -\varepsilon + \mu & -\lambda^* \\
 \hline
 \Delta^* & 0 & -\lambda & \varepsilon + \mu \\
 \hline
 \end{array}
 \end{array} \left\{ 2 \cdot |8_n| \right.$$

$$E_{\pm, \sigma\pm}^{\text{BdG}} = \pm \left(\sqrt{\varepsilon^2 + |\lambda|^2} + \alpha \cdot \sqrt{\mu^2 + |\Delta|^2} \right) \equiv \pm E_{\alpha}$$



BdG solution: Single-site example

② BdG: $\hat{H} = \frac{1}{2} \hat{\Psi}^\dagger H_{\text{BdG}} \hat{\Psi}$, where $\hat{\Psi}^\dagger = (c_\uparrow, c_\downarrow, c_\uparrow^\dagger, c_\downarrow^\dagger)$ is fermion spinor $\{\hat{\Psi}_i, \hat{\Psi}_j^\dagger\} = \delta_{ij}$

$H_{\text{BdG}} \chi_{a\pm} = \pm E_a \chi_{a\pm}; (\chi \in \mathbb{C}^4) \Rightarrow \hat{H} = \frac{1}{2} \sum_{a\pm} \pm E_a \hat{\chi}_{a\pm}^\dagger \hat{\chi}_{a\pm}$, where

Bogoliubon: $\boxed{\hat{\chi}_{a\pm}^\dagger} = \chi_{a\pm} \cdot \hat{\Psi}^\dagger = \chi_{a\pm}^1 \boxed{c_\uparrow^\dagger} + \chi_{a\pm}^2 \boxed{c_\downarrow^\dagger} + \chi_{a\pm}^3 \boxed{c_\uparrow} + \chi_{a\pm}^4 \boxed{c_\downarrow}$; $\{\hat{\chi}_A, \hat{\chi}_B^\dagger\} = \delta_{AB}$

(fermion)

electron "u" (red arrow pointing to $c_\uparrow^\dagger$)
hole "v" (blue arrow pointing to $c_\downarrow$)

BdG solution: Single-site example

② BdG: $\hat{H} = \frac{1}{2} \hat{\Psi}^\dagger \text{Hodg} \hat{\Psi}$, where $\hat{\Psi}^\dagger = (c_\uparrow, c_\downarrow, c_\uparrow^\dagger, c_\downarrow^\dagger)$ is fermion spinor $\{\hat{\Psi}_i, \hat{\Psi}_j^\dagger\} = \delta_{ij}$

$$\text{Hodg} \chi_{a\pm} = \pm E_a \chi_{a\pm} \Rightarrow \hat{H} = \frac{1}{2} \sum_{a\pm} \pm E_a \hat{\chi}_{a\pm}^\dagger \hat{\chi}_{a\pm}, \text{ where}$$

• Bogoliubon: $\begin{bmatrix} \chi_{a+}^\dagger \\ \chi_{a+} \end{bmatrix} = \chi_{a\pm} \cdot \hat{\Psi}^\dagger = \chi_{a+}^1 \begin{bmatrix} c_\uparrow^\dagger \\ c_\downarrow^\dagger \end{bmatrix} + \chi_{a+}^2 \begin{bmatrix} c_\uparrow^\dagger \\ c_\downarrow^\dagger \end{bmatrix} + \chi_{a+}^3 \begin{bmatrix} c_\uparrow \\ c_\downarrow \end{bmatrix} + \chi_{a+}^4 \begin{bmatrix} c_\uparrow \\ c_\downarrow \end{bmatrix}$; $\{\hat{\chi}_A, \hat{\chi}_B^\dagger\} = \delta_{AB}$
(fermion) electron "u" hole "v"

• Particle-Hole (PH) constraint: $(\hat{\Psi}_{1/2})^\dagger = \hat{\Psi}_{3/4}$, with $\tau_x = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\Psi_i^\dagger = \tau_x^{ij} \Psi_j$
(doubling)

$$\left[\hat{H} = \frac{1}{2} \hat{\Psi}^\dagger \text{Hodg} \hat{\Psi} = \frac{1}{2} (\tau_x \hat{\Psi})^\dagger \text{Hodg} (\tau_x \hat{\Psi}) = \frac{1}{2} \hat{\Psi}^\dagger (-\tau_x \text{Hodg} \tau_x) \hat{\Psi} \right]$$

$$\Rightarrow \text{Hodg}_B = -P \text{Hodg}_A P^{-1}, \text{ with } P \equiv \tau_x K \Rightarrow \text{Hodg} \chi_{a+} = +E_a \chi_{a+} \Rightarrow \text{Hodg}(P \chi_{a+}) = -E_a P \chi_{a+}$$

BdG solution: Single-site example

② BdG: $\hat{H} = \frac{1}{2} \hat{\Psi}^\dagger H_{\text{BdG}} \hat{\Psi}$, where $\hat{\Psi}^\dagger = (\underline{c}_\uparrow, \underline{c}_\downarrow, \underline{c}_\uparrow^\dagger, \underline{c}_\downarrow^\dagger)$ is fermion spinor $\{\hat{\Psi}_i, \hat{\Psi}_j^\dagger\} = \delta_{ij}$

$$H_{\text{BdG}} \chi_{a\pm} = \pm E_a \chi_{a\pm} \Rightarrow \hat{H} = \frac{1}{2} \sum_{a\pm} \pm E_a \hat{\chi}_{a\pm}^\dagger \hat{\chi}_{a\pm}, \text{ where}$$

• Bogoliubon: $\hat{\chi}_{a\pm}^\dagger = \chi_{a\pm}^\dagger \cdot \hat{\Psi}^\dagger = \chi_{a\pm}^\dagger \begin{bmatrix} \underline{c}_\uparrow^\dagger \\ \underline{c}_\downarrow^\dagger \end{bmatrix} + \chi_{a\pm}^2 \begin{bmatrix} \underline{c}_\uparrow \\ \underline{c}_\downarrow \end{bmatrix} + \chi_{a\pm}^3 \begin{bmatrix} \underline{c}_\uparrow \\ \underline{c}_\downarrow \end{bmatrix} + \chi_{a\pm}^4 \begin{bmatrix} \underline{c}_\uparrow^\dagger \\ \underline{c}_\downarrow^\dagger \end{bmatrix}$; $\{\hat{\chi}_A, \hat{\chi}_B^\dagger\} = \delta_{AB}$
(fermion) electron "u" hole "v"

• Particle-Hole (PH) constraint: $(\hat{\Psi}_{1/2})^\dagger = \hat{\Psi}_{3/4}$, with $\tau_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\Psi_i^\dagger = \tau_1^\dagger \Psi_i$
(doubling)

$$\left[\hat{H} = \frac{1}{2} \hat{\Psi}^\dagger H_{\text{BdG}} \hat{\Psi} = \frac{1}{2} (\tau_1 \hat{\Psi})^\dagger H_{\text{BdG}} (\tau_1 \hat{\Psi}) = \frac{1}{2} \hat{\Psi}^\dagger (-\tau_1 H_{\text{BdG}} \tau_1) \hat{\Psi} \right]$$

$$\Rightarrow H_{\text{BdG}} = -P H_{\text{BdG}} P^{-1}, \text{ with } P \equiv \tau_x K \Rightarrow H_{\text{BdG}} \chi_{a+} = +E_a \chi_{a+} \Rightarrow H_{\text{BdG}} (P \chi_{a+}) = -E_a P \chi_{a+}$$

$$\textcircled{1} \chi_{a-} = \tau_x \chi_{a+}^* \quad \textcircled{2} E_{-a} = -E_{+a} \quad \textcircled{3} \hat{\chi}_{a-}^\dagger = \hat{\chi}_{a+}^\dagger \quad [\chi_{a+}^* \cdot \hat{\Psi} = \chi_{a+}^* \tau_x \hat{\Psi}^\dagger = \chi_{a-} \hat{\Psi}^\dagger]$$

$$\Rightarrow \left[\hat{H} = \frac{1}{2} \sum_a (+E_a \hat{\chi}_{a+}^\dagger \hat{\chi}_{a+} - E_a \hat{\chi}_{a-}^\dagger \hat{\chi}_{a-}) = \sum_a |E_a| \hat{\chi}_{a+}^\dagger \hat{\chi}_{a+} + \text{const} \right]$$

BdG structure: Single-site example

● Bogoliubov free fermion structure:

① $|GS\rangle, \hat{\gamma}_{a=1}^+ |GS\rangle, \hat{\gamma}_{a=2}^+ |GS\rangle, \hat{\gamma}_{a=1}^+ \hat{\gamma}_{a=2}^+ |GS\rangle$: Fock states $2^{|S|}$ from $|S|$ fermionic excitations

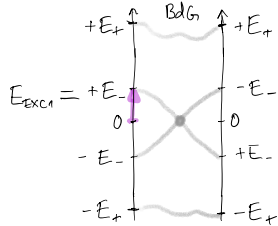
② $|GS\rangle = \text{vacuum of (+) Bogoliubons}$: $\hat{\gamma}_{a+} |GS\rangle \equiv 0, \forall a$

Build $|GS\rangle \equiv \prod_a \hat{\gamma}_{a+}^+ |\psi_0\rangle$, where $|\psi_0\rangle = |\text{vac}\rangle$ or $c_\sigma^+ |\text{vac}\rangle$, so that $|GS\rangle \neq 0$.
 $\Rightarrow$ BCS-like : $\hat{\gamma}_{a+}^+ |\psi_0\rangle = \sum_{\sigma} (u_{\sigma} c_{\sigma}^+ + v_{\sigma} c_{\sigma}) |\psi_0\rangle \sim (v_{\sigma} + u_{\sigma} c_{\sigma}^+ c_{\sigma}^+) |\tilde{\psi}_0\rangle$

③ Fermion parity $\hat{F} \sim c^{\dagger}c + c^{\dagger}c^{\dagger} + cc$ mixes $\begin{cases} \text{only } N = 0, 2, 4, \dots \\ \text{only } N = 1, 3, 5, \dots \end{cases}$ (Z_2 charge due to $c_{\sigma}^{\dagger} \rightarrow -c_{\sigma}^{\dagger}$)
 $\hat{F} \equiv (-1)^{\hat{N}} = \pm 1$

Parity and topology: Single-site example

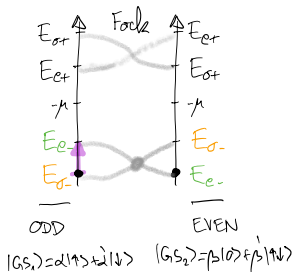
Gap-closing adiabatic transitions



Parity switch:

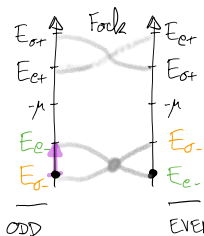
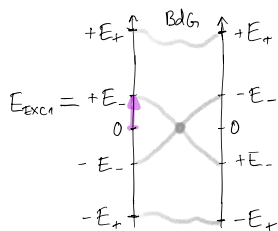
$$|GS_1\rangle \xrightarrow{\downarrow} |EXC_1\rangle = \hat{N}_{exc}^+ |GS_1\rangle = |GS_2\rangle$$

Fermion excitation
collapses $\rightarrow$ parity switch.



Parity and topology: Single-site example

Gap-closing adiabatic transitions



$$|GS_1\rangle = \alpha|\uparrow\rangle\alpha|\downarrow\rangle \quad |GS_2\rangle = \beta|\uparrow\rangle\beta|\downarrow\rangle$$

Parity switch:

$$|GS_1\rangle \xrightarrow{\downarrow} |EXC_1\rangle = \sum_{\alpha\alpha_2} \alpha_{\alpha\alpha_2}^+ |GS_1\rangle = |GS_2\rangle$$

Fermion excitation collapses $\rightarrow$ parity switch.

Parity = Topological Invariant

From H_{BdG} ? "Sign change" of E_a ?

$$\text{ALMOST: } F_{GS1} \cdot F_{GS2} = (\text{sgn Pf } X_1) \cdot (\text{sgn Pf } X_2)$$

Majorana basis $\lambda_{1\sigma} = C_{\sigma} + C_{\sigma}^+$
 $\lambda_{2\sigma} = i(C_{\sigma} - C_{\sigma}^+)$

$$\hat{H} = \frac{1}{2} \hat{\Psi}^+ H_{BdG} \hat{\Psi} = \frac{1}{2} i \hat{\lambda} X \hat{\lambda}$$

$$X^T = -X \Rightarrow X \simeq \begin{array}{c|c} E_a & \\ \hline -E_a & E_a \end{array}$$

$$\text{Pf } X = E_a \cdot E_a =$$

interesting in $d > 0$ dimensions.

BdG theory in general: setup

Second quantized Hamiltonian: $\hat{H} = \sum_{k,a,b}^P (\xi_k^{ab} - \mu \delta_{ab}) c_{ka}^\dagger c_{kb} + \frac{1}{2} \sum_{k,a,b}^P (\Delta_k^{ab} c_{ka}^\dagger c_{-k,b}^\dagger + \Delta_k^{ab*} c_{-k,b} c_{ka})$

Key idea: identify fermionic quasiparticles

$a, b = 1 \dots p$ P degrees of freedom in unit cell

- Nambu spinor:

$$\boxed{\Psi_k} = \begin{pmatrix} c_{k1} \\ \vdots \\ c_{kp} \\ \vdots \\ c_{-k1}^\dagger \\ \vdots \\ c_{-kp}^\dagger \end{pmatrix} \left. \begin{array}{l} \text{electrons} \\ \text{holes} \end{array} \right\} \Rightarrow \boxed{\Psi_k^\dagger} = \left(\underbrace{c_{k1}^\dagger, \dots, c_{kp}^\dagger}_{\text{electrons}}, \underbrace{c_{-k1}, \dots, c_{-kp}}_{\text{holes}} \right)_{2p}$$

- Indeed fermions:

$$\{\psi_{ka}, \psi_{k'a'}\} = \{\psi_{ka}^\dagger, \psi_{k'a'}^\dagger\} = 0$$

$$\{\psi_{ka}, \psi_{k'a'}^\dagger\} = \delta_{kk'} \delta_{aa'}$$

NOTE: Fourier space

$$\psi_k = \frac{1}{\sqrt{N}} \sum_{\alpha} e^{i k \alpha} \begin{pmatrix} c_{\alpha 1} \\ c_{\alpha p} \\ \vdots \\ c_{\alpha 1}^\dagger \\ \vdots \\ c_{\alpha p}^\dagger \end{pmatrix}$$

BdG theory: recipe

Goal: Rewrite $\hat{H} \equiv \frac{1}{2} \sum_{k,i,j} \psi_{ki}^\dagger H_{ki}^{ij} \psi_{kj} + \text{const} \leftarrow i,j=1 \dots 2p \text{ (c&d h)}$

RECIPE for BdG matrix (first quantized)

$$(H_{\text{BdG}}) \quad H_k = \begin{pmatrix} \overset{e}{\xi_k} & \overset{h}{\Delta_k} \\ \underset{h}{\Delta_k^\dagger} & -\xi_{-k}^\dagger \end{pmatrix}_{2p \times 2p}; \quad [\xi_k]_{p \times p} = \xi_k^{ab} - \mu, \quad a,b=1 \dots p$$

$$[\Delta_k]_{p \times p} = \frac{1}{2} (\Delta_k^{ab} - \Delta_{-k}^{ba}), \quad a,b=1 \dots p$$

Fermion constraint: $\Delta_k \equiv -\Delta_{-k}^\dagger$

$$\left[\text{because } \sum_{k,a,b} \Delta_k^{ab} c_{ka}^\dagger c_{-kb}^\dagger = \sum_{k,a,b} -\Delta_{-k}^{ab} c_{-kb}^\dagger c_{ka}^\dagger \xrightarrow[k \leftrightarrow -k]{a \leftrightarrow b} \sum_{k,a,b} (-\Delta_{-k}^{ba}) c_{ka}^\dagger c_{-kb}^\dagger \right]$$

BdG theory: solution

Bogoliubons: $\hat{H} \equiv \frac{1}{2} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} H_{\mathbf{k}} \Psi_{\mathbf{k}} = \frac{1}{2} \sum_{\mathbf{k}} \sum_{i=1}^{2p} E_{\mathbf{k}}^{(i)} \gamma_{\mathbf{k}}^{(i)\dagger} \gamma_{\mathbf{k}}^{(i)}$, $i=1 \dots 2p$

• 2p free Bogoliubov bands $E_{\mathbf{k}}^{(i)}$, $i=1 \dots 2p$

Bogoliubov fermion

BdG theory: solution

Bogoliubons: $\hat{H} \equiv \frac{1}{2} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger H_{\mathbf{k}} \Psi_{\mathbf{k}} = \frac{1}{2} \sum_{\mathbf{k}} \sum_{i=1}^{2p} E_{\mathbf{k}}^{(i)} \gamma_{\mathbf{k}}^{(i)} \gamma_{\mathbf{k}}^{(i)\dagger}, \quad i=1 \dots 2p$

- 2p free Bogoliubov bands $E_{\mathbf{k}}^{(i)}, i=1 \dots 2p$ Bogoliubov fermion

RECIPE: $H_{\mathbf{k}} \chi_{\mathbf{k}}^{(i)} = E_{\mathbf{k}}^{(i)} \chi_{\mathbf{k}}^{(i)} ; \chi_{\mathbf{k}}^{(i)} = \begin{pmatrix} u_{\mathbf{k}1}^{(i)} \\ \vdots \\ u_{\mathbf{k}p}^{(i)} \\ v_{\mathbf{k}1}^{(i)} \\ \vdots \\ v_{\mathbf{k}p}^{(i)} \end{pmatrix}$ 2p complex numbers

Bogoliubon: $\gamma_{\mathbf{k}}^{(i)\dagger} \equiv \sum_{a=1}^{2p} \chi_{\mathbf{k}a}^{(i)} \psi_{\mathbf{k}a}^\dagger = \sum_{a=1}^p \left(u_{\mathbf{k}a}^{(i)} c_{\mathbf{k}a}^\dagger + v_{\mathbf{k}a}^{(i)} c_{-\mathbf{k}a} \right)$

BdG theory: PHS constraint

Bogoliubons are NOT independent!

$$\psi_k \equiv \begin{pmatrix} \underbrace{c_{k1}}_{\text{e}} \vdots c_{kp} \\ \underbrace{c_{-k1}^\dagger} \vdots c_{-kp}^\dagger \end{pmatrix} \xrightarrow{\text{green arrow}} \psi_{k,p+1}^\dagger = \psi_{k,p+1}$$

$$\text{DEFINE: } \tau_x = \begin{pmatrix} \text{e} & \text{h} \\ 0 & 1 \end{pmatrix} \text{e} = \tau_x \otimes \mathbb{1}_p = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ 1 & & & 1 \end{pmatrix}_{2p \times 2p}$$

$\Rightarrow$ Particle-Hole Symmetry (constraint): $\psi_k^\dagger = (\tau_x \psi_{-k})^\dagger$ (second quantized)

$$\Rightarrow \tau_x H_{-k}^\dagger \tau_x = \tau_x H_{-k}^* \tau_x = -H_k \quad (\text{first quantized})$$

REMINDER:

$$H_k = \begin{pmatrix} \text{e} & \text{h} \\ \frac{\epsilon}{\hbar} \tau_k & \Delta_k \\ \text{h} & \Delta_k^\dagger \\ \Delta_k^\dagger & -\frac{\epsilon}{\hbar} \tau_k^\dagger \end{pmatrix}_{2p \times 2p}$$

$$P \equiv \tau_x K$$

$$P H_{-k} P^{-1} = -H_k \quad (\text{first quantized})$$

BdG theory: Interpretation

Bogoliubon doubling = PHS:

1st quant.: ① $(k, E_k^{(i)}) \Rightarrow (-k, -E_k^{(i)})$ ② $\chi_{-k}^{(i-)} = \tau_x \chi_k^{(i+)*} \Rightarrow$ 2nd g. ③ $\chi_{-k}^{(i-)+} = \chi_k^{(i+)}$

• Division into $E^{(i_+)} > 0$ and $E^{(i_-)} < 0$ at each k ; $i_+, i_- = 1 \dots p$

BdG theory: Interpretation

Bogoliubon doubling = PHS:

1st quant. : ① $(k, E_k^{(i)}) \Rightarrow (-k, -E_k^{(i)})$ ② $\chi_{-k}^{(i-)} = \tau_x \chi_k^{(i+)*} \Rightarrow$ 2nd g. ③ $\gamma_{-k}^{(i-)+} = \gamma_k^{(i+)}$

- Division into $E^{(i)} > 0$ and $E^{(i)} < 0$ at each k ; $i_+, i_- = 1 \dots p$

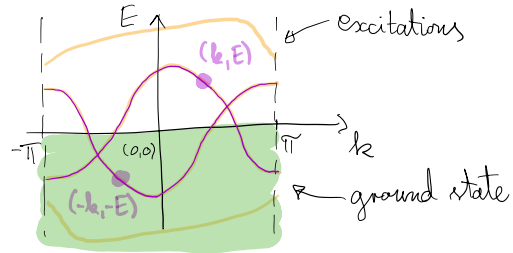
$$\Rightarrow \hat{H} = \frac{1}{2} \sum_k \sum_{i_-}^{2p} E_k^{(i_-)} \gamma_k^{(i_-)+} \gamma_k^{(i_-)} = \sum_k \sum_{i_+}^p |E_k^{(i_+)}| \gamma_k^{(i_+)+} \gamma_k^{(i_+)} + \text{const}$$

- GS is vacuum of positive Bogoliubons; $\gamma_k^{(i_+)} |GS\rangle \equiv 0, \forall k, i_+ = 1 \dots p$
- Bogoliubon excitations: $\gamma_k^{(i_+)+} |GS\rangle, \dots, E_k^{(i_+)} > 0$

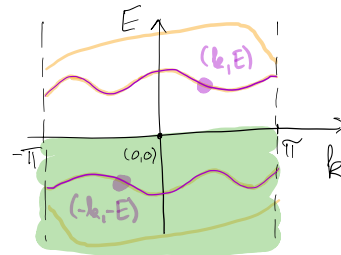
$$\left[\frac{1}{2} \sum_k \sum_{i_-}^{2p} E_k^{(i_-)} \gamma_k^{(i_-)+} \gamma_k^{(i_-)} \xrightarrow{k \rightarrow -k} \frac{1}{2} \sum_k \sum_{i_+}^p \overbrace{E_k^{(i_+)}}^{E_k^{(i_+)}} (-\gamma_k^{(i_+)+} \gamma_k^{(i_+)} + 1) \right]$$

BdG theory: Implications

BdG bands



HERE: GAPPED (T)SC



Band topology

Kitaev chain, PBC

1) Spinless electron model



$$\text{Real space: } \hat{H} = -\frac{1}{2} \sum_{\alpha} (t C_{\alpha}^{\dagger} C_{\alpha+1} + \text{h.c.}) - \mu \sum_{\alpha} C_{\alpha}^{\dagger} C_{\alpha} + \frac{1}{2} \sum_{\alpha} (\bar{\Delta} C_{\alpha}^{\dagger} C_{\alpha+1}^{\dagger} + \text{h.c.})$$

$$\text{Momentum: } \hat{H} = \sum_{\mathbf{k}} (-t \cos k - \mu) C_{\mathbf{k}}^{\dagger} C_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}} (\bar{\Delta} e^{i\mathbf{k}} C_{\mathbf{k}}^{\dagger} C_{-\mathbf{k}}^{\dagger} + \bar{\Delta}^* e^{i\mathbf{k}} C_{-\mathbf{k}} C_{\mathbf{k}})$$

BdG (RECIPE:) (assume $t > 0, \bar{\Delta} \in \mathbb{R}$)

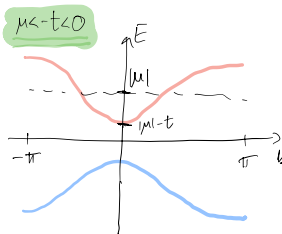
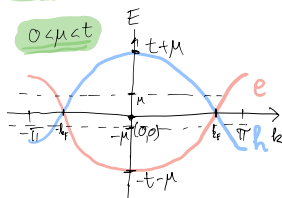
$$\psi_{\mathbf{k}} \equiv \begin{pmatrix} C_{\mathbf{k}} \\ C_{-\mathbf{k}}^{\dagger} \end{pmatrix}; \quad \tilde{\gamma}_{\mathbf{k}} = -t \cos k - \mu; \quad \Delta_{\mathbf{k}} \equiv \frac{1}{2} (\bar{\Delta} e^{i\mathbf{k}} - \bar{\Delta} e^{i\mathbf{k}}) = -i \bar{\Delta} \sin k$$

$$\Rightarrow H_{\mathbf{k}} = \frac{\tilde{\gamma}_{\mathbf{k}} \Delta_{\mathbf{k}}}{i \bar{\Delta} \sin k} \Rightarrow E_{\mathbf{k}}^{\pm} = \pm \sqrt{\tilde{\gamma}_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} = \pm \sqrt{(t \cos k + \mu)^2 + |\bar{\Delta}|^2 \sin^2 k}$$

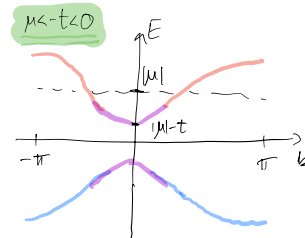
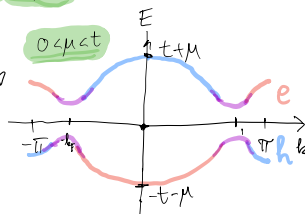
Kitaev chain, BdG bands

Mixing electrons and holes

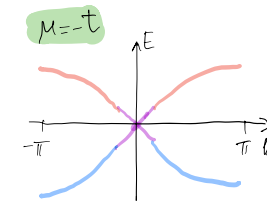
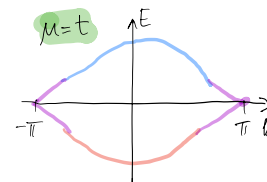
$\Delta \equiv 0$



$\Delta \neq 0$

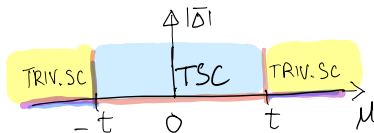


$$H_k = \begin{vmatrix} -t \cos k - \mu & -i \Delta \sin k \\ i \Delta^* \sin k & t \cos k + \mu \end{vmatrix}$$



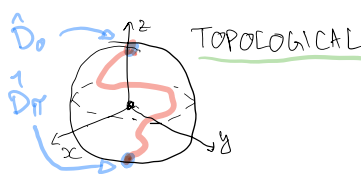
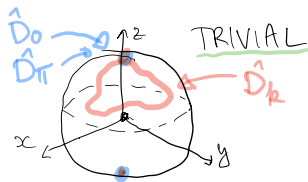
Kitaev chain, topology

Phase diagram



$$H_k = \begin{vmatrix} -t \cos k - \mu & -i \Delta \sin k \\ i \Delta^* \sin k & t \cos k + \mu \end{vmatrix}$$

Bulk topology: $H_k = \vec{D}_k \cdot \vec{\sigma}$; At $k=0, \pi$, $\Delta_k=0 \Rightarrow \hat{D}_k = \text{sgn}(\vec{z}_k) \cdot \hat{z}$



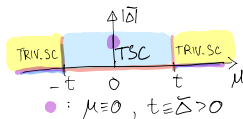
$\mathbb{Z}_2$ topological invariant: $W = \text{sgn}(\vec{z}_0) \cdot \text{sgn}(\vec{z}_\pi) = \begin{cases} -1, & |\mu| < t \\ +1, & |\mu| > t \end{cases}$
(for two bands)

Kitaev chain, open

Edge states

$$\alpha = 1 \text{ --- } 2 \text{ --- } 3 \text{ --- } \dots \text{ --- } N-1 \text{ --- } N$$

$$\hat{H} \equiv -\frac{1}{2} \sum_{\alpha}^{N-1} (t C_{\alpha}^{\dagger} C_{\alpha+1} + \text{h.c.}) - \mu \sum_{\alpha}^N C_{\alpha}^{\dagger} C_{\alpha} + \frac{1}{2} \sum_{\alpha}^{N-1} (\Delta C_{\alpha}^{\dagger} C_{\alpha+1}^{\dagger} + \text{h.c.})$$



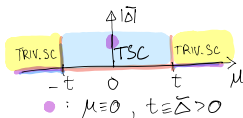
$$\hat{H}_T = \frac{t}{2} \sum_{\alpha=1}^{N-1} (-C_{\alpha}^{\dagger} C_{\alpha+1} - C_{\alpha+1}^{\dagger} C_{\alpha} + C_{\alpha}^{\dagger} C_{\alpha+1}^{\dagger} + C_{\alpha+1} C_{\alpha})$$

Kitaev chain, open

Edge states

$$\alpha = 1 \text{ --- } 2 \text{ --- } 3 \text{ --- } \dots \text{ --- } N-1 \text{ --- } N$$

$$\hat{H} \equiv -\frac{1}{2} \sum_{\alpha}^{N-1} (t c_{\alpha}^{\dagger} c_{\alpha+1} + \text{h.c.}) - \mu \sum_{\alpha}^{N-1} c_{\alpha}^{\dagger} c_{\alpha} + \frac{1}{2} \sum_{\alpha}^{N-1} (\tilde{\Delta} c_{\alpha}^{\dagger} c_{\alpha+1}^{\dagger} + \text{h.c.})$$



$$\hat{H}_T = \frac{t}{2} \sum_{\alpha=1}^{N-1} (-c_{\alpha}^{\dagger} c_{\alpha+1} - c_{\alpha+1}^{\dagger} c_{\alpha} + c_{\alpha}^{\dagger} c_{\alpha+1}^{\dagger} + c_{\alpha+1}^{\dagger} c_{\alpha})$$

Majorana fermions

$$\lambda_{\alpha R} \equiv c_{\alpha} + c_{\alpha}^{\dagger}$$

$$\lambda_{\alpha L} \equiv i(c_{\alpha} - c_{\alpha}^{\dagger})$$

$$\lambda_{\alpha R}^{\dagger} = \lambda_{\alpha R}$$

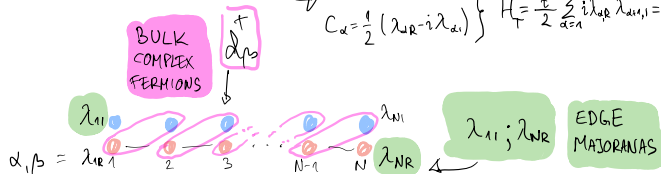
$$\lambda_{\alpha L}^{\dagger} = \lambda_{\alpha L}$$

"Real" fermion, not "complex"

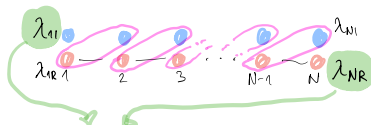
$$c_{\alpha}^{\dagger} = \frac{1}{2} (\lambda_{\alpha R} + i \lambda_{\alpha L})$$

$$c_{\alpha} = \frac{1}{2} (\lambda_{\alpha R} - i \lambda_{\alpha L})$$

$$\hat{H}_T = \frac{t}{2} \sum_{\alpha=1}^{N-1} i \lambda_{\alpha R} \lambda_{\alpha+1, L} = -t \sum_{\beta=1}^{N-1} (d_{\beta}^{\dagger} d_{\beta} - \frac{1}{2}), \quad \lambda_{1L}, \lambda_{NR} \text{ do not appear}$$



Majorana Bound States (MBS)



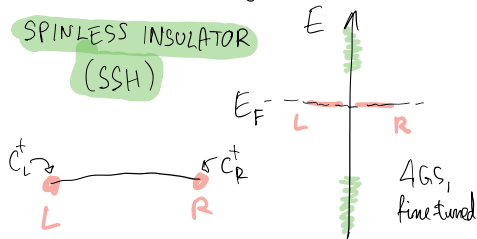
(our chain) $\alpha = 1 - 2 - 3 \dots N-1 - N$

$d_0^+ \equiv \frac{1}{2}(\lambda_{NR} + i\lambda_{11}) = \frac{1}{2}(c_N - c_1 + c_N^\dagger + c_1^\dagger)$: COMPLEX NON-LOCAL FERMION

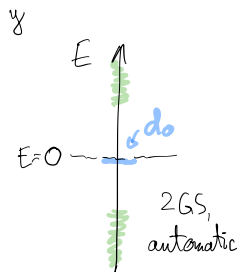
Consequences

- ① Ground State (GS) degeneracy: $\{|GS\rangle, d_0^+ |GS\rangle\}$
- ② Non-locality $\rightarrow$ non-Abelian anyon

SPINLESS INSULATOR (SSH)



TOPOLOGICAL SC (KITAEV CHAIN)



Pairing: Electron spin

Cooper pair: orbitals and spins

$$\Delta_{\mathbf{k}a\mathbf{b}}^{\sigma\sigma'} C_{\mathbf{k}a\sigma}^{\dagger} C_{\mathbf{k}b\sigma'}^{\dagger} |\text{vac}\rangle = \Delta_{\mathbf{k}a\mathbf{b}}^{\sigma\sigma'} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes |\sigma\sigma'\rangle; \sigma, \sigma' = \uparrow, \downarrow \text{ for } S_z = \pm \frac{1}{2}$$

orbital spin $a, b = 1 \dots r$ for orbitals

Adding two spins $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$

$$\sum_{\sigma, \sigma'} \Delta_{\mathbf{k}a\mathbf{b}}^{\sigma\sigma'} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes |\sigma\sigma'\rangle = \left(\frac{\Delta^{\uparrow\downarrow} - \Delta^{\downarrow\uparrow}}{2} |\mathbf{k}a; -\mathbf{k}b\rangle \right) \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) : S_z = 0 \} S = 0 \text{ [ODD] in } \sigma \leftrightarrow \sigma'$$

$$+ \left(\Delta^{\uparrow\uparrow} |\mathbf{k}a; -\mathbf{k}b\rangle \right) \otimes (|\uparrow\uparrow\rangle) : S_z = +1$$

$$+ \left(\Delta^{\downarrow\downarrow} |\mathbf{k}a; -\mathbf{k}b\rangle \right) \otimes (|\downarrow\downarrow\rangle) : S_z = -1$$

$$+ \left(\frac{\Delta^{\uparrow\downarrow} + \Delta^{\downarrow\uparrow}}{2} |\mathbf{k}a; -\mathbf{k}b\rangle \right) \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) : S_z = 0 \} S = 1 \text{ [EVEN] in } \sigma \leftrightarrow \sigma'$$

Fermion constraint: $|A_1 A_2\rangle \otimes |\downarrow_1 \downarrow_2\rangle = -|A_2 A_1\rangle \otimes |\downarrow_2 \downarrow_1\rangle \Rightarrow \Delta_{\mathbf{k}a\mathbf{b}} = -\Delta_{-\mathbf{k}b\mathbf{a}}$

↗ EVEN

↘ ODD

Pairing: Electron spin

Cooper pair: orbitals and spins

$$\Delta_{\mathbf{k}\sigma\sigma'}^{\sigma\sigma'} c_{\mathbf{k}\sigma\sigma'}^{\dagger} c_{-\mathbf{k}\sigma\sigma'}^{\dagger} |vac\rangle = \Delta_{\mathbf{k}\sigma\sigma'}^{\sigma\sigma'} |\underbrace{\mathbf{k}\sigma; -\mathbf{k}\sigma}_{\text{orbital}} \otimes \underbrace{|\sigma\sigma'\rangle}_{\text{spin}}\rangle; \sigma, \sigma' = \uparrow, \downarrow \text{ for } S_z = \pm \frac{1}{2}$$

$a, b = 1 \dots \mathcal{N}$ for orbitals

Adding two spins $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$

$$\sum_{\sigma, \sigma'}^{\uparrow, \downarrow} \Delta_{\mathbf{k}\sigma\sigma'}^{\sigma\sigma'} |\mathbf{k}\sigma; -\mathbf{k}\sigma'\rangle \otimes |\sigma\sigma'\rangle = \left(\frac{\Delta^{\uparrow\uparrow} - \Delta^{\downarrow\downarrow}}{2} |\mathbf{k}\sigma; -\mathbf{k}\sigma'\rangle \otimes (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) : S_z = 0 \right\} S = 0 \text{ [ODD] in } \sigma \leftrightarrow \sigma'$$

$$+ \left(\Delta^{\uparrow\uparrow} |\mathbf{k}\sigma; -\mathbf{k}\sigma'\rangle \otimes |\uparrow\uparrow\rangle \right) : S_z = +1$$

$$+ \left(\Delta^{\downarrow\downarrow} |\mathbf{k}\sigma; -\mathbf{k}\sigma'\rangle \otimes |\downarrow\downarrow\rangle \right) : S_z = -1$$

$$+ \left(\frac{\Delta^{\uparrow\downarrow} + \Delta^{\downarrow\uparrow}}{2} |\mathbf{k}\sigma; -\mathbf{k}\sigma'\rangle \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) : S_z = 0 \right\} S = 1 \text{ [EVEN] in } \sigma \leftrightarrow \sigma'$$

Fermion constraint: $|A_1 A_2\rangle \otimes |S_1 S_2\rangle = -|A_2 A_1\rangle \otimes |S_2 S_1\rangle \Rightarrow \Delta_{\mathbf{k}\sigma\sigma'} = -\Delta_{-\mathbf{k}\sigma'\sigma}$

EVEN
ODD

Kitaev chain: $C_{\mathbf{k}} \equiv C_{\mathbf{k}\uparrow}$ (spin polarized) $\Rightarrow$ pairing is triplet, odd in $\mathbf{k}$ ($\propto \sin \mathbf{k}$)

(PROBLEM) Materials? MBS $\uparrow\downarrow\uparrow \rightarrow$ gapped out

Pairing: Electron spin

Cooper pair: orbitals and spins

$$\Delta_{\mathbf{k}ab}^{\sigma\sigma'} c_{\mathbf{k}a\sigma}^\dagger c_{-\mathbf{k}b\sigma'}^\dagger |\text{vac}\rangle = \Delta_{\mathbf{k}ab}^{\sigma\sigma'} |\underbrace{\mathbf{k}a; -\mathbf{k}b}_{\text{orbital}} \otimes \underbrace{|\sigma\sigma'\rangle}_{\text{spin}}; \sigma, \sigma' = \uparrow, \downarrow \text{ for } S_z = \pm \frac{1}{2}$$

$a, b = 1 \dots r$ for orbitals

Adding two spins $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$

$$\sum_{\sigma, \sigma'} \Delta_{\mathbf{k}ab}^{\sigma\sigma'} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes |\sigma\sigma'\rangle = \left(\frac{\Delta_{\mathbf{k}}^{\uparrow\uparrow} - \Delta_{\mathbf{k}}^{\downarrow\downarrow}}{2} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) : S_z = 0 \right\} S = 0 \quad \boxed{\text{ODD}} \text{ in } \sigma \leftrightarrow \sigma'$$

$$+ \left(\Delta_{\mathbf{k}}^{\uparrow\downarrow} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes (|\uparrow\downarrow\rangle) : S_z = +1 \right)$$

$$+ \left(\Delta_{\mathbf{k}}^{\downarrow\uparrow} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes (|\downarrow\uparrow\rangle) : S_z = -1 \right)$$

$$+ \left(\frac{\Delta_{\mathbf{k}}^{\uparrow\downarrow} + \Delta_{\mathbf{k}}^{\downarrow\uparrow}}{2} |\mathbf{k}a; -\mathbf{k}b\rangle \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) : S_z = 0 \right) \left. \vphantom{\sum_{\sigma, \sigma'}} \right\} S = 1 \quad \boxed{\text{EVEN}} \text{ in } \sigma \leftrightarrow \sigma'$$

Fermion constraint: $|A_1 A_2\rangle \otimes |A_1 A_2\rangle = -|A_2 A_1\rangle \otimes |A_2 A_1\rangle \Rightarrow \Delta_{\mathbf{k}ab} = -\Delta_{-\mathbf{k}ba}$

EVEN
ODD

RECIPE:
DEFINITION
OF $\Psi, \vec{\sigma}$

$$[\Delta_{\mathbf{k}ab}]_{ss'} \equiv \left(\begin{array}{c|c} -dx + idy & d_z + \phi \\ \hline d_z - \phi & dx + idy \end{array} \right)_{ss'} = \left[\left(\phi_{\mathbf{k}}^{ab} \mathbb{1} + \vec{d}_{\mathbf{k}}^{ab} \cdot \vec{\sigma} \right) i\sigma_y \right]_{ss'}; \left\{ \begin{array}{l} \phi_{\mathbf{k}} = \phi_{\mathbf{k}}^T \\ \vec{d}_{\mathbf{k}} = -\vec{d}_{\mathbf{k}}^T \end{array} \right.$$

Pairing: Symmetries

- SC is a spontaneously symmetry-broken phase $\Rightarrow$ Landau theory

Normal state $G_N = (U(1) \times TR) \times SG \xrightarrow{T \leftrightarrow T_c} G_{SC} < G_N$. $\Delta_{\mathbf{k}}^{s,d}$ is order parameter, labeled by IRREPS of G_N .

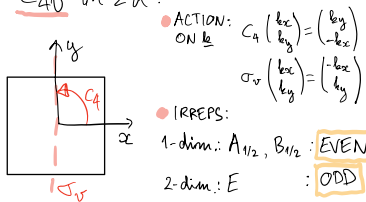
- Inversion symmetry

if $I_{inv} \in G_N$, then $I_{inv} \Delta I_{inv}^{-1} = \begin{cases} +\Delta, \text{EVEN} \Rightarrow \phi \text{ (SINGLET)} \\ -\Delta, \text{ODD} \Rightarrow \vec{d} \text{ (TRIPLT)} \end{cases}$

SOC
if $I_{inv} \notin G_N$, can mix $\phi, \vec{d}$

- Rotation symmetry (EXAMPLE)

C_{4v} in 2d:



IRREP BASIS FUNCTIONS:

E.g., for tight-binding problem,
on Bravais lattice $\{a\hat{x}, a\hat{y}\}$,
at nearest neighbor level:

$$A_1: \begin{cases} f_{\mathbf{k}}^{(A)} = \cos(k_x a) + \cos(k_y a) \\ f_{\mathbf{k}}^{(E,1)} = \sin(k_x a) \\ f_{\mathbf{k}}^{(E,2)} = \sin(k_y a) \end{cases}$$

• SINGLET SC ORDER PARAMETER
 $\Phi_{\mathbf{k}} = \eta^{(A)} f_{\mathbf{k}}^{(A)}$, $\eta^{(A)} \in \mathbb{C}$
"S-wave"

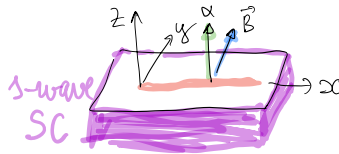
• TRIPLT SC ORDER PARAMETER
 $\vec{d}_{\mathbf{k}} = \eta^{(E,1)} f_{\mathbf{k}}^{(E,1)} + \eta^{(E,2)} f_{\mathbf{k}}^{(E,2)}$, $(\eta^{(E,1)}, \eta^{(E,2)}) \in \mathbb{C}^2$
"P-wave"

- Chiral SC: In SC such as $\vec{d} = \begin{pmatrix} p_x \\ p_y \end{pmatrix}$, system likes $p_x \neq i p_y$.

Realize MBS: Rashba wire

- Solution: Magic of Spin-Orbit Coupling (SOC)
- (ONE) RECIPE: Balance of singlet s-wave, SOC, and magnetic field.

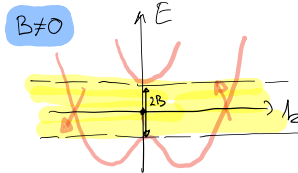
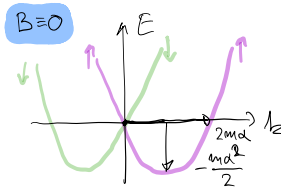
● Rashba SOC wire model:



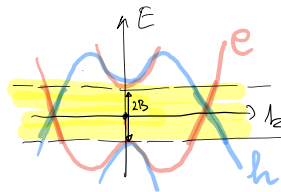
Realize MBS: Rashba wire

Bulk (PBC) Rashba wire: $\psi_k = \begin{pmatrix} C_{k\uparrow} \\ C_{k\downarrow} \\ C_{k\uparrow}^\dagger \\ C_{k\downarrow}^\dagger \end{pmatrix} \Rightarrow \begin{cases} \tilde{\epsilon}_k = \frac{k^2}{2m} - \alpha k \sigma_z + B \sigma_y - \mu \\ \Delta_k = \bar{\Delta} i \sigma_2 \text{ SINGLET } s\text{-wave} \leftarrow (\bar{\Delta} C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger + \text{h.c.}) \end{cases}$

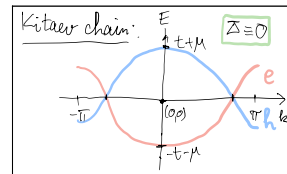
ξ_k ONLY
(not BdG)



BdG
 $\bar{\Delta} \equiv 0$
($\mu \neq 0$)



ONE BAND
IF
 $|\mu|, \bar{\Delta} < B$



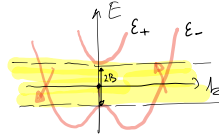
Realize MBS: SOC bands + s-wave pairing

- Triplet pairing introduced by SOC

$$H_k = \begin{pmatrix} \tilde{\zeta}_k & \Delta_k \\ \Delta_k^\dagger & -\tilde{\zeta}_k^\dagger \end{pmatrix}_{4 \times 4}; \psi_k = \begin{pmatrix} C_{k\uparrow} \\ C_{k\downarrow} \\ C_{k\uparrow}^\dagger \\ C_{k\downarrow}^\dagger \end{pmatrix} \rightarrow \text{Eigenbasis of } \tilde{\zeta}_k: \tilde{H}_k = \begin{pmatrix} \epsilon_{k+} & 0 & \tilde{\Delta}_+ & \tilde{\Delta}_- \\ 0 & \epsilon_{k-} & \tilde{\Delta}_+^\dagger & \tilde{\Delta}_-^\dagger \\ \tilde{\Delta}_+^\dagger & \tilde{\Delta}_-^\dagger & -\epsilon_{k+} & 0 \\ \tilde{\Delta}_+ & \tilde{\Delta}_- & 0 & -\epsilon_{k-} \end{pmatrix}; \tilde{\psi}_k = \begin{pmatrix} d_{k+} \\ d_{k-} \\ d_{k+}^\dagger \\ d_{k-}^\dagger \end{pmatrix}$$

INTRABAND $\Delta_{++} = \Delta_{--} = -\frac{i}{2} \cdot \tilde{\Delta} \cdot \frac{\alpha k}{\sqrt{(\alpha k)^2 + B^2}}: \text{ODD in } k_z$

INTERBAND $\Delta_{+-} = -\Delta_{-+} = -\frac{i}{2} \cdot \tilde{\Delta} \cdot \frac{B}{\sqrt{(\alpha k)^2 + B^2}}: \text{EVEN in } k_z$



Realize MBS: SOC bands + s-wave pairing

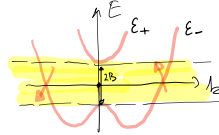
- Triplet pairing introduced by SOC

$$H_k = \begin{pmatrix} \tilde{z}_k & \Delta_k \\ \Delta_k^\dagger & -\tilde{z}_k^\dagger \end{pmatrix}; \Psi_k = \begin{pmatrix} C_{k\uparrow} \\ C_{k\downarrow} \\ C_{k\uparrow}^\dagger \\ C_{k\downarrow}^\dagger \end{pmatrix} \rightarrow \text{Eigenbasis of } \tilde{z}_k: \tilde{H}_k = \begin{pmatrix} \epsilon_{k+} & 0 \\ 0 & \epsilon_{k-} \\ \Delta^+ & -\epsilon_{k+} & 0 \\ 0 & -\epsilon_{k-} \end{pmatrix}; \tilde{\Psi}_k = \begin{pmatrix} d_{k+} \\ d_{k-} \\ d_{k+}^\dagger \\ d_{k-}^\dagger \end{pmatrix}$$

(helicity basis)

INTRABAND $\Delta_{++} = \Delta_{--} = -\frac{i}{2} \tilde{\Delta} \frac{\alpha k}{\sqrt{(\alpha k)^2 + B^2}} : \text{ODD in } k$

INTERBAND $\Delta_{+-} = -\Delta_{-+} = -\frac{i}{2} \tilde{\Delta} \frac{B}{\sqrt{(\alpha k)^2 + B^2}} : \text{EVEN in } k$



- Effectively a Kitaev chain in topo SC phase: $-\sqrt{\mu^2 + \tilde{\Delta}^2} < B < \sqrt{\mu^2 + \tilde{\Delta}^2}$ (full solution)

Controlled by $\mu, B, \tilde{\Delta} \Rightarrow$ gating, fields... control of MBS position

SOC works hard: split bands & allows singlet to be efficient.

GENERAL: Topo-SC from Δ_k or $\tilde{z}_k : \Delta_s C_{k\uparrow}^\dagger C_{k\downarrow}^\dagger \leadsto \Delta_s \psi_{k\uparrow}^* \psi_{k\downarrow}^* d_{k\downarrow}^\dagger d_{k\downarrow}^\dagger$
(BdG)

Classes of gapped SCs

● Strong TSC - from 10-fold table

$$H_{\mathbf{k}} = \begin{pmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^\dagger & -\xi_{\mathbf{k}}^\dagger \end{pmatrix}_{2 \times 2} ; \psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\uparrow}^\dagger \\ c_{\mathbf{k}\downarrow} \\ c_{\mathbf{k}\downarrow}^\dagger \end{pmatrix}$$

$SU(2)$
spin-rotation
symmetry

class	T^2	P^2	S^2	$d=0$	1	2	3
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2^{\text{CS}}$	$\mathbb{Z}^{\text{CI}}$	
DIII	-1	+1	+1		$\mathbb{Z}_2^{\text{CS}}$	$\mathbb{Z}_2^{\text{FI}}$	$\mathbb{Z}^{\text{VI}}$
C	0	-1	0			$2\mathbb{Z}$	
CI	+1	-1	+1				$2\mathbb{Z}$

Gapped SCs: d=1, class D

● Kitaev chain class! Has only the PHS constraint: $\tau_x H_k \tau_x = -H_{-k}$

class	T^2	P^2	S^2	$d=0$	1	2	3
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\mathbb{Z}$
DIII	-1	+1	+1		$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
C	0	-1	0			$2\mathbb{Z}$	
CII	+1	-1	+1				$2\mathbb{Z}$

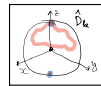
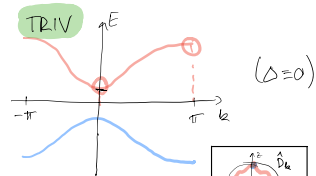
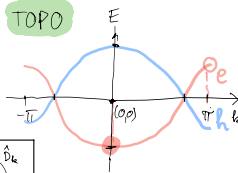
● Topological invariant

① Take Berry connection: $A_k^{ij} \equiv i\chi_k^{(i)\dagger} \cdot \partial_k \chi_k^{(j)}$, where $H_k \chi_k^{(i)} = E_k^{(i)} \chi_k^{(i)}$

② Chern-Simons integral $CS = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{i=1}^P A_k^{ii} \in \frac{\mathbb{Z}}{2}$ for filled BdG bands, $E_k^{(i)} < 0$

$$\Rightarrow \mathbb{Z}_2 : W \equiv e^{2\pi i \cdot CS} = \text{sgn}[\text{Pf}(X_{k=\pi}) \cdot \text{Pf}(X_{k=0})] = \pm 1 \begin{cases} \text{TRIV. SC} \\ \text{TOPO. SC} \end{cases}$$

For one electron band ($p=1$):
Electron filling @ $k=0$ vs. $k=\pi$



Gapped SCs: d=1, class DIII

• Spinful Time-Reversal Symmetry: $\sigma_y H_{k_2} \sigma_y = H_{-k_2}$

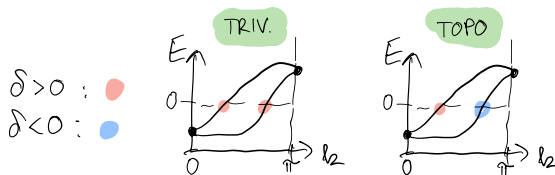
• Topological invariant $\mathbb{Z}_2: W_k = \pm 1 \begin{cases} \text{TRIV. SC} \\ \text{TOPO. SC} \end{cases}$

class	T^2	P^2	S^2	± 0	1	2	3
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2^2$	
DIII	-1	+1	+1		$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2^2$
C	0	-1	0			$\mathbb{Z}_2$	
CII	+1	-1	+1				$\mathbb{Z}_2^2$

• Key simplification: $|\Delta| \ll E_F$, topology should depend on Fermi surface (FS) and Δ

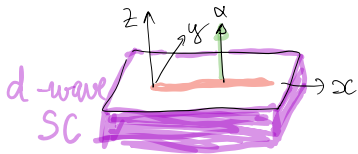
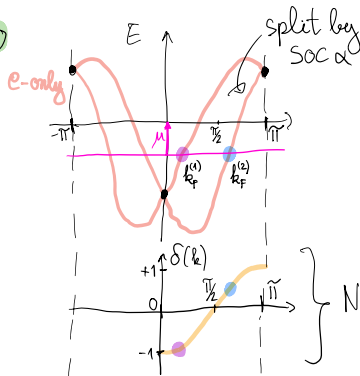
$N_{1d} \equiv \prod_s \text{sgn}(\delta_{k_F^{(s)}}) = W_k$, s labels all Fermi points $0 < k_F^{(s)} < \pi$.

$\delta_{k_F^{(s)}} \equiv \chi_{k_F^{(s)}}^{\dagger} (T \Delta_k^{\dagger}) \chi_{k_F^{(s)}} \in \mathbb{R} \rightarrow$ "sign of pairing"



Rashba wire to realize DIII TSC

Rashba wire + d-wave SC, NO B-field


$$\Delta \equiv 0$$


- s-wave: $C_{x\uparrow}^+ C_{x\downarrow}^+ \rightarrow C_{k\uparrow}^+ C_{-k\downarrow}^+$
- d-wave: $C_{x+1\uparrow}^+ C_{x\downarrow}^+ - C_{x+1\downarrow}^+ C_{x\uparrow}^+ \rightarrow \cos k \cdot C_{k\uparrow}^+ C_{-k\downarrow}^+$

$$\begin{aligned} \xi_k &= \frac{\hbar^2}{2m} - \underline{\alpha \hbar \sigma_z} - \mu \\ \Delta_k &= \underline{\bar{\Delta} \cos k(i\sigma_y)} \end{aligned} \quad \text{SINGLET d-wave}$$

- Precise solution: TSC for $1\text{M}\Omega$.
(Kramers pair of MBS at each end.)

$$N_{1d} = \text{sgn}[\delta(k_F^{(1)}) \cdot \delta(k_F^{(2)})] = -1 \text{ if } |\mu| < \alpha$$

Gapped SCs: d=2, class D

- Time-reversal broken. Has only the PHS constraint: $T_x H_k T_x = -H_k$

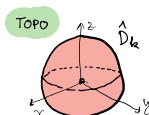
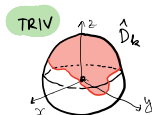
class	T^2	P^2	S^2	± 0	1	2	3
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
DIII	-1	+1	+1		$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}^{(2)}$
C	0	-1	0			$\mathbb{Z}$	
CI	+1	-1	-1				$2\mathbb{Z}$

- Topological invariant: The usual Chern number $Ch \in \mathbb{Z}$

- Some other forms

EXAMPLE: $H_k = \begin{pmatrix} \xi_k & \Delta(\sin k_x - i \sin k_y) \\ \Delta(\sin k_x + i \sin k_y) & -\xi_k \end{pmatrix} \Rightarrow \vec{D}_k = (D_x, D_y, D_z) = (\Delta \sin k_x, \Delta \sin k_y, \xi_k)$

For one electron band ($p=i$), $H_k = \vec{D}_k \cdot \vec{\tau}$, and $Ch = \# \text{wraps of } \vec{D}_k$



- TSC in this class is "chiral", and is expected when SC pairing is chiral, e.g., $p_x \pm i p_y$, $dx^2 - y^2 \pm i dx dy$.

EXERCISE
TOMORROW

Gapped SCs: d=2, class DIII

Spinful Time-Reversal Symmetry: $\sigma_y H_{\mathbf{k}}^* \sigma_y = H_{-\mathbf{k}}$

class	T^2	P^2	S^2	$\pm D$	1	2	3
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2^2$	
DIII	-1	+1	+1		$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^4$
C	0	-1	0			$\mathbb{Z}_2$	
CI	+1	-1	+1				$\mathbb{Z}_2^2$

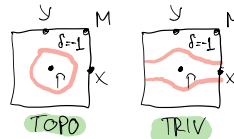
Topological invariant: $\mathbb{Z}_2$: $FK = \pm 1 \begin{cases} \text{TRIV. SC} \\ \text{TOPO. SC} \end{cases}$

Key simplification: IF $\Delta \ll E_F$:

$$N_{2d} \equiv \prod_s \text{sgn}(\delta_s)^{m_s} = FK, \quad s \text{ labels all Fermi lines}$$

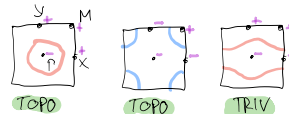
$m_s = \# \text{ TRIM enclosed by } s\text{-th Fermi line}$

$$\delta_s \equiv \chi_{\mathbf{k}_F}^{(d_s)} + (\Gamma \Delta_{\mathbf{k}}^*) \chi_{\mathbf{k}_F}^{(d_s)} \in \mathbb{R} \rightarrow \text{"sign of pairing"}$$



Another simplification: If $\xi_{\mathbf{k}}$ has inversion, and Δ is pure triplet, $p=1$

$$N_{2d} = (-1)^{p_0}, \quad \text{where } p_0 = \# \text{ connected components of Fermi line}$$

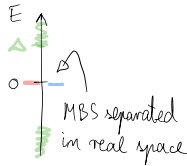


Point defects: Majorana Bound State

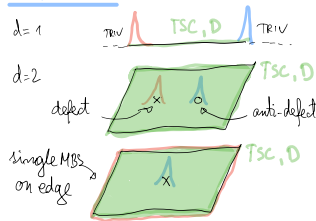
class	T^2	P^2	S^2	$d=1$			
D	0	1	0	$\mathbb{Z}_2$ 	$\mathbb{Z}_2$ 	$\mathbb{Z}_2$ 	$\rightarrow$ Majorana Bound State (MBS)
DIII	-1	1	1	$\mathbb{Z}_2$ 	$\mathbb{Z}_2$ 	$\mathbb{Z}_2$ 	$\rightarrow$ Kramers pair of MBS
C	0	-1	0				
CI	+1	-1	1				

① MBS: class D ($\mathbb{Z}_2$)

ENERGY:

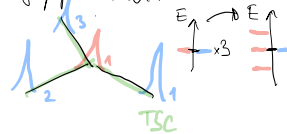


REALSPACE:



TOPOLOGICAL PROTECTION

Locally, odd vs. even
of MBS is distinguished.
In TSC, all except one
red and one blue can be
gapped out.



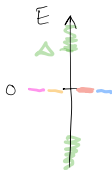
NOTE: Fundamentally, we don't need the blue partner.

Point defects: Majorana Bound State

class	T^2	P^2	S^2	$d=1$	$d=2$	$d=3$	
D	0	+1	0	$\mathbb{Z}_2^{CS_1}$	$\mathbb{Z}_2^{CS_2}$	$\mathbb{Z}_2^{CS_3}$	← Majorana Bound State (MBS)
DIII	-1	+1	+1	$\mathbb{Z}_2^{CS_1}$	$\mathbb{Z}_2^{CS_2}$	$\mathbb{Z}_2^{CS_3}$	← Kramers pair of MBS
C	0	-1	0				
CI	+1	-1	+1				

② Kramers MBS, class DIII ($\mathbb{Z}_2$)

ENERGY:



REALSPACE:



$$\lambda_1 = \sum_{\alpha} \chi_{\alpha} \psi_{\alpha}$$

$$\lambda_1' = \sum_{\alpha} (\tau x_{\alpha})_{\alpha} \psi_{\alpha}$$

λ_1, λ_1' are independent!

Kramers theorem: $T^2 = -1 \Rightarrow \chi_{\alpha}^{\dagger} (\tau x_{\alpha}) = 0$
(Wigner)

TOPOLOGICAL PROTECTION

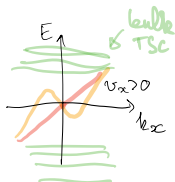
Topology distinguishes
odd vs. even # of K. pairs
If # K. p. = odd, one
pair is protected.

Line defects: Chiral Majorana Mode

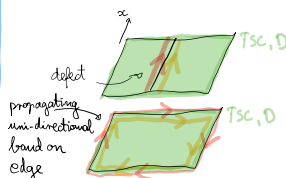
class	T^2	P^2	S^2	$d=1$			
D	0	+1	0		$\mathbb{Z}$ C_2	$\mathbb{Z}$ C_2	← Chiral Majorana Mode (cMM)
DIII	-1	+1	+1		$\mathbb{Z}_2$ F_4	$\mathbb{Z}_2$ F_4	← Helical MM (hMM)
C	0	-1	0		$2\mathbb{Z}$ $2C_2$	$2\mathbb{Z}$ $2C_2$	← Chiral Dirac Mode
CI	+1	-1	+1				

① Chiral MM, class D ($\mathbb{Z}$)

ENERGY:



REALSPACE:



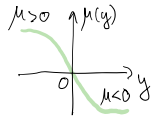
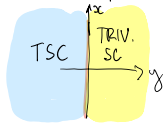
TOPOLOGICAL PROTECTION

$\mathbb{Z}$ is $(\# \text{ modes } v_x > 0) - (\# \text{ modes } v_x < 0)$.

cMM cannot hybridise with itself or other cMM of same chirality.

An example of Chiral Majorana Mode

Take spinless (chiral) p-ip SC in 2d



In bulk, $\mu > 0$ is TSC/TRIV SC.

Here, $\Delta(k_x - i k_y) \rightarrow \bar{\Delta}(k_x - 2y)$.

Neglect $\frac{(\nabla^2)^2}{2m}$, due to slow variation of $\mu \Rightarrow H_{\text{BdG}} = \frac{-\mu(y)}{\bar{\Delta}(k_x + 2y)} \frac{\bar{\Delta}(k_x - 2y)}{\mu(y)}$

Solutions localized around $y=0$:

1st quant: $\chi_{k_x, y} \sim e^{+\frac{1}{2} \int dy \mu(y)} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

with $E = \bar{\Delta} k_x$ } chiral MM

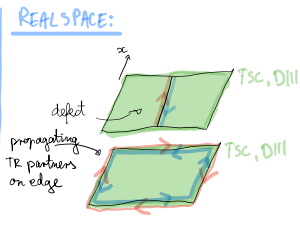
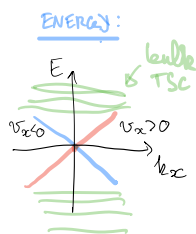
2nd quant: $\chi_{k_x, y} \sim |f(y)| (C_{k_x, y} + C_{k_x, y}^+)$

NOTE: For p+ip pairing, $E = -\Delta k_x$ and $\begin{pmatrix} 1 \\ 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

Line defects: Helical Majorana Mode

class	T^2	P^2	S^2	$d=1$			
D	0	+1	0		$\mathbb{Z}$ C_2	$\mathbb{Z}$ C_2	← Chiral Majorana Mode (cMM)
DIII	-1	+1	+1		$\mathbb{Z}_2$ FK_1	$\mathbb{Z}_2$ FK_2	← Helical MM (hMM)
C	0	-1	0		$2\mathbb{Z}$ $2C_2$	$2\mathbb{Z}$ $2C_2$	← Chiral Dirac Mode
CI	+1	-1	+1				

② Helical MM, class DIII ($\mathbb{Z}_2$)



TOPOLOGICAL PROTECTION

Distinguishes odd vs. even pairs $\cancel{\lambda}$. The λ of one pair can hybridize with $\cancel{\lambda}$ of another pair, so only 1 pair protected.

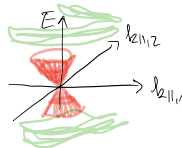
$$\text{Kramers pair: } T\lambda_b T^{-1} = \lambda_{b\downarrow}$$

Planar defects



class	T^2	p^2	S^2	$d=1$	2	3
D	0	+1	0			
DIII	-1	+1	+1			$\mathbb{Z}$ ^{v_3}
C	0	-1	0			
CI	+1	-1	+1			$2\mathbb{Z}$ ^{$2v_3$}

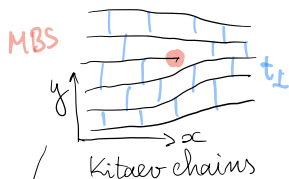
Surface mode of 3d TSC in class D is a "cone of Majorana's".



MBS from weak topology

- In 2d class D, MBS without chiral SC?

Kitaev wires:



- As $t_{\perp}$ grows $\rightarrow$ 2d system with $Ch=0$.
MBS remains? Weak Topology:

class	T^2	P^2	S^2	$d=0$	1	2
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
					w	Ch

Weak indices $\vec{G}_w = (w_x, w_y)$.

- $\vec{G}_w = (0, 1) \Rightarrow$
- Edge state along y
 - MBS on dislocation $\vec{b} = \hat{y}$.

Experimental Signatures

- ① Zero-bias conductance peak in STS/tunnel junction
- ② Quantized thermal Hall conductivity
- ③ Thermal conductivity and spin current
- ④ Anomalous Josephson effect
- ⑤ Transport through wire

Where to search for topological SC?

Theorems?

- 1 Possible (not necessary): (1) odd pairing, (2) gapped; (3) count of FS pockets.
(1) is automatic in spin-split bands; (2) in 2d chiral SC
- 2 MBS only with broken spin-rotations $\Rightarrow$ Odd pairing and SOC help.

Candidate systems?

INTRINSIC

- Heavy fermions UTe_2, UPt_3 (TRS breaking)...
- $SmRuO_4$ disproven p+ip after 20+ years
- Fe-based: $FeSe_{1-x}Te_x$... (vortex MBS)
- Doped TIs: $Cu_xBi_2Se_3$...
- TMDs, van der Waals (ABC graphene...)

EXTRINSIC

- 1d proximity residues
- 2d TI + s-wave SC
- Defect engineering...

BEYOND:

- Crystalline TSC: doping TCI ($LaNiGa_2$)
- Weak TSC, even with even pairing
- Gapless, chiral-even pairing ...