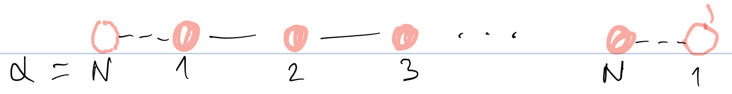
PART 1: BdG, KITAEV CHAIN

Consider a 1d model – the Kitaev chain:



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

$\Delta \in \mathbb{C}$ is pairing function, to be discussed later.

$c_{\alpha} \equiv \frac{1}{\sqrt{N}}\sum_{k} e^{-ik\alpha} c_{k} \Rightarrow c_{\alpha}^{+} = \frac{1}{\sqrt{N}}\sum_{k} e^{ik\alpha} c_{k}^{+}$ momentum k; lattice constant $= 1$.

PBC : $e^{ik(Na)} = 1 \Rightarrow k = \frac{2\pi}{Na} \cdot m$; $m \in \mathbb{Z}$

BZ : $K = 2\pi \Rightarrow k \in [-\pi, \pi) = 1BZ$

NOTE : $\sum_{n=1}^{N} e^{ikn} = N \sum_{\ell=-\infty}^{+\infty} \delta_{k, \ell \cdot 2\pi}$

for $k \in 1BZ$: $= N \delta_{k,0}$

$$\hat{H} = -\frac{1}{2}\sum_{k}\left(t c_{k}^{+} c_{k} e^{-ik} + h.c.\right) - \mu \sum_{k} c_{k}^{+} c_{k} + \frac{1}{2}\sum_{k}\left(\Delta e^{-ik} c_{k}^{+} c_{-k}^{+} + h.c.\right)$$

$$= \sum_{k}\left(-t\cos k - \mu\right) c_{k}^{+} c_{k} + \frac{1}{2}\sum_{k}\left(\Delta e^{-ik} c_{k}^{+} c_{-k}^{+} + \Delta^{*} e^{+ik} c_{-k} c_{k}\right)$$

1.A Bogoliubov–de Gennes theory

Uncover the excitation structure in $\hat{H}$ using that electrons and holes are fermions. Let's do general $\hat{H}$ with k representing a d-dimensional momentum vector, and having $a = 1 \ldots P$ degrees of freedom in unit-cell, which may include spin ↑,↓.

$$\hat{H} \equiv \sum_{k,a,b}\left(\varepsilon_{k}^{ab} - \mu \delta_{ab}\right) c_{ka}^{+} c_{kb} + \frac{1}{2}\sum_{k,a,b}\left(\Delta_{k}^{ab} c_{ka}^{+} c_{-kb}^{+} + \Delta_{k}^{ab*} c_{-kb} c_{ka}\right)$$

NOTE: $\varepsilon_{k}^{ab} = \varepsilon_{k}^{ba*}$

Key idea „Namber spinor":

$$\Psi_{k} \equiv \begin{pmatrix} c_{k1} \\ \vdots \\ c_{kP} \\ \hline c_{-k1}^{+} \\ \vdots \\ c_{-kP}^{+} \end{pmatrix} \begin{matrix} \left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\} e \\ \left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\} h \end{matrix} \Rightarrow \Psi_{k}^{+} = (\underbrace{c_{k1}^{+}, \ldots, c_{kP}^{+}}_{\text{electron}} | \underbrace{c_{-k1}, \ldots, c_{-kP}}_{\text{hole}})$$

NOTE: $\Psi_{k} = \frac{1}{\sqrt{N}}\sum_{\alpha} e^{ik\alpha} \begin{pmatrix} c_{\alpha 1} \\ \vdots \\ c_{\alpha P} \\ \hline c_{\alpha 1}^{+} \\ \vdots \\ c_{\alpha P}^{+} \end{pmatrix}$

$\Rightarrow \{\Psi_{ka}, \Psi_{k'a'}\} = \{\Psi_{ka}^{+}, \Psi_{k'a'}^{+}\} = 0$; $\{\Psi_{ka}, \Psi_{k'a'}^{+}\} = \delta_{kk'}\delta_{aa'} \Rightarrow \Psi_{ka}$ are <u>FERMIONS</u>.

$$\hat{H} \equiv \frac{1}{2} \Psi_k^{\dagger} H_k \Psi_k = \frac{1}{2} \Psi^{\dagger}_{ka} H_k^{ab} \Psi_{kb}$$

$[H_k]_{2p\times 2p}$ is the BdG Hamiltonian (matrix), representing $\hat{H}$ as fermionic bilinear.

1.A1 How to find H_k matrix?

"Undo" the ordering of electrons and holes: $c_i^{\dagger} c_j \to \frac{1}{2}\{(c_i)^{\dagger}(c_j) + [\delta_{ij} - (c_j^{\dagger})^{\dagger}(c_i^{\dagger})]\}$

Need to care about k too: $\hat{H} \equiv \sum_{k,a,b} \xi_k^{ab} c^{\dagger}_{ka} c_{kb} + \frac{1}{2}\sum_{k,a,b}(\Delta_k^{ab} c^{\dagger}_{ka} c^{\dagger}_{-kb} + h.c.)$

NOTE:
$\xi_k^{ab} \equiv \varepsilon_k^{ab} - \mu\delta_{ab}$

① $$\sum_{kab} \xi_k^{ab} c^{\dagger}_{ka} c_{kb} = \frac{1}{2}\sum_{kab}\{\xi_k^{ab}(c_{ka})^{\dagger}(c_{kb}) + \xi_k^{ab}\delta_{ab} - \underbrace{\xi_k^{ab}(c_{kb}^{\dagger})^{\dagger}(c_{ka}^{\dagger})}_{\substack{k\to -k \text{ in sum} \\ a\leftrightarrow b}}\} =$$

$$= \sum_{kab} \frac{1}{2}\left\{\xi_k^{ab}(c_{ka})^{\dagger}(c_{kb}) - \xi_{-k}^{ba}(c^{\dagger}_{-ka})^{\dagger}(c^{\dagger}_{-kb})\right\} + \frac{1}{2}\sum_k \mathrm{Tr}\, \xi_k$$

② $$\frac{1}{2}\sum_{kab} \Delta_k^{ab} c^{\dagger}_{ka} c^{\dagger}_{-kb} = \frac{1}{2}\sum_{kab}\Delta_k^{ab}(c_{ka})^{\dagger}(c^{\dagger}_{-kb})$$

Since $\{c_i^{\dagger}, c_j^{\dagger}\} = 0, \forall i,j$, we get a fermionic constraint:

$$\sum_{kab} \Delta_k^{ab} c^{\dagger}_{ka} c^{\dagger}_{-kb} = \sum_{kab} -\Delta_k^{ab} c^{\dagger}_{-kb} c^{\dagger}_{ka} = \sum_{kab} -\Delta_{-k}^{ba} c^{\dagger}_{ka} c^{\dagger}_{-kb} \Rightarrow \Delta_k^{ab} = -\Delta_{-k}^{ba} \Rightarrow$$

$$\Rightarrow \Delta_k \to \frac{1}{2}(\Delta_k - \Delta^{T}_{-k})$$

$$\Rightarrow H_k = \begin{array}{c|c|c} & e & h \\ \hline e & \xi_k & \Delta_k \\ \hline h & \Delta_k^{\dagger} & -\xi^{T}_{-k} \end{array} ; \left\{ \begin{array}{l} \xi_k^{\dagger} = \xi_k \\ \Delta_k = -\Delta^{T}_{-k} \end{array} \right\} ; \hat{H} = \frac{1}{2}\Psi_k^{\dagger} H_k \Psi_k + \frac{1}{2}\sum_k \mathrm{Tr}\,\xi_k$$

Hermiticity

Hermiticity

fermions

1.A2 BdG doubling: $[\xi, \Delta]_{p\times p} \to [H_k]_{2p\times 2p} \Rightarrow$ PARTICLE-HOLE CONSTRAINT "(PHS)"

τ_i = Pauli matrices acting on $\begin{pmatrix} e \\ h \end{pmatrix} \Rightarrow \Psi^{\dagger}_{ka} = (\tau_x \Psi_{-k})_a = \tau_x^{ab}\Psi_{-kb}$

$$\hat{H} = \frac{1}{2}\sum_{kab} \Psi^{\dagger}_{ka} H_k^{ab} \Psi_{kb} = \frac{1}{2}\sum_{kabcd}(\tau_x^{ac}\Psi_{-kc}) H_k^{ab} (\tau_x^{bd}\Psi^{\dagger}_{-kd}) = \frac{1}{2}\sum_{kcd}[\tau_x^{T} H_k \tau_x]_{cd} \Psi_{-kc}\Psi^{\dagger}_{-kd}$$

$$\overset{k\to -k}{=} \frac{1}{2}\sum_{kcd}[\tau_x H_{-k}\tau_x]_{cd}(\delta_{cd} - \Psi^{\dagger}_{kd}\Psi_{kc}) = \frac{1}{2}\sum_{kcd}\Psi^{\dagger}_{kd}(-)[\tau_x H_{-k}\tau_x]^{T}_{dc}\Psi_{kc} + \frac{1}{2}\sum_k \mathrm{Tr}(\tau_x H_{-k}\tau_x) =$$

$$= \frac{1}{2}\sum_k \Psi_k^{\dagger}(-\tau_x H^{T}_{-k}\tau_x)\Psi_k + \frac{1}{2}\sum_k \mathrm{Tr}(H_k)$$

NOTE: $\sum_k \mathrm{Tr}(H_k) = \sum_k \left[\mathrm{Tr}\,\xi_k + \mathrm{Tr}\left(-\xi^T_{-k}\right)\right] = \sum_k \left(\mathrm{Tr}\,\xi_k - \mathrm{Tr}\,\xi_{-k}\right) = \sum_k (\text{odd in } k) = 0$

$\Rightarrow$ BdG Particle-Hole Symmetry (PHS): $\underline{H_k = -\tau_x H^T_{-k} \tau_x}$

$\Rightarrow$ <u>an automatic constraint</u>

- On matrix level, $P \equiv \tau_x K$, with K = complex conjugation in k-basis (does not flip k)

$P^{-1} = P$, and note $H^\dagger_k = H_k \Rightarrow H^T_k = H^*_k$

$\Rightarrow PH_kP^{-1} = -H_{-k}$

- Spectrum symmetry for matrix $[H_k]_{2p\times 2p}$ acting on columns $\chi = \begin{pmatrix}\chi_1\\ \vdots \\ \chi_{2p}\end{pmatrix} \in \mathbb{C}^{2p}$

i-th eigen: $H_k \chi^{(i)}_k \equiv E_{ki}\chi^{(i)}_k \Rightarrow P\left(H_k \underbrace{(P^{-1}P)}_{1_{2p}} \chi^{(i)}_k\right) = P\left(E_{ki}\chi^{(i)}_k\right)$

$\Rightarrow \left(PH_kP^{-1}\right)\left(P\chi^{(i)}_k\right) = E^*_{ki}\left(P\chi^{(i)}_k\right) \Rightarrow -H_{-k}\left(P\chi^{(i)}_k\right) = E_{ki}\left(P\chi^{(i)}_k\right)$

$\Rightarrow$ ① IF $\chi^{(i)}_k$ @ $(k \neq -k, E_{ki})$ THEN $\tau_x \chi^{(i)*}_k$ @ $(-k, E_{ki})$. THE E_{ki} can be 0.

② IF $\underset{(\mathrm{TRIM})}{k} = -k \equiv \Gamma_a$, THEN $\chi^{(i)}_{\Gamma_a}$ @ $(\Gamma_a, E_{\Gamma_a i} \neq 0) \Rightarrow \tau_x \chi^{(i)*}_{\Gamma_a}$ @ $(\Gamma_a, -E_{\Gamma_a i} \neq 0)$.

③ IF $k = \Gamma_a$, $\chi^{(i)}_{\Gamma_a}$ @ $(\Gamma_a, E_{\Gamma_a i} \equiv 0)$, THEN $\tau_x \chi^{(i)*}_{\Gamma_a}$ could be $\sim \chi^{(i)}_{\Gamma_a}$

Since $\dim(H_k) = 2p$ = even, each band $E_i(k)$ inverted to $-E_i(-k)$, and zero energy states at TRIMs also come in pairs. <u>IMPORTANT!</u> (LATER)

1.A3 Physics of BdG doubling

Diagonalization $H^{ab}_k = \sum_{i=1}^{2p} E_{ki}\,\chi^{(i)}_{k,a}\,\chi^{(i)*}_{k,b} \Rightarrow$

$$\hat{H} = \frac{1}{2}\sum_{kab} \Psi^\dagger_{ka} H^{ab}_k \Psi_{kb} = \frac{1}{2}\sum_{kab}\sum_i \Psi^\dagger_{ka}\chi^{(i)}_{ka} E_{ki}\,\chi^{(i)*}_{k,b}\Psi_{kb} =$$

$$= \frac{1}{2}\sum_{k,i}\left(\sum_a \chi^{(i)*}_{k,a}\Psi_{ka}\right)^\dagger E_{ki}\left(\sum_b \chi^{(i)*}_{k,b}\Psi_{kb}\right) \equiv \frac{1}{2}\sum_{k,i} E_{ki}\,\gamma^{(i)\dagger}_k \gamma^{(i)}_k$$

$\gamma^{(i)}_k \equiv \sum_a \chi^{(i)*}_{ka}\cdot\Psi_{ka}$, $i = 1..2p$, are fermions! $\{\gamma^{(i)}_k, \gamma^{(j)\dagger}_{k'}\} = \delta_{kk'}\left(\sum_a \chi^{(i)*}_{ka}\chi^{(j)}_{ka}\right) = \delta_{kk'}\delta_{ij}$

PHS: $\tilde{\gamma}^{(i)}_{-k} \equiv \sum_{ab}\left(\tau^{ab}_x \chi^{(i)*}_{kb}\right)^* \Psi_{-ka} = \sum_{ab} \chi^{(i)}_{kb}\left(\tau^{ba}_x \Psi_{-ka}\right) = \sum_{ab}\chi^{(i)}_{kb}\,\Psi^\dagger_{kb} = \gamma^{(i)\dagger}_k$

$\Rightarrow$ At each k, pick $i_+ = 1,\dots,p$ so that $E_{ki_+}>0$, $\gamma_k^{(i_+)} = \sum_a \chi_{ka}^{(i)*}\psi_{ka}$,
while label the rest $\gamma_k^{(i_-)}$ having $E_{k,i_-}<0$, then we know that for each (k,i_+) there is its pair $(-k,i_-)$ such that

PHS: ① $E_{-k,i_-} = -E_{k,i_+} < 0$; ② $\chi_{-k}^{(i_-)} = \tau_x \chi_k^{(i_+)*}$; ③ $\gamma_{-k}^{(i_-)\dagger} = \gamma_{+k}^{(i_+)}$ $\Rightarrow$

$$\hat{H} = \frac{1}{2}\sum_{k,i_+=1}^{p} E_{ki_+}\gamma_k^{(i_+)\dagger}\gamma_k^{(i_+)} + \frac{1}{2}\sum_{k,i_-=1}^{p} E_{ki_-}\gamma_k^{(i_-)\dagger}\gamma_k^{(i_-)} =$$

$$= \frac{1}{2}\sum_{k,i_+} E_{ki_+}\gamma_k^{(i_+)\dagger}\gamma_k^{(i_+)} + \frac{1}{2}\sum_{k,i_+}\left(-E_{-k,i_+}\right)\underbrace{\gamma_{-k}^{(i_+)}\gamma_{-k}^{(i_+)\dagger}}_{\text{fermions}} =$$

$$= \sum_k \sum_{i_+=1}^{p} |E_{ki_+}|\gamma_k^{(i_+)\dagger}\gamma_k^{(i_+)} + \frac{1}{2}\sum_k\left(\mathrm{Tr}\,\xi_k - \sum_{i_+=1}^{p}|E_{k,i_+}|\right)$$

reinstated const $= \frac{1}{2}\mathrm{Tr}\,\xi_k$

"Free fermions" = "Bogoliubons":

ⓐ $|GS\rangle$ is vacuum of $\gamma_k^{(i_+)}$: $\gamma_k^{(i_+)}|GS\rangle \equiv 0$, $\forall k; i_+ = 1,\dots,p$

$$\hat{H}|GS\rangle = -\frac{1}{2}\sum_{k,i}|E_{k,i_+}| \equiv E_{GS}$$

Since $\gamma_k^{(i_+)}|GS\rangle \equiv 0$, $|GS\rangle \sim \gamma_k^{(i_+)}|\psi_0\rangle$, with unknown $|\psi_0\rangle$ in Fock space

so $|GS\rangle = \prod_k \prod_{i_+=1}^{p}\gamma_k^{(i_+)}|\psi_0\rangle \overset{PHS}{=} \prod_k \prod_{i_-=1}^{p}\gamma_{-k}^{(i_-)\dagger}|\psi_0\rangle =$ "Fermi sea" of $E_{ki_-}<0$.

ⓑ Bogoliubon excitations: $\gamma_k^{(i_+)\dagger}|GS\rangle$, with excitation energy $E_{ki_+}>0$

$\gamma_k^{(i_+)\dagger}\gamma_{k'}^{(i'_+)\dagger}|GS\rangle$, with $E_{ki_+}+E_{k'i'_+}$

...

ⓒ Electrons and holes?

FERMION PARITY: $\hat{H}$ preserves #electrons (mod 2) in Fock space

$c^\dagger c|\tilde{N},l\rangle \sim |\tilde{N},m\rangle$; $c^\dagger c^\dagger|\tilde{N},l\rangle \sim |\tilde{N}+2,m\rangle$; $cc|\tilde{N},l\rangle \sim |\tilde{N}-2,m\rangle$

for some states l,m in subspace of $\tilde{N}$ electrons ($|\tilde{N},l\rangle$; $|\tilde{N},m\rangle$).

Particle conservation $U(1)$ symmetry $c \to e^{i\varphi}c$; $c^\dagger \to e^{-i\varphi}c^\dagger$ is broken to $\mathbb{Z}_2$ symmetry in $\hat{H}$: $c \to -c$; $c^\dagger \to -c^\dagger$ by pairing, since $\Delta c^\dagger c^\dagger \to \Delta(-c^\dagger)(-c^\dagger) = \Delta c^\dagger c^\dagger$.

NOTE:
# of DoF N
is independent
of #electron $\tilde{N}$.

- The $|GS\rangle$, as any eigenstate of $\hat{H}$, has either even or odd # electrons, $\Pi_{GS} = 0, 1$.
  $|GS\rangle = \omega_0 |vac\rangle + \omega_2 c^+ c^+ |vac\rangle + \cdots$ or $|GS\rangle = \omega_1 c^+ |vac\rangle + \omega_3 c^+ c^+ c^+ |vac\rangle + \cdots$
  Hence to get $|GS\rangle = \prod_k \prod_{i=1}^{p} \gamma_k^{(i)+} |\Psi_0\rangle$, the $|\Psi_0\rangle$ has to be any Fock state of correct parity $(\Pi_{\Psi_0} + p \cdot N)(\mathrm{mod}\ 2) = \Pi_{GS}$.
  number of positive bands ↗ ↖ number of sites (or momenta)

- Bogoliubon: $\chi_k^{(i_+)} = (u_{k1}^{(i_+)}, \ldots, u_{kp}^{(i_+)} ; v_{k1}^{(i_+)}, \ldots, v_{kp}^{(i_+)})^T \in \mathbb{C}^{2P}$; PHS: $v_{ka}^{(i_+)} = u_{-ka}^{(i_-)*}$, $E_{k,i_+} = -E_{-k,i_-}$
  $\gamma_k^{(i_+)+} |GS\rangle = \left[\sum_{a=1}^{p} \left(u_{k,a}^{(i_+)} c_{ka}^+ + v_{k,a}^{(i_+)} c_{-ka} \right) \right] |GS\rangle$ has opposite parity than $|GS\rangle$.

BCS GROUND STATE?

For simplicity let's take a single band $(p=1)$ $\hat{H}$ in 1 dimension (e.g. Kitaev chain) such that $\Pi_{GS} = N(m2)$, then we can take $|\Psi_0\rangle = \prod_k c_k^+ |vac\rangle$; $\chi_k^{(1+)} = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$; $\chi_k^{(1-)} = \begin{pmatrix} \bar{u}_k \\ \bar{v}_k \end{pmatrix}$

PHS: $\begin{pmatrix} v_{-k}^* \\ u_{-k}^* \end{pmatrix} = \begin{pmatrix} \bar{u}_k \\ \bar{v}_k \end{pmatrix}$; orthonormality (or fermion algebra) at k $\begin{cases} (\bar{u}_k^*, \bar{v}_k^*) \begin{pmatrix} u_k \\ v_k \end{pmatrix} = 0 \\ |u_k|^2 + |v_k|^2 = 1 \end{cases}$ $\Rightarrow$ $\bar{v}_k = \pm u_k^*$, $\bar{u}_k = \mp v_k^*$, so $u_{-k} = \pm u_k$, $v_{-k} = \mp v_k$

$\Rightarrow |GS\rangle \sim \prod_k \gamma_k^{(+)} c_k^+ |vac\rangle = \prod_k (u_k^* + v_k^* c_{-k}^+ c_k^+) |vac\rangle \sim |BCS\rangle$

- IF @ $k = k_0$, $\Delta_{k_0} = 0$, no need for BdG there: $|GS\rangle = \begin{cases} c_{k_0}^+ |GS'(k \neq k_0)\rangle \\ |GS'(k \neq k_0)\rangle \end{cases}$
  which in BdG becomes $\chi_{k_0}^{(+)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

SUMMARY 1.A: BdG method reveals a „Fermi sea" ground state (BCS), with Bogoliubon fermionic excitations (coherent superpositions of electrons and holes). The price is a redundancy („PHS") so that only $E > 0$ bands are Bogoliubon excitations. Bulk gap to ground state is measured from $E = 0$. Bogoliubon's don't have fixed charge, but carry fermion parity ($\mathbb{Z}_2$ symmetry $c^+ \to -c^+$), which is conserved in BdG (i.e., 2e pairing).

$\boxed{1.B}$ Back to Kitaev chain with PBC:

$$\overset{}{\circ}\text{- - -}\bullet\text{—}\bullet\text{—}\bullet\;\cdots\;\bullet\text{- - -}\circ$$
$$\alpha = N \quad 1 \quad 2 \quad 3 \quad \quad N \quad 1$$

$$\hat{H} \equiv -\frac{1}{2}\sum_\alpha \left(t c^\dagger_\alpha c_{\alpha+1} + h.c.\right) - \mu \sum_\alpha c^\dagger_\alpha c_\alpha + \frac{1}{2}\sum_\alpha \left(\Delta c^\dagger_\alpha c^\dagger_{\alpha+1} + h.c.\right)$$

$$\hat{H} = \sum_k \underbrace{(-t\cos k - \mu)}_{\equiv \xi_k} c^\dagger_k c_k + \frac{1}{2}\sum_k \left(\underbrace{\Delta e^{-ik}}_{\equiv \Delta_k} c^\dagger_k c^\dagger_{-k} + \Delta^* e^{+ik} c_{-k} c_k\right)$$

ASSUME $t > 0$, $\Delta \in \mathbb{C}$; $\Delta_k \to \frac{1}{2}(\Delta_k - \Delta_{-k}) \Rightarrow \Delta_k \to -i\Delta \sin k$

BdG: $\Psi_k = \begin{pmatrix} c_k \\ c^\dagger_{-k} \end{pmatrix} \Rightarrow \hat{H} = \frac{1}{2}\sum_k \Psi^\dagger_k H_k \Psi_k + \frac{1}{2}\sum_k \xi_k$

$$H_k = \begin{array}{c|c} \xi_k & -i\Delta \sin k \\ \hline i\Delta^* \sin k & -\xi_k \end{array} \Rightarrow E_{k\pm} = \pm\sqrt{\xi_k^2 + |\Delta_k|^2} = \pm\sqrt{(t\cos k + \mu)^2 + |\Delta|^2 \sin^2 k}$$

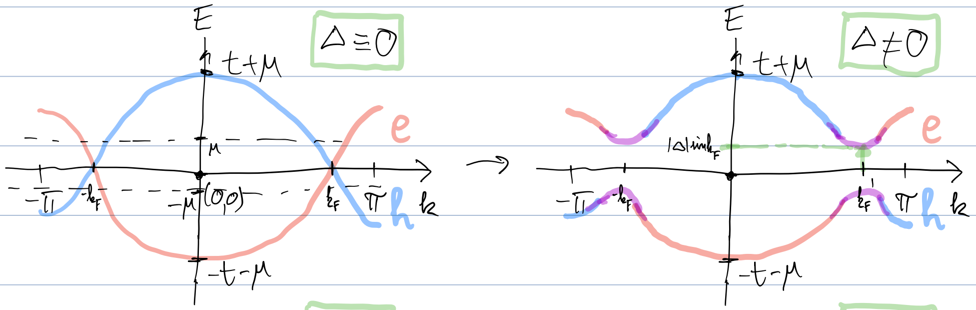
- Bulkgap closing $E_k \equiv 0 \Rightarrow (t\cos k + \mu = 0) \wedge (|\Delta| \sin k \equiv 0)$

① $|\mu| > t \to$ gapped

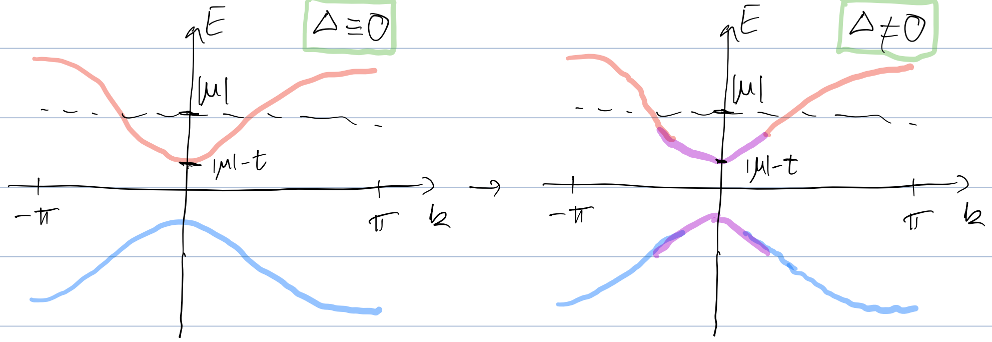
② $\mu = \pm t \to$ closing @ $k = \pi$ $(k = 0)$

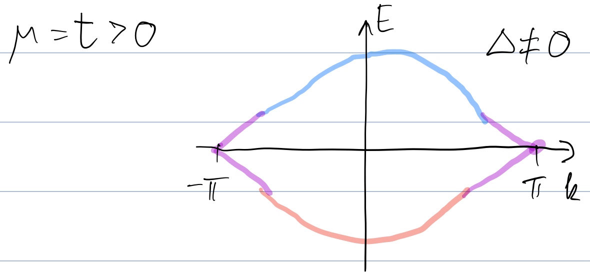
③ $|\mu| < t \to$ closing @ $k = \pm k_F$ if $|\Delta| = 0$

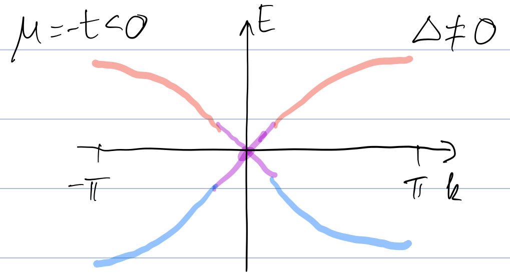
$0 < \mu < t$



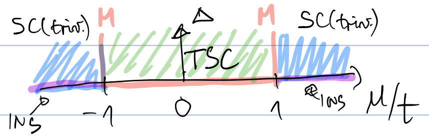
$\mu < -t < 0$







- Phase diagram :



- Ground state : $K \equiv 0, \pi$; $\Delta_K = 0 \Rightarrow |GS\rangle = \begin{cases} \mu < -t & , |GS'\rangle \\ -t < \mu < t & , c^+_{k=0}|GS'\rangle \\ t < \mu & , c^+_{k=\pi} c^+_{k=0}|GS'\rangle \end{cases}$

$$|GS'\rangle \equiv \prod_{k \neq 0,\pi} \gamma^{(+)}_k c^+_k |vac\rangle = \prod_{k \neq 0,\pi} (u^*_k - v^*_k c^+_k c^+_{-k})|vac\rangle$$

$\boxed{\text{NOTE: } u_{-k} = u_k \, ; \, v_{-k} = -v_k}$

- Electron-hole balance in Bogoliubon band: $\Delta = |\Delta| e^{i\varphi}$

$$X^{(+)}_k = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \frac{\xi_k}{E_k}} \\ i e^{-i\varphi} \cdot \mathrm{sgn}(k) \sqrt{1 - \frac{\xi_k}{E_k}} \end{pmatrix} \equiv \begin{pmatrix} u_k \\ v_k \end{pmatrix} \Rightarrow \gamma^{(+)+}_k = u_k \underline{c^+_k} + v_k \underline{c_{-k}}$$

- k values where : $E_k >> |\Delta_k| \Rightarrow \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta_k|^2}} \simeq \mathrm{sgn}(\xi_k) \Rightarrow \begin{pmatrix} |u_k| \\ |v_k| \end{pmatrix} \simeq \underline{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}$ or $\underline{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}$

- k near gap opening : $|\xi_k| << |\Delta_k| \Rightarrow \frac{\xi_k}{E_k} \simeq \frac{\xi_k}{|\Delta_k|} << 1 \Rightarrow \begin{pmatrix} |u_k| \\ |v_k| \end{pmatrix} \simeq \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$E_{gap} \simeq E_{k_F} = |\Delta_{k_F}| = |\Delta| \sin k_F$

precisely $\left.\frac{\partial E_k}{\partial k}\right|_{k'_F} \equiv 0 \Rightarrow \frac{1}{2E_{k'_F}} \cdot \left(2\xi_{k'_F} \cdot \left.\frac{\partial \xi}{\partial k}\right|_{k'_F} + 2\Delta_{k'_F} \cdot \left.\frac{\partial \Delta}{\partial k}\right|_{k'_F}\right) \equiv 0 \Rightarrow (tc + \mu)(-ts) \equiv -|\Delta|^2 s \cdot c$

$\Rightarrow t^2 \cancel{s} c + \mu t \cancel{s} \equiv |\Delta|^2 \cancel{s} c \Rightarrow c(t^2 - |\Delta|^2) = -\mu t \Rightarrow \cos k'_F = \frac{\mu t}{|\Delta|^2 - t^2}$

$\Rightarrow \cos k'_F = \frac{t^2}{t^2 - \Delta^2} \cos k_F \Rightarrow |\sin k'_F|^2 = |\sin k_F|^2 \cdot \frac{t^4}{(t^2-\Delta^2)^2} + 1 - \frac{t^4}{(t^2-\Delta^2)^2}$

$$\Rightarrow E_{gap} = E_{k'_F} = \sqrt{(t \cdot c_{k'_F} + \mu)^2 + |\Delta|^2 s^2_{k'_F}} = \sqrt{\mu^2 \left(1 - \frac{t^2}{t^2 - \Delta^2}\right) + |\Delta|^2 s^2_{k'_F}} = |\Delta| s_{k'_F} \sqrt{1 + \frac{\mu}{(|\Delta|^2 - t^2) s^2_{k'_F}}}$$

NOTE: $|\Delta| \equiv t \Rightarrow k_F = \pi \Rightarrow E_{gap} = |\mu - t| = |\mu - |\Delta||$

1.C Bulk topology of Kitaev chain

1 For 1 BdG band $(p=1)$, H^{BdG} is 2x2 → bulk invariant from sphere

$$M_{2\times2} = \begin{pmatrix} A & B \\ B^* & C \end{pmatrix} = D_0 \mathbb{1}_2 + \vec{D}\cdot\vec{\sigma} \qquad \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)$$

$$H_k = \begin{array}{c|c} -t\cos k - \mu & -i\Delta \sin k \\ \hline i\Delta^* \sin k & +t\cos k + \mu \end{array} = (-t\cos k - \mu)\sigma_3 + Re(\Delta)\cdot \sin k\, \sigma_2 + Im(\Delta) \sin k \cdot \sigma_1 = \vec{D}_k \cdot \vec{\sigma}$$

$E_{k\pm} = \pm|\vec{D}_k|$ so if gapped $\left(\min_k E_{k+} > 0\right)$ then $|\vec{D}_k| \neq 0, \forall k$

Topology: smoothly deform H_k to flatten bands:

$Q_k \equiv H_k / E_{k+} \Rightarrow \hat{D}_k \equiv \vec{D}_k / |\vec{D}_k| \Rightarrow |\hat{D}_k| = 1$

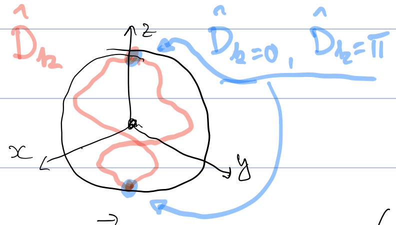
PHS constrains H^{BdG}: $\tau_x H^T_{-k} \tau_x = -H_k$, here $\tau_i = \sigma_i$.

For TRIM $k \equiv K$, $K = -K + 2\pi n \Rightarrow \sigma_x H^T_K \sigma_x = -H_K \Rightarrow \sigma_1 Q^T_K \sigma_1 = -Q_K$

$\Rightarrow \sigma_1 (\hat{D}_{K,1} \sigma_1^T + \hat{D}_{K,2} \sigma_2^T + \hat{D}_{K,3} \sigma_3^T) \sigma_1 = -\hat{D}_K \cdot \vec{\sigma}$

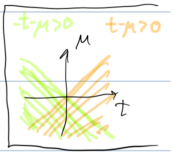
$\Rightarrow \hat{D}_{K,1} = 0 \wedge \hat{D}_{K,2} = 0$

Here $K = 0, \pi \Rightarrow \hat{D}_{k=0} = s_0 \hat{z} \wedge \hat{D}_{k=\pi} = s_\pi \cdot \hat{z}$, $s_K = sgn(D_{K,3})$



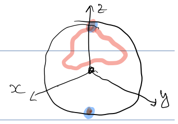
$\hat{D}_k$ contractible to point on sphere or not,

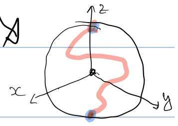
$(\pm)^\nu = s_0 \cdot s_\pi = \pm 1 \leftarrow \mathbb{Z}_2$ topology



Here $\vec{D}_K = D_{K,3}\sigma_3 = (-t\cos K - \mu)\sigma_3$

$\Rightarrow s_K = sgn(D_{K,3}) \Rightarrow \left\{ \begin{array}{l} s_0 = sgn(-t-\mu) \\ s_\pi = sgn(t-\mu) \end{array} \right\} s_0 \cdot s_\pi = \begin{cases} +1, & |\mu|>|t| \rightarrow \\ -1, & |\mu|<|t| \end{cases}$



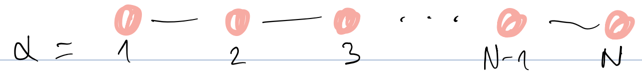


→ TO BE DEMONSTRATED INTERACTIVELY

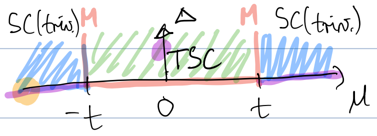
2 (2a) $(\pm)^\nu = Pf[H_{k=0}] \cdot Pf[H_{k=\pi}]$ to be explained

(2b) Topologically $\begin{cases} \text{non-trivial}, & \text{when 2 Fermi points} \\ \text{trivial}, & \text{when 0 Fermi points} \end{cases}$

$\boxed{1.D}$ Bulk-edge correspondence: Open Kitaev chain



$$\hat{H} \equiv -\frac{1}{2}\sum_\alpha \left(t\, c_\alpha^+ c_{\alpha+1} + h.c.\right) - \mu \sum_\alpha c_\alpha^+ c_\alpha + \frac{1}{2}\sum_\alpha \left(\Delta\, c_\alpha^+ c_{\alpha+1}^+ + h.c.\right)$$



: Compare trivial vs. topo SC at two special cases

$$\begin{cases} \text{●} : \mu < 0,\ t \equiv \Delta \equiv 0 \\ \text{●} : \mu \equiv 0,\ t \equiv \Delta > 0 \end{cases}$$

$\boxed{\text{●} : \mu < 0,\ t \equiv \Delta \equiv 0}$ Connected to $\mu \to -\infty$, trivial insulator with vanishing pairing.

$$\hat{H} = +|\mu| \sum_{\alpha=1}^{N} c_\alpha^+ c_\alpha \Rightarrow |GS\rangle = |vac\rangle :$$ EMPTY WIRE

$\boxed{\text{●} : \mu \equiv 0,\ t \equiv \Delta > 0}$

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

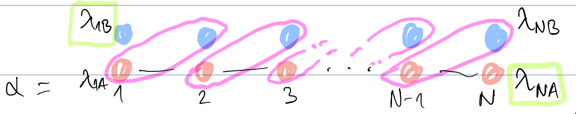
→ INTRODUCE MAJORANA OPERATORS

$$\lambda_{\alpha A} \equiv c_\alpha + c_\alpha^+ \ ;\ \lambda_{\alpha B} \equiv i\left(c_\alpha - c_\alpha^+\right) \Rightarrow \begin{cases} \boxed{\lambda_{\alpha A}^+ = \lambda_{\alpha A} \ ;\ \lambda_{\alpha B}^+ = \lambda_{\alpha B}} \\ \{\lambda_{\alpha D}, \lambda_{\beta F}\} = 2\delta_{\alpha\beta}\delta_{DF} \end{cases}$$

Majorana is it's own anti-particle, is a fermion, and a special Bogoliubon.
(NOTE: $(c^+)^2 = 0$, $\lambda^2 = 1$)

$$\Rightarrow \left.\begin{aligned} c_\alpha &= \frac{1}{2}\left(\lambda_{\alpha A} - i\lambda_{\alpha B}\right) \\ c_\alpha^+ &= \frac{1}{2}\left(\lambda_{\alpha A} + i\lambda_{\alpha B}\right) \end{aligned}\right\}$$ λ is „half electron",
a „real" fermion
(not „complex")

$$\Rightarrow \hat{H} = \frac{t}{8}\sum_{\alpha=1}^{N-1} -\left(\lambda_{\alpha A} + i\lambda_{\alpha B}\right)\left(\lambda_{\alpha+1 A} - i\lambda_{\alpha+1 B}\right) - \left(\lambda_{\alpha+1 A} + i\lambda_{\alpha+1 B}\right)\left(\lambda_{\alpha A} - i\lambda_{\alpha B}\right)$$
$$+\left(\lambda_{\alpha A} + i\lambda_{\alpha B}\right)\left(\lambda_{\alpha+1 A} + i\lambda_{\alpha+1 B}\right) + \left(\lambda_{\alpha+1 A} - i\lambda_{\alpha+1 B}\right)\left(\lambda_{\alpha A} - i\lambda_{\alpha B}\right) =$$
$$= \frac{t}{8}\sum_{\alpha=1}^{N-1} 4i\, \lambda_{\alpha A} \lambda_{\alpha+1 B} = \frac{i}{2}\sum_{\alpha=1}^{N-1} \lambda_{\alpha A} \lambda_{\alpha+1 B}$$



DEFINE: COMPLEX FERMIONS

$$\left.\begin{aligned} d_\beta &\equiv \frac{1}{2}\left(\lambda_{\beta A} - i\lambda_{\beta+1 B}\right) \\ d_\beta^+ &= \frac{1}{2}\left(\lambda_{\beta A} + i\lambda_{\beta+1 B}\right) \end{aligned}\right\} \beta = 1 \ldots N-1$$

$$\{d_\beta, d_{\beta'}\} = \delta_{\beta\beta'}\frac{1}{4}(2-2)=0 \quad ; \quad \{d_\beta, d_{\beta'}^+\} = \delta_{\beta\beta'}\frac{1}{4}(2+2) = \delta_{\beta\beta'}$$

$$\hat{H} = \frac{it}{2}\sum_{\beta=1}^{N-1}(d_\beta + d_\beta^+)\, i(d_\beta - d_\beta^+) = -t\sum_{\beta=1}^{N-1}\left(d_\beta^+ d_\beta - \frac{1}{2}\right)$$

$|GS\rangle = |vac\rangle_d$, i.e. $d_\beta |vac\rangle_d \equiv 0$, $\beta = 1 \dots N-1$

BUT λ_{1B} & λ_{NA} are NOT in $\hat{H}$.

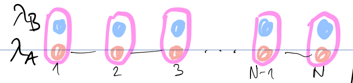
→ DEFINE NON-LOCAL COMPLEX FERMION : $d_0^+ \equiv \frac{1}{2}(\lambda_{NA} + i\lambda_{1B}) = \frac{1}{2}(C_N + C_N^+ - C_1 + C_1^+)$

Has zero energy ⇒ $\boxed{\text{GS DEGENERACY}}$: $\{|GS\rangle, d_0^+|GS\rangle\}$: parity even and odd

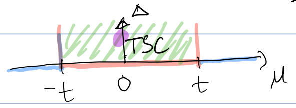
CONFIRM: $[d_0^+, \hat{H}] = 0 \therefore \sum_{\alpha=1}^{N-1}(\lambda_{\alpha A}\lambda_{\alpha+1B})\lambda_{1B} = \lambda_{1B}\sum_{\alpha=1}^{N-1}(-\lambda_{\alpha A})(-\lambda_{\alpha+1B})$

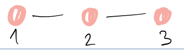
$\hat{H} d_0^+ |\psi_n\rangle = d_0^+ \hat{H} |\psi_n\rangle = d_0^+ E_n |\psi_n\rangle$ ⇒ DEGENERACY E_n : $\begin{cases} |\psi_n\rangle \\ d_0^+|\psi_n\rangle \end{cases}$

NOTE: Trivial insulator $-\mu\sum c_\alpha^+ c_\alpha$ →



GENERALLY IN TSC PHASE: exponentially decaying wavefunction of single Majorana per edge.





→ $\lambda_A^{left} \sim \sum_{\alpha=1}^{\infty} e^{-\alpha/\xi}\lambda_{\alpha A}$ (half-infinite chain's edge)

⇒ Small hybridization in finite chain $E_r \sim e^{-N/\xi}$

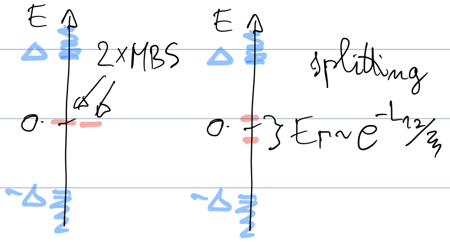
$\hat{H}_{eff}^{split} = i2E_r\,\lambda_B^{right}\lambda_A^{left} = E_r\, d_{edge}^+ d_{edge} + const$

→ TO BE DEMONSTRATED INTERACTIVELY

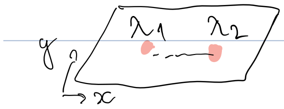
1.E TopoSC and Majorana Bound States (MBS)

① SC: Pointlike Bogoliubon at E=0 is a Majorana

remember: ±E pairs



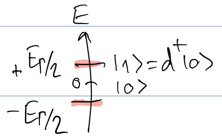
② TSC: Non-local information – spatially separated MBS pinned at $E=0$



$d^\dagger = \frac{1}{2}(\lambda_1 + i\lambda_2) \Rightarrow GS: \{ |0\rangle, |1\rangle = d^\dagger|0\rangle = \frac{1}{2}\underbrace{(\lambda_1 + i\lambda_2)}_{\text{non local}}|0\rangle \}$

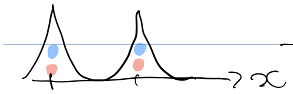
Parity: $P = (-1)^{\hat{N}_d}$ given by $\hat{N}_d = d^\dagger d = \frac{1}{2}(1 - i\lambda_1\lambda_2)$: NON-LOCAL detection

We neglect the splitting. If $\hat{H}_{eff}^{split} \neq 0 \Rightarrow$



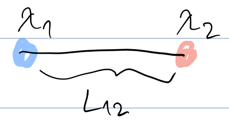
- Compare to trivial Bound State(s)

$\Psi^\dagger(x) \sim \lambda_1(x) + i\lambda_2(x)$, both $\lambda_{1,2}$ at x_1

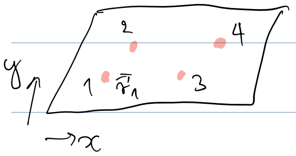


→ still can't isolate, e.g. $●_1$ and $●_2$.

Kitaev chain



③ Topological Quantum Computation



$\lambda_1, \lambda_2, \lambda_3, \lambda_4 \Rightarrow d_a^\dagger, d_b^\dagger$ non-local

$4\,GS\ (|00\rangle, |01\rangle, |10\rangle, |11\rangle)$ with N_a and N_b marking the first and second entry

At fixed total parity $P = (-1)^{d_a + d_b} = \text{const} \Rightarrow 2GS = \begin{cases} \{|0,0\rangle, |1,1\rangle\}, & \text{if even} \\ \{|10\rangle, |01\rangle\}, & \text{if odd} \end{cases}$

Any operation preserving P must be even, $\sim(\lambda_i\lambda_j)^n$, with $i \neq j$, as $\lambda_i^2 = 1$, so it must act non-locally $(\vec{r}_i \neq \vec{r}_j)$.

The doublet GS still non-locally encoded by all 4 MBS ⇒ topological qubit.

- How to manipulate linear combination in doublet?

BRAIDING MBS (revisited later)

⇒ MBS are non-Abelian anyons: their braiding mixes states in doublet, allows gate operations on GS qubit.

NOTE: $2N$ MBS ⇒ N d's ⇒ $\#GS = 2^{N-1}$ at fixed P.

⇒ Each MBS grows the „qubit" Hilbert space by factor $\sqrt{2}$ ⇒ non-Ab. anyon.

$\boxed{1.F}$ Mean-field SC — the source of BdG

Consider a general electron-electron interaction term for electrons in momentum basis, $c_{\underline{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{\underline{r}} e^{i\underline{k}\cdot\underline{r}} c_{\underline{r}\sigma}$, with spin $\sigma = \uparrow, \downarrow$.

$$\hat{H}_V = \sum_{\substack{\underline{P},\underline{k},\underline{k}' \\ \sigma,\sigma',\lambda,\lambda'}} V^{\sigma,\sigma',\lambda,\lambda'}_{\underline{k},\underline{k}',\underline{P}} \; c^\dagger_{\underline{k}'+\frac{\underline{P}}{2},\lambda} c^\dagger_{-\underline{k}'+\frac{\underline{P}}{2},\lambda'} \; c_{-\underline{k}+\frac{\underline{P}}{2},\sigma} c_{\underline{k}+\frac{\underline{P}}{2},\sigma'}.$$

There are 3 momenta due to global translation symmetry, and these summation variables are reshuffled to help with the next step.

The SC state is characterized by an „anomalous" expectation value

$$\langle c_{-\underline{k}+\frac{\underline{P}}{2},\sigma} c_{+\underline{k}+\frac{\underline{P}}{2},\sigma'} \rangle_{GS} \neq 0 \text{ for some } \underline{k}, \underline{P}, \sigma, \sigma'.$$

The ground state contains (Cooper) pairs of electrons. In a SC in which the center of mass of the Cooper pair is not moving, i.e. a SC homogeneous in space, $\underline{P} \equiv 0$. Now we keep only interactions with $\underline{P}=0$, and do a mean-field decoupling in Cooper channel:

$$c_{-\underline{k},\sigma} c_{\underline{k},\sigma'} = \underbrace{\langle c_{-\underline{k}\sigma} c_{\underline{k}\sigma'} \rangle}_{\equiv F_{\underline{k}\sigma\sigma'}} + \underbrace{\left(c_{-\underline{k}\sigma} c_{\underline{k}\sigma'} - \langle c_{-\underline{k}\sigma} c_{\underline{k}\sigma'} \rangle \right)}_{\equiv \delta_{\underline{k}\sigma\sigma'}}$$

$$\Rightarrow c^\dagger_{\underline{k}'\lambda} c^\dagger_{-\underline{k}'\lambda'} = (c_{-\underline{k}'\lambda'} c_{\underline{k}'\lambda})^\dagger = F^*_{\underline{k}'\lambda'\lambda} + \delta^\dagger_{\underline{k}'\lambda'\lambda}$$

MF: neglect fluctuations

$$\Rightarrow \hat{H}_V = \sum V^{\sigma\sigma'\lambda\lambda'}_{\underline{k},\underline{k}',0} \left(F^*_{\underline{k}'\lambda'\lambda} + \delta^\dagger_{\underline{k}'\lambda'\lambda} \right)\left(F_{\underline{k}\sigma\sigma'} + \delta_{\underline{k}\sigma\sigma'} \right) =$$

$$= \sum V^{\sigma\sigma'\lambda\lambda'}_{\underline{k},\underline{k}',0} \left(F^*_{\underline{k}'\lambda'\lambda} \delta_{\underline{k}\sigma\sigma'} + F_{\underline{k}\sigma\sigma'} \delta^\dagger_{\underline{k}'\lambda'\lambda} \right) + \underbrace{\sum V^{\sigma\sigma'\lambda\lambda}_{\underline{k},\underline{k}',0} F^*_{\underline{k}'\lambda'\lambda} F_{\underline{k}\sigma\sigma'}}_{\text{const}} + \underbrace{\cancel{\sum V^{\sigma\sigma'\lambda\lambda'}_{\underline{k},\underline{k}',0} \delta^\dagger_{\underline{k}'\lambda'\lambda} \delta_{\underline{k}\sigma\sigma'}}}_{0}$$

$$= \sum V^{\sigma\sigma'\lambda\lambda'}_{\underline{k},\underline{k}',0} \left(F^*_{\underline{k}'\lambda'\lambda} c_{-\underline{k}\sigma} c_{\underline{k}\sigma'} + F_{\underline{k}\sigma\sigma'} c^\dagger_{\underline{k}'\lambda} c^\dagger_{-\underline{k}'\lambda'} \right) \quad \text{(neglected another constant)}$$

Define the pairing function („wavefunction of Cooper pair"):

$\Delta^{\sigma\sigma'}_{\underline{k}} \equiv \sum_{\underline{k}',\lambda,\lambda'} V^{\lambda\lambda'\sigma\sigma'}_{\underline{k}',\underline{k},0} \langle c_{-\underline{k}'\lambda} c_{\underline{k}'\lambda'} \rangle$, and now use that V is constrained such that $\hat{H}_V^\dagger = \hat{H}_V$.

$$\Rightarrow \hat{H}_V = \sum_{\underline{k}\sigma\sigma'} \left(\Delta^{\sigma\sigma'}_{\underline{k}} c^\dagger_{\underline{k}\sigma} c^\dagger_{-\underline{k}\sigma'} + (\Delta^{\sigma\sigma'}_{\underline{k}})^* c_{-\underline{k}\sigma'} c_{\underline{k}\sigma} \right).$$

1.G Beyond mean-field SC and BdG

① __Issues__: The „order parameter" Δ is not gauge invariant $(c \to e^{i\varphi} c \Rightarrow \Delta \to e^{i2\varphi}\Delta)$. The mean-field decoupling to $\Delta c^+ c^+$ forces the $|GS\rangle$ to have superposition of many N (# of electrons), puzzling in a system with fixed N.

② __Answers__: A gauge-invariant order parameter of a SC can be built, but it is non-local. This is related to the fact that a SC (any, e.g., simple s-wave, trivial in the band topology) is topologically ordered, with fractionalized gapped excitations (neutral π-flux...). Hence, a general treatment of band topology is difficult.

In practice one can fix the number of Cooper pairs to N: $|GS\rangle = \left(\sum_i f_i c_i^+ c_{-i}^+\right)^N |vac\rangle$, with f_i playing the role of v/u, which is similar to the projection to 2N-electron states $|GS\rangle = P_{2N} |GS_{BdG}\rangle$. Variational studies for small N show that the $|GS_{BdG}\rangle$ is highly successful in reproducing SC correlations at weak coupling

happy to have the limited but effective __linear__ BdG theory. We can measure SC correlations at fixed N simply,

$$\langle (f_i c_i^+ c_{-i}^+)(f_i^* c_{-i} c_i)\rangle_N \sim \langle \Delta\Delta^+\rangle,$$ which is also gauge invariant.

③ __Impact on BdG topology__: An exactly solvable, fixed N, interacting (non-mean-field) model of a spinless SC chain was solved [Ortiz2014].

$$\hat{H} = -t\sum c_n^+ c_{n+1} + h.c. - \frac{4g_0}{L} I^+ I \; ; \; I = \sum_{m<n} \eta(n-m)\, c_n c_m \; ; \; c_{n+L} = e^{i\phi/2} c_n$$

ϕ is flux in PBC ring

→ Kitaev phase: $\eta(s) = FT(\sin\frac{k}{2})$, gives $g = g_c$ transition.

→ Fermion parity in GS: $K(\phi) = \frac{1}{2} E_{GS}(2N+1,\phi) + \frac{1}{2} E_{GS}(2N-1,\phi) - E_{GS}(2N,\phi)$ is a key quantity distinguishing phases. Many-body „zero-mode" can be defined. $Q \equiv \mathrm{sgn}[K(0)\cdot K(h/2e)]$ is an invariant, mimicking BdG class D in 1d.

PART 2: PAIRING IN REALITY — SPIN

2.A Realistic pairing

2.A1 What we learned in BdG theory:

System with p degrees of freedom per unit-cell (labeled by lattice vector $\underline{R}$) has 2p Nambu fermions at momentum $\underline{k}$ ($N = \#$unit-cells)

$$\boxed{\Psi_{\underline{k}}} \equiv \begin{pmatrix} c_{\underline{k}1} \\ \vdots \\ c_{\underline{k}p} \\ \hdashline c^{\dagger}_{-\underline{k}1} \\ \vdots \\ c^{\dagger}_{-\underline{k}p} \end{pmatrix} \begin{matrix} \left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\} e \\ \left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\} h \end{matrix} \Rightarrow \Psi^{\dagger}_{\underline{k}} = (\underbrace{c^{\dagger}_{\underline{k}1}, \dots, c^{\dagger}_{\underline{k}p}}_{\text{electron}} \,\vdots\, \underbrace{c_{-\underline{k}1}, \dots, c_{-\underline{k}p}}_{\text{hole}}) ; \quad \Psi_{\underline{k}} = \frac{1}{\sqrt{N}} \sum_{\underline{R}} e^{i\underline{k}\cdot\underline{R}} \begin{pmatrix} c_{\underline{R}1} \\ \vdots \\ c_{\underline{R}p} \\ \hdashline c^{\dagger}_{\underline{R}1} \\ \vdots \\ c^{\dagger}_{\underline{R}p} \end{pmatrix}$$

$$\Rightarrow \{\Psi_{\underline{k}a}, \Psi_{\underline{k}'a'}\} = \{\Psi^{\dagger}_{\underline{k}a}, \Psi^{\dagger}_{\underline{k}'a'}\} = 0 ; \quad \{\Psi_{\underline{k}a}, \Psi^{\dagger}_{\underline{k}'a'}\} = \delta_{\underline{k}\underline{k}'}\delta_{aa'}$$

$$\boxed{\hat{H}} = \sum_{\underline{k}} \sum_{a,b}^{p} \xi^{ab}_{\underline{k}} c^{\dagger}_{\underline{k}a} c_{\underline{k}b} + \frac{1}{2} \sum_{\underline{k}} \sum_{a,b}^{p} \left(\Delta^{ab}_{\underline{k}} c^{\dagger}_{\underline{k}a} c^{\dagger}_{-\underline{k}b} + \Delta^{ab*}_{\underline{k}} c_{-\underline{k}b} c_{\underline{k}a} \right)$$

with matrices $[\xi_{\underline{k}}]_{ab} = \varepsilon^{ab}_{\underline{k}} - \mu\delta_{ab}$, and $[\Delta_{\underline{k}}]_{ab} = \Delta^{ab}_{\underline{k}} \in \mathbb{C}$:

$$\boxed{H_{\underline{k}}} = \begin{array}{c|cc} & e & h \\ \hline e & \xi_{\underline{k}} & \Delta_{\underline{k}} \\ h & \Delta^{\dagger}_{\underline{k}} & -\xi^{T}_{-\underline{k}} \end{array} ; \quad \begin{cases} \xi^{\dagger}_{\underline{k}} = \xi_{\underline{k}} \leftarrow \text{Hermiticity} \\ \Delta_{\underline{k}} = -\Delta^{T}_{-\underline{k}} \leftarrow \text{fermions} \end{cases} ; \quad \hat{H} = \frac{1}{2} \Psi^{\dagger}_{\underline{k}} H_{\underline{k}} \Psi_{\underline{k}} + \frac{1}{2} \sum_{\underline{k}} \mathrm{Tr}(\xi_{\underline{k}})$$

where fermion constraint $\Delta_{\underline{k}} = -\Delta^{T}_{-\underline{k}}$ comes from $c^{\dagger}_{\underline{k}a} c^{\dagger}_{-\underline{k}b} = -c^{\dagger}_{-\underline{k}b} c^{\dagger}_{\underline{k}a}$.

2.A2 Electron spin: $S = \frac{1}{2}$

Instead of general case of effective degrees of freedom $c^{\dagger}_{\underline{k}a}$, $a = 1 \dots p$, (e.g. some bands projected in some energy range), we want to consider a more elementary case where the spin is specified:

$c^{\dagger}_{\underline{k}a\sigma}$, spin label $\sigma = \uparrow, \downarrow$ for $S_z = \pm\frac{1}{2}$, or as algebra index $\sigma = 1, 2$; other d.o.f. $a = 1 \dots r$ (e.g., orbitals in unit-cell). Connecting to above general case we can imagine $p = 2 \cdot r$. We can order as:

$$\Psi_k \equiv \left(\begin{array}{c} c_{k1\uparrow} \\ c_{k1\downarrow} \\ \vdots \\ c_{kr\downarrow} \\ \hline c^+_{-k1\uparrow} \\ c^+_{-k1\downarrow} \\ \vdots \\ c^+_{-kr\downarrow} \end{array}\right)$$

, but doesn't matter much, as we will use the separation of indices $a\sigma \to (a,\sigma)$, and hence any matrix (e.g. H_k) acting on column-vector Ψ_k can be written as a tensor product $\hat{M}_{2r\times 2r} = \hat{m}_{r\times r} \otimes \hat{S}_{2\times 2}$ where $\hat{m}$ acts as $\hat{m}\Psi_k = \sum_b m_{ab} \Psi_{kb\sigma}$, and $\hat{S}\Psi_k = \sum_{\sigma'} S_{\sigma\sigma'} \Psi_{ka\sigma'}$.

In spin space, any matrix is $\hat{S} = \Lambda_0 \cdot \mathbb{1}_2 + \vec{\Lambda}\cdot\vec{\sigma}$; $\Lambda_i \in \mathbb{C}$, $i = 0,1,2,3$.

→ Pairing term, general with spin $\Delta^{\sigma\sigma'}_{kab} c^+_{ka\sigma} c^+_{-kb\sigma'}$ is a Cooper pair, a two-electron state is created $\Delta^{AB} c^+_A c^+_B |vac\rangle = \Delta^{AB} |AB\rangle$, with total spin $\frac{1}{2}\otimes\frac{1}{2} = 0 \oplus 1$. Hence, based on action of spin rotations we should label the singlet ($S=0$) and triplet ($S=1$) components.

$$\underbrace{\Delta^{\sigma\sigma'}_{kab}}_{=\tilde{\Delta}_{\sigma\sigma'}} c^+_{ka\sigma} c^+_{-kb\sigma'} = \left(c^+_{ka\uparrow}, c^+_{ka\downarrow}\right) \begin{pmatrix} \tilde{\Delta}_{\uparrow\uparrow} & \tilde{\Delta}_{\uparrow\downarrow} \\ \tilde{\Delta}_{\downarrow\uparrow} & \tilde{\Delta}_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} c^+_{-kb\uparrow} \\ c^+_{-kb\downarrow} \end{pmatrix} =$$

$$= \frac{\tilde{\Delta}_{\uparrow\downarrow} - \tilde{\Delta}_{\downarrow\uparrow}}{2} \left(c^+_{ka\uparrow} c^+_{-kb\downarrow} - c^+_{ka\downarrow} c^+_{-kb\uparrow}\right) + \quad : S_z = 0 \,\}\, S = 0 \quad \text{(ODD in exchange of spin)}$$

$$+ \tilde{\Delta}_{\uparrow\uparrow} c^+_{ka\uparrow} c^+_{-kb\uparrow} + \quad : S_z = +1$$

$$+ \tilde{\Delta}_{\downarrow\downarrow} c_{ka\downarrow} c_{-kb\downarrow}{}^+ \quad : S_z = -1$$

$$+ \frac{\tilde{\Delta}_{\uparrow\downarrow} + \tilde{\Delta}_{\downarrow\uparrow}}{2} \left(c^+_{ka\uparrow} c^+_{-kb\downarrow} + c^+_{ka\downarrow} c^+_{-kb\uparrow}\right) \quad : S_z = 0$$

$$\left.\right\} S = 1 \text{ (EVEN)}$$

Introduce scalar ϕ and vector $\vec{d}$ for singlet and triplet, with conventional

$$\phi \equiv \frac{\Delta_{\uparrow\downarrow} - \Delta_{\downarrow\uparrow}}{2}; \quad d_z \equiv \frac{\Delta_{\uparrow\downarrow} + \Delta_{\downarrow\uparrow}}{2}; \quad d_x \equiv \frac{\Delta_{\downarrow\downarrow} - \Delta_{\uparrow\uparrow}}{2}; \quad d_y \equiv \frac{1}{i}\frac{\Delta_{\uparrow\uparrow} + \Delta_{\downarrow\downarrow}}{2}$$

$|S,S_z\rangle$: $|0,0\rangle$ $\quad |1,0\rangle \quad \frac{1}{2}(|1,-1\rangle - |1,1\rangle) \quad -\frac{i}{2}(|1,1\rangle + |1,-1\rangle)$

so that the matrix $[\tilde{\Delta}]_{ss'} = \left[(\phi\mathbb{1}_2 + \vec{d}\cdot\vec{\sigma})(i\sigma_y)\right]_{ss'}$, $s,s' = 1,2$ for $\uparrow,\downarrow$,

or $\tilde{\Delta} = \begin{array}{c|c} -d_x + i d_y & d_z + \psi \\ \hline d_z - \psi & d_x + i d_y \end{array}$. The "$i\sigma_2$" factor is not intuitive, but standard.

Putting back other indices, $\Delta^{ss'}_{kab} = \left[(\phi^{ab}_k \mathbb{1}_2 + \vec{d}^{ab}_k \cdot \vec{\sigma})(i\sigma_2)\right]_{ss'}$, so that ϕ, $\vec{d}$ are k-dependent $r\times r$ matrices: $[\hat{\phi}_k]_{r\times r}$, $[\hat{\vec{d}}_k]_{r\times r}$.

2.A3 Constraints and symmetries

2.A3.1 Fermion constraint

$$\Delta_{\underline{k}} = -\Delta^T_{-\underline{k}} \Rightarrow \Delta^T_{\underline{k}} = \hat{\phi}^T_{\underline{k}}\, i\sigma_2^T + (i\sigma_2)^T\, \hat{\vec{d}}^T_{\underline{k}} \cdot \vec{\sigma}^T = -\hat{\phi}^T_{\underline{k}}(i\sigma_2) + \hat{\vec{d}}^T_{\underline{k}} \cdot \vec{\sigma}(i\sigma_2) \equiv -\Delta_{-\underline{k}}$$

$$\Rightarrow \begin{cases} \hat{\phi}_{\underline{k}} = \hat{\phi}^T_{-\underline{k}} \\ \hat{\vec{d}}_{\underline{k}} = -\hat{\vec{d}}^T_{-\underline{k}} \end{cases} \Bigg| \text{ in case of single „orbital" } (\tau \equiv 1): \begin{cases} \phi_{\underline{k}} = \phi_{-\underline{k}} \\ \vec{d}_{\underline{k}} = -\vec{d}_{-\underline{k}} \end{cases}.$$

Singlet pairing (ϕ) is even in $\underline{k}$, triplet ($\vec{d}$) is odd in $\underline{k}$.
The parity of orbital part ($\phi, \vec{d}$) compensates parity of spin part.
Always true, we do NOT assume any symmetry here.

2.A3.2 Symmetries

The normal state Hamiltonian ($\xi_{\underline{k}}$) obeys certain symmetries, say a group G_N. The SC state will at least break the global phase $U(1)$ symmetry $c_i \to e^{i\varphi} c_i$ (conventional SC), but may break more symmetries of G_N (unconventional SC). In either case, we should label the SC order parameters by IRREPs of G_N, and a spontaneous choice of an IRREP determines the symmetry broken SC state and the new symmetry group G_{SC}, as always in Landau theory. Note that SC topology is determined (protected) by G_{SC}.

- Inversion symmetry: Separation of singlet and triplet

Spatial inversion symmetry in G_N forces the SC state to be purely even or odd (two IRREPS of inversion). Since inversion does NOT act on spin (as on any angular/magnetic moment), it only does $\underline{k} \to -\underline{k}$, hence if pairing function is purely even or odd $\Rightarrow$ purely $S=0$ or $S=1$.
Hence a triplet SC ($S=1 \Rightarrow \underline{k}$-odd) spontaneously breaks inversion, $I \notin G_{SC}$.
Breaking of inversion in G_N allows pairing with both $\phi \neq 0$, $\vec{d} \neq 0$.

- Rotation symmetry

For a rotation R: $\Delta_{\underline{k}}^{(\Gamma,i)} \xrightarrow{R} U_R \Delta_{R^{-1}\underline{k}}^{(\Gamma,i)} U_R^{\dagger} = \sum_{j=1}^{|\Gamma|} \Delta_{\underline{k}}^{(\Gamma,j)}$,

where Γ is an IRREP of dimension $|\Gamma|$, and $i,j = 1 \dots |\Gamma|$ are its components.

→ Continuum in 3d (SO(3)) : IRREPS are labeled by angular momentum $\Gamma \equiv l$ of dimension $|\Gamma| = 2l+1$, and hence a pairing in Γ is:

$$\phi_{\underline{k}}^{(l)} = \sum_{m=-l}^{l} \eta_m^{(l)} Y_{lm}(\hat{k}) \ , \ l = 0, 2, 4 \dots$$

$$\vec{d}_{\underline{k}}^{(l)} = \sum_{m=-l}^{l} \vec{\eta}_m^{(l)} Y_{lm}(\hat{k}) \ , \ l = 1, 3, 5 \dots$$

(3 dimensions)

with spherical harmonics $Y_{lm}(\hat{k})$ that are even (odd) in $\underline{k}$ for l even (odd).

The $\eta_m^{(l)} \in \mathbb{C}$, $m = -l \dots l$ or vectors $\vec{\eta}_m^{(l)} \in \mathbb{C}^3$, $m = -l, \dots, l$ are the SC order param.

We call these as atomic orbitals: „s-wave", „p-wave" … for $l = 0, 1 \dots$

→ Continuum in 2d: rotations around $\hat{z}$-axis and vertical mirrors (O(2)), we have the label L, with basis functions $F(\hat{k})$ of the ort $\hat{k}$, and matching:

L	$F(\hat{k})$	$\tilde{F}(\hat{k})$		
0	1	1	$\longleftrightarrow (l=0, m=0)$	$\leftrightarrow$ „s-wave"
1	$\hat{k}_x, \hat{k}_y$	$\hat{k}_x \pm i \hat{k}_y$	$\longleftrightarrow (l=1, m=\pm 1)$	$\leftrightarrow$ „p-wave"
2	$\hat{k}_x^2 - \hat{k}_y^2, \hat{k}_x \cdot \hat{k}_y$	$\hat{k}_x^2 - \hat{k}_y^2 \pm i \hat{k}_x \hat{k}_y$	$\longleftrightarrow (l=2, m=\pm 2)$	$\leftrightarrow$ „d-wave"
⋮	⋮	⋮	⋮	⋮

- Spin-rotation symmetry : Spin-Orbit Coupling (SOC)

In triplet pairing term we can rotate purely the spin, without touching the orbital space $\underline{k}$:

$$\vec{d}_{\underline{k}} \xrightarrow{SO(3)_{spin}} (R_s \vec{d})_{\underline{k}} \Rightarrow \left[\vec{\eta}_m^{(l)}\right]_\alpha \rightarrow \sum_{\alpha,\beta=1}^{3} R_{s,\alpha\beta}\, \eta_{m,\beta}^{(l)},$$

and the basis of vector space $\vec{\eta}$ is unrelated to orbital space $\underline{k}$.

With strong SOC, only joint rotations are possible in group $SO(3)_{\underline{k}} \times SO(3)_{spin}$,

so $\vec{d}_{\underline{k}}^{\Gamma} = \sum_i \vec{\eta}^{\Gamma,i} F(\hat{k}) \longrightarrow \sum_i \eta^{\Gamma,i} \left(F_x(\hat{k}) \hat{x} + F_y(\hat{k}) \hat{y} + F_z(\hat{k}) \hat{z} \right)$, with

$\hat{x}, \hat{y}, \hat{z}$ orts in $\underline{k}$-space.

– Crystal : Point Group (PG) symmetry

O(3) group in 3d is reduced to a subgroup PG, whose IRREPS are Γ_a, so for weak SOC:

$$\Phi_{\underline{k}}^{(\Gamma_e)} = \sum_{i=1}^{|\Gamma_e|} \eta_i^{(\Gamma_e)} f_i^{(\Gamma_e)}(\underline{k})$$

$$\vec{d}_{\underline{k}}^{(\Gamma_o)} = \sum_{i=1}^{|\Gamma_o|} \vec{\eta}_i^{(\Gamma_o)} f_i^{(\Gamma_o)}(\underline{k}) ,$$

where for any IRREP $\Gamma_e(\Gamma_o)$, the basis functions must be even(odd) under $\underline{k} \to -\underline{k}$.
„gerade" „ungerade"

→ **Basis functions** for IRREPS of PG of crystal with Bravais lattice generated by vectors $\underline{a}_1, \ldots, \underline{a}_d$ in d dimensions, are easily built from Fourier components:

for Γ_e: $\cos\left(\sum_{j=1}^{d} n_j \underline{k}\cdot\underline{a}_j\right)$, $n_j \in \mathbb{Z}$

for Γ_o: $\sin\left(\sum_j n_j \underline{k}\cdot\underline{a}_j\right)$

Each harmonic n is generated in tight-binding models by hopping of range n unit-cells.

In a small-$\underline{k}$ development around a High-Symmetry Point (HSP) in BZ, a useful list of generating functions for the $f_i(\underline{k})$ is $\underline{k}\cdot\underline{a}_i$, $(\underline{k}\cdot a_i)\cdot\underline{k}\cdot\underline{a}_j)$, ...

We abuse language by still using „s-wave", etc.

E.g.: 2d, $C_{4v} = \{e, C_4, C_4^2, C_4^3\} \otimes \{e, \sigma_v\}$; $C_4\begin{pmatrix}k_x\\k_y\end{pmatrix} = \begin{pmatrix}k_y\\-k_x\end{pmatrix}$; $\sigma_v\begin{pmatrix}k_x\\k_y\end{pmatrix} = \begin{pmatrix}-k_x\\k_y\end{pmatrix}$

IRREP A_0 (trivial, even) : $f^{(A_0)}(\underline{k}) = \alpha_1(\cos(k_x)+\cos(k_y)) +$
$+\alpha_2(\cos(k_x+k_y)+\cos(k_x-k_y)) +$
$+\alpha_3(\cos(2k_x)+\cos(2k_y)) + \ldots$

⇒ „s-wave"

IRREP E_u (2-dim, odd) : $f_1^{(E_u)}(\underline{k}) = \alpha_1 \sin k_x + \alpha_2 \sin(2k_x) \ldots$

⇒ „p-wave" $f_2^{(E_u)}(\underline{k}) = \alpha_1 \sin k_y + \alpha_2 \sin(2k_y) \ldots$

– Degeneracy of multi-dimensional IRREPS

The SC order parameter should spontaneously choose the linear combination in the degenerate space, and hence finalize the symmetry breaking. E.g., in C_{4v} example, $\begin{pmatrix} d_{\underline{k},x} \\ d_{\underline{k},y} \end{pmatrix} = \begin{pmatrix} \beta_{1x} \\ \beta_{1y} \end{pmatrix} f_1^{(E_u)}(\underline{k}) + \begin{pmatrix} \beta_{2x} \\ \beta_{2y} \end{pmatrix} f_2^{(E_u)}(\underline{k})$.

The general theory of Ginzburg-Landau free energy functionals $F(\eta_i^{(\Gamma_a)})$ says that the ground state will be such a linear combination that the remaining (unbroken) symmetry G_{SC} is maximal. E.g. $\eta_1^{(E_u)}$ is invariant under $C_2 = \{e, \sigma_v^{(y)}\}$, while $\frac{3}{5}\eta_1^{(E_u)} + \frac{4}{5}\eta_2^{(E_2)}$ is only invariant under $C_1 = \{e\}$.

$\Rightarrow$ We must consider ALL the symmetries of the paired state.

– U(1) phase symmetry

Recall that $\Delta_{\underline{k}}$ is not invariant under global (not gauge) $U(1)$,

$c_i \to e^{i\varphi} c_i \Rightarrow c_i^{+} \to e^{-i\varphi} c_i^{+} \Rightarrow \Delta_{\underline{k}} \to e^{-i2\varphi} \Delta_{\underline{k}}$ (2 electrons $\Rightarrow$ charge is 2)

We should consider the entire group $\boxed{U(1)} \times TRS \times PG \times SO(3)_{spin}$ (weak SOC).

In particular, $e^{i\varphi} \in U(1)$ transformations may compensate some PG ones.

E.g., $\sigma_v f_1^{(E_u)}(\underline{k}) = - f_1^{(E_u)}(\underline{k})$, but $(e^{i\varphi_1} \cdot \sigma_v) f_1^{(E_u)}(\underline{k}) = + f_1^{(E_u)}(\underline{k})$ for $\varphi_1 \equiv \pi$.

Key physical consequences:

① SC in 1-dim IRREP doesn't break TRS. That's because for all 1-dim Γ_a of any PG, $f^{(\Gamma_a)}(-\underline{k})^* = e^{i\varphi_{\Gamma_a}} f^{(\Gamma_a)}(\underline{k})$, and $T' \equiv e^{-i\varphi_{\Gamma_a}} T$ physically the same as T.

② SC in 2-dim IRREP will often prefer to form a CHIRAL state, $\boxed{f_1^{(\Gamma_a)}(\underline{k}) \pm i f_2^{(\Gamma_a)}(\underline{k})}$ (either singlet or triplet)

③ There are two partner states ($\pm$), spontaneously chosen, may form domains.

④ Chiral SC breaks TRS ($f \in \mathbb{C}$).

⑤ Physical „explanation" in 2d: even if f_1 and f_2 have nodes, $|f_1 \pm i f_2|^2 = |f_1|^2 + |f_2|^2 \neq 0$ in $BZ \setminus \{TRIM\}$, and SC is gapped ($E_{\underline{k}\pm} = \pm\sqrt{\xi_{\underline{k}}^2 + |\Delta_{\underline{k}}|^2}$).

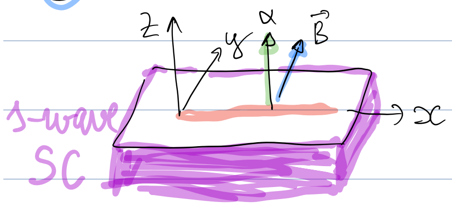
(Think $\sin k_x \pm i \sin k_y$. Nodes of f_2 are rotated w.r.t. to nodes of f_1.)

Full gap lowers energy of GS, so it's preferred.

2.B Realizing Kitaev chain in a spinful wire

Now we can understand that in K.C. $\Delta c_i^\dagger c_{i+1}^\dagger \to \Delta e^{-ik} c_k^\dagger c_{-k}^\dagger$, $\Delta e^{-ik} \longrightarrow \Delta_k - \Delta_{-k} \sim i\Delta \sin k$ is odd in k, as it should be, since spinless $(c_k, c_{-k}^\dagger) \simeq (c_{k\uparrow}, c_{-k\uparrow}^\dagger)$ gives triplet Δ.

① Rashba wire



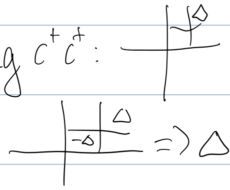
$$\hat{H} = \int dx \sum_{s,s'}^{\uparrow,\downarrow} c_{xs}^\dagger \left(-\frac{\partial_x^2}{2m} - \mu - \underline{\alpha (i\sigma_z)\partial_x} + \underline{B\sigma_y} \right)_{ss'} c_{xs'}$$

$$+ \int dx \left(\underset{\uparrow \atop \Delta \in \mathbb{R}}{\Delta} c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger + h.c. \right)$$

Rashba SOC $(\vec{k} \times \vec{\sigma})$

Bulk (PBC) wire : $\hat{H} = \sum_k c_{ks}^\dagger \Big(\underbrace{\frac{k^2}{2m} - \mu}_{\varepsilon_k} - \alpha \sigma_z k + B\sigma_y \Big)_{ss'} c_{ks'} + \sum_k \left(\Delta c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c. \right)$

$$\Psi_k \equiv \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ \hline c_{-k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix} ; \quad \xi_k = \varepsilon_k - \alpha\sigma_z k + B\sigma_y ;$$



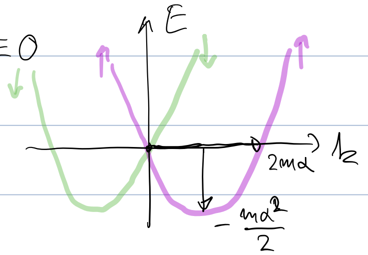
Pairing $c^\dagger c^\dagger$: $\to$

$\to \frac{1}{2}$ $\Rightarrow \Delta_k = i\sigma_2 \Delta$

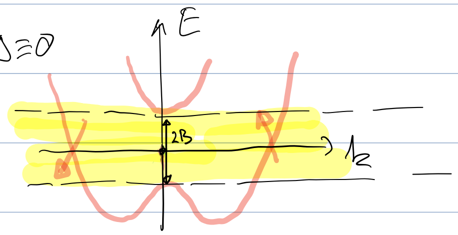
$$H_k = \left(\begin{array}{c|c} \xi_k & \Delta_k \\ \hline \Delta_k^\dagger & -\xi_{-k}^T \end{array} \right) = \varepsilon_k \tau_z - \alpha k \sigma_z + B\sigma_y - \Delta \tau_y \sigma_y$$

① $\Delta \equiv 0$, $B \equiv 0$

$(\mu \equiv 0)$



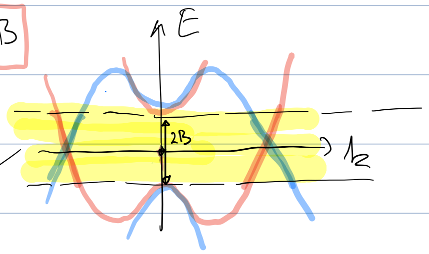
② $\Delta \equiv 0$

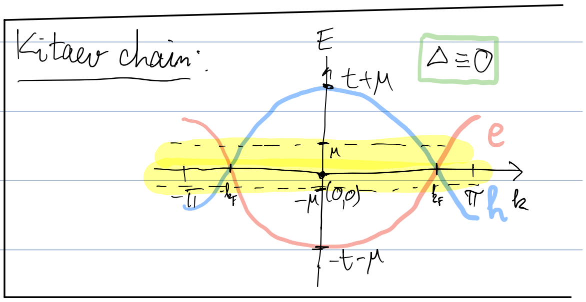


③ $\boxed{|\mu| = 0 < B}$

$\Delta \equiv 0$

$\approx$ one band & if $\boxed{\Delta < B}$




Kitaev chain:

$\boxed{\Delta \equiv 0}$

$\Rightarrow$ Should be effectively spinless (single band) triplet SC if „$|\mu|, \Delta < B$".

Let's see how this pairing arises.

Go to band basis („helicity basis" of SOC):

$$H^{wire}_{\underline{k}} = \varepsilon_k - \alpha\sigma_z k + B\sigma_y \Rightarrow \begin{cases} E_{k\pm} = \varepsilon_k \pm \sqrt{(\alpha k)^2 + B^2} \\ H_k \psi_{k\pm} = E_{k\pm}\psi_{k\pm} \Rightarrow \psi_{k\pm} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1 \pm \frac{D_z}{|D|}} \\ \pm \frac{D_+}{|D_+|} \cdot \sqrt{1 \mp \frac{D_z}{|D|}} \end{pmatrix} \end{cases}$$

② $\leftarrow$

$$\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} = \begin{pmatrix} \psi_{+,1} & \psi_{-,1} \\ \psi_{+,2} & \psi_{-,2} \end{pmatrix} \begin{pmatrix} d_{k+} \\ d_{k-} \end{pmatrix} \Rightarrow$$

$$D_+ \equiv D_x + iD_y \,;\; \vec{D} = (0, B, -\alpha k) \longrightarrow$$

$$\Rightarrow c^+_{k\uparrow} c^+_{\underline{k}\downarrow} = (\psi^*_{+,1} d^+_{k+} + \psi^*_{-,1} d^+_{k-})(\psi^*_{+,2}(-k) d^+_{\underline{k}+} + \psi^*_{-,2}(-k) d^+_{\underline{k}-}) =$$

$$= \underline{\psi_{+,1}(k)^* \psi_{+,2}(-k)^*} d^+_{k,+} d^+_{-k,+} + \underline{\psi^*_{-,1}(k)\psi^*_{-,2}(-k)} d^+_{k,-} d^+_{-k,-} \quad \leftarrow \text{INTRABAND}$$

$$+ \underline{\psi^*_{+,1}(k)\psi^*_{-,2}(-k)} d^+_{k,+} d^+_{-k,-} + \psi^*_{-,1}\psi^*_{+,2}(-k) d^+_{k,-} d^+_{-k,+} \quad \leftarrow \text{INTERBAND}$$

$$\psi^*_{\pm,1}(k)\psi_{\pm,2}(-k)^* = \frac{1}{2}\left(1 \pm \frac{(-\alpha k)}{\sqrt{(\alpha k)^2 + B^2}}\right)(\pm)(-i) = \frac{-i\alpha k}{2\sqrt{(\alpha k)^2 + B^2}} \Rightarrow \begin{cases} \Delta_{++} = \Delta_{--} = \frac{-i\alpha k \Delta}{2\sqrt{(\alpha k)^2 + B^2}} : \text{ODD} \\ \Delta_{+-} = -\Delta_{-+} = -\frac{i}{2}\frac{B\Delta}{\sqrt{(\alpha k)^2 + B^2}} : \text{EVEN} \end{cases}$$

$\to = 0$, fermion; $B > 0$

$$\psi^*_{+,1}(k)\psi^*_{-,2}(-k) = \frac{1}{2}\sqrt{\frac{B^2}{(\alpha k)^2 + B^2}}(-)i = -\frac{i}{2}\frac{B}{\sqrt{(\alpha k)^2 + B^2}}$$

$$H_{\underline{k}} = E_{k+} d^+_{k+} d_{k+} + E_{k-} d^+_{k-} d_{k-} + \frac{1}{2}(\Delta c^+_{k\uparrow} c^+_{-k\downarrow} + h.c.) =$$

$$= E_{k+} d^+_{k+} d_{k+} + E_{k-} d^+_{k-} d_{k-} + \frac{\Delta_{++}}{2}(d^+_{k,+} d^+_{-k,+} + d^+_{k,-} d^+_{-k,-}) + h.c. + \Delta_{+-} d^+_{k,+} d^+_{-k,-} + h.c.$$

- IF $|\mu|, |\Delta| \ll B$ we project to lower band (−), which has p-wave pairing as Kitaev chain, and is hence topological.

$\to$ TO BE DEMONSTRATED INTERACTIVELY

- Solving BdG just above gives one bulkgap closing @ $k=0$, and topo SC phase is for $\boxed{B > \sqrt{\Delta^2 + \mu^2}}$ confirming our expectation $|\mu|, |\Delta| < B$.
- Topo SC state controlled by μ, B, Δ, i.e. gating, field, so MBS can be created and moved at edges between topo and triv. wire.

- We engineer Kitaev chain by mixing SOC, B, and s-wave.
  ⇒ giant effort in community
- SOC works hard: splits bands, allows s-wave in band.
- Topo-SC created by non-trivial bands and trivial pairing.

Other candidate heterostructures, e.g. 2DTI edges + s-wave

PART 3: CLASSES OF GAPPED SC

BULK SC STRONG TOPOLOGY (AZ classes)

class	T^2	P^2	S^2	$d=0$	1	2	3
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$ CS	$\mathbb{Z}$ Ch	
DIII	-1	+1	+1		$\mathbb{Z}_2$ $\widetilde{CS}$	$\mathbb{Z}_2$ FK	$\mathbb{Z}$ V_3
C	0	-1	0			$2\mathbb{Z}$	
CI	+1	-1	+1				$2\mathbb{Z}$

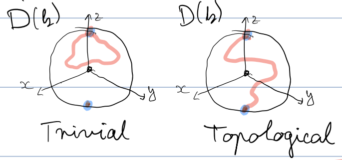
The invariants take various forms (additionally, with fixed # of bands), so we focus on presenting just some examples of them in physical dimensions, emphasizing differences.

3.A One dimension (1d)

3.A1 Class D ($d=1$)

Has only PHS, $\tau_x H_k^T \tau_x = -H_{-k}$, invariant is $\mathbb{Z}_2$.

Kitaev chain is key example, being single band, $H_k = \vec{D}_k \cdot \vec{\sigma}$, we saw



Trivial Topological

. More generally, PHS quantizes the:

Chern-Simons $\boxed{\mathbb{Z}_2}$ invariant: $\boxed{CS_1 = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{\alpha}^{occ.} A_k^{\alpha\alpha}}$; $A_k^{\alpha\beta} \equiv \chi_k^{(\alpha)*} \cdot \partial_k \chi_k^{(\beta)}$

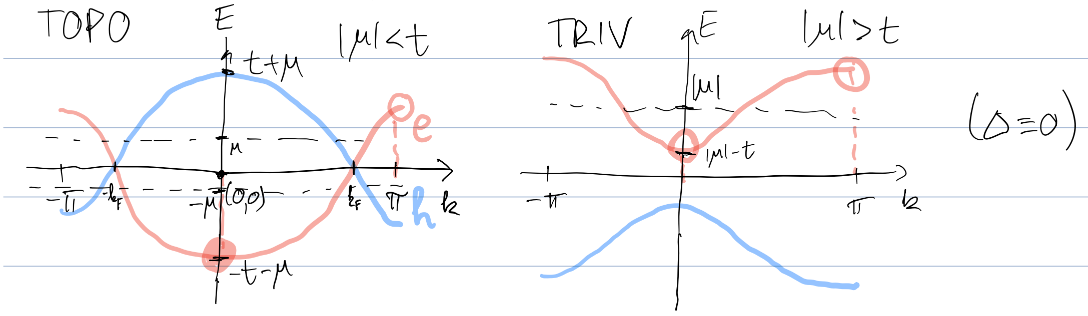
$H_k \chi_k^\alpha = E_{k\alpha} \chi_k^\alpha$

We only take occupied bands (BdG negative): $[H_k]_{2N\times 2N} \Rightarrow \alpha = \{(1-), \ldots (N-)\}$.

$$PHS \Rightarrow \boxed{e^{iCS_1}} = \pm 1 \left({}^{\text{triv}}/_{\text{topo}} \right) = \frac{\det[U_{k=\pi}]}{\det[U_{k=0}]} \underline{\underline{PHS}} \boxed{\mathrm{Sgn}\{ Pf[X_{k=\pi}] \cdot Pf[X_{k=0}] \}}, \quad ①$$

where unitary $[U_k]_{2N\times 2N} = \left(\begin{pmatrix} \chi_k^{(1-)} \end{pmatrix} \cdots \begin{pmatrix} \chi_k^{(2N-)} \end{pmatrix} \right)$, and $H_{K=0,\pi} = \frac{1}{2} \sum_{\alpha,\beta}^{2N} \lambda_{K\alpha} (i X_K^{\alpha\beta}) \lambda_{K\beta}$; $\{\lambda_{K\alpha}, \lambda_{K\beta}\} = 2\delta_{\alpha\beta}$

→ In Kitaev PBC chain, the $\mathrm{Pf}[X_K]$ measures if the electron state is filled at K, remember, the triplet $\Delta_k \sim \sin k = 0$ at TRIM $k \simeq -k \equiv K = 0, \pi$



- In case of threading flux, $e^{iCS_1} = \mathrm{Parity}(\phi=0) \cdot \mathrm{Parity}(\phi = \frac{h}{2e})$.

DETAILS:

What is X_K? Iff $k \simeq -k \equiv K$ (k is a TRIM), PHS is $(\tau_x \psi_K^{+})^T = \psi_{-K} = \psi_K$ a constraint at K alone. There are now Majorana's

$\lambda_{K\alpha} \equiv c_{K\alpha} + c_{K\alpha}^{+}$; $\lambda_{K,\alpha+N} \equiv i(c_{K\alpha} - c_{K\alpha}^{+})$; $\alpha = 1 \ldots N$; $\Rightarrow \{\lambda_{K\alpha}, \lambda_{K\beta}\} = 2\delta_{\alpha\beta}$; $\alpha, \beta = 1 \ldots 2N$.

In that basis, $H_K = \frac{1}{2} \sum_{\alpha,\beta}^{2N} \lambda_{K\alpha} (i X_K^{\alpha\beta}) \lambda_{K\beta}$; so that $X_K^{\alpha\beta} \in \mathbb{R}$, $X_K^{\beta\alpha} = -X_K^{\alpha\beta}$.

X_K is skew-symmetric so can be reduced to $\begin{pmatrix} \begin{matrix} 0 & E_{K1} \\ -E_{K1} & 0 \end{matrix} & \\ & \begin{matrix} 0 & E_{K2} \\ -E_{K2} & 0 \end{matrix} \\ & & \ddots \end{pmatrix}_{2N \times 2N}$, with

$\mathrm{Pf} X_K = \prod_{a=1}^{N} E_{Ka} \Rightarrow \det X_K = (\mathrm{Pf} X_K)^2$, where E_{Ka} are the BdG energies.

$\mathrm{Pf} X_K$ changes sign when an E_{Ka} changes sign, i.e. when parity changes at K, i.e., when electron state changes occupation.

In general at TRIM, the $\lambda_{K\alpha}$ gives:
$$X_K = \frac{1}{2} \left(\begin{array}{c|c} \mathrm{Im}(\xi_K + \Delta_K) & -\mathrm{Re}(\xi_K - \Delta_K) \\ \hline \mathrm{Re}(\xi_K + \Delta_K) & \mathrm{Im}(\xi_K - \Delta_K) \end{array} \right)_{2N \times 2N}$$

For Kitaev chain, triplet $\Delta_K = 0$; $\xi_K = t\cos K - \mu \in \mathbb{R}$, so $\mathrm{Pf}[X_K] = -\xi_K$

$\Rightarrow e^{iCS_1} = \mathrm{sgn}\{(t-\mu)(-t-\mu)\} = \begin{cases} -1, & t > |\mu| \\ +1, & t < |\mu|. \end{cases}$

Proof of ①: PHS relates $\mathcal{A}_k^{(a-)(b-)}$ to $\mathcal{A}_{-k}^{(a+)(b+)}$, so $\int_{-\pi}^{\pi} dk\, \mathcal{A}_k^{(a-)(a-)} \to \int_0^{\pi} dk \left(\mathcal{A}_k^{(a-)(a-)} + \mathcal{A}_k^{(a+)(a+)} \right)$, while summing over all $(a\pm)$ allows $\mathcal{A}_k(\chi_k) \to U_k$, giving $e^{iCS_1} = \frac{\det U_\pi}{\det U_0}$.

Now changing to Majorana basis, "diagonalizing" X_K with $O_K \in O(2N)$, gives the Pf.

3.A2 Class DIII (d=1)

Has PHS, and spinful TRS: $\sigma_y H_k^* \sigma_y = H_{-k}$, so also chirality $S \sim P \cdot T$ automatically.

The $\mathbb{Z}_2$ invariant $\boxed{\widetilde{CS}_1 = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_{\alpha=(a-)}^{N} A_k^{\alpha\alpha} \ (\mathrm{mod}\ 2)}$.

Here TRS quantizes the CS integral differently than PHS.

Reducing to a quantity at TRIMs gives expressions that are challenging for practical use.

EXAMPLE: $T = i\sigma_2 K$, $P = \tau_1 K \Rightarrow S = \tau_1 \sigma_2$ chirality, $S^2 = \mathbb{1}_{2N}$.

In S eigenbasis, $S = \begin{array}{c|c} \mathbb{1}_N & \\ \hline & -\mathbb{1}_N \end{array}$, $H_k = \begin{pmatrix} 0 & h_k \\ h_k^\dagger & 0 \end{pmatrix}$, $T = \begin{array}{c|c} & \mathbb{1}_N \\ \hline -\mathbb{1}_N & \end{array} K$.

TRS $\Rightarrow h_k = -h_{-k}^T$. Also for flattened Hamiltonian $Q_k = \begin{pmatrix} 0 & g_k \\ g_k^\dagger & 0 \end{pmatrix}$, $g_k = -g_{-k}^T$.

$\Rightarrow \boxed{(-1)^{\widetilde{CS}_1} = \frac{\mathrm{Pf}[g_\pi]}{\sqrt{\det g_\pi}} \Big/ \frac{\mathrm{Pf}[g_0]}{\sqrt{\det g_0}}}$, must choose $\sqrt{\ }$ branch so that it is continuous from $k=0$ to $k=\pi$. (HARD)

3.A2.1 Simplification at weak pairing

Simplification: The SC gap opens at the Fermi Surface (FS) - in 1d, Fermi points — i.e., at $\xi_k = \varepsilon_k - \mu \equiv 0$. Hence for weak pairing, $\Delta/|k_F| \ll 1$, the topology should depend on the FS and Δ only

$$\boxed{N_{1d} \equiv \prod_s \mathrm{sgn}(\delta_{k_F^{(s)}}) = \widetilde{CS}_1},$$

where s labels all Fermi points $0 < k_F^{(s)} < \pi$, while

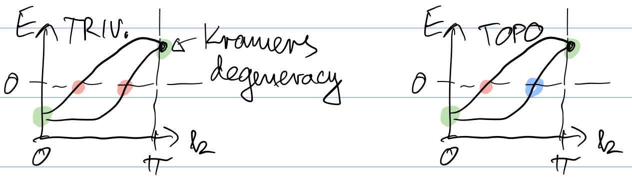
$\delta_{k_F^{(s)}} \equiv \langle k_F^{(s)}, \alpha_s | T \Delta_k^\dagger | k_F^{(s)}, \alpha_s \rangle \in \mathbb{R}$, where the band α_s defines the Fermi point s.

→ Consequently, odd # crossings @ $E=0$ with $\delta<0$ each gives Topo SC.

EXAMPLE:

$\delta > 0$: ●

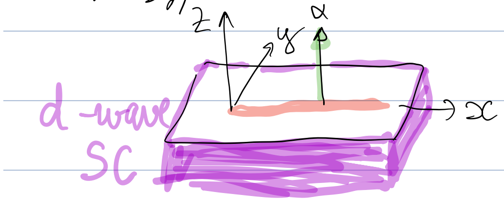
$\delta < 0$: ●



NOTE: Isn't sign of Δ_k meaningless? $c^\dagger \to e^{-i\varphi} c^\dagger \Rightarrow \Delta \to e^{2i\varphi}\Delta$; BUT matrix element between $|1\rangle$ and $T|1\rangle$ is meaningful: $\langle 1|\Delta|1\rangle \to (\langle 1|e^{i\varphi})(e^{2i\varphi}\Delta)(e^{-i\varphi}|1\rangle) = e^{2i\varphi}\langle 1|\Delta|1\rangle$, BUT $\langle 1| \overbrace{i\sigma_2 K}^{T} (\Delta|2\rangle)$ is OK.

$\boxed{3.A2.2}$ Model wire to realize DIII topology:

Rashba wire + d-wave
(no B!)

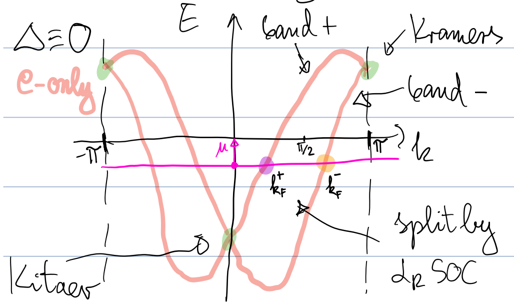


$$\hat{H} = -\frac{1}{2}t\sum_{j\sigma}\left(c^{\dagger}_{j+1,\sigma}c_{j,\sigma} + h.c.\right) - \mu c^{\dagger}_{j\sigma}c_{j\sigma}$$
$$-\frac{\hat{1}}{2}\alpha_R\sum_{j,\sigma,\sigma'}\left(c^{\dagger}_{j+1,\sigma}(i\sigma_y)^{\sigma\sigma'}c_{j,\sigma'} + h.c.\right)$$
$$+\frac{1}{2}\sum_{j}\left(\Delta\left(c^{\dagger}_{j+1,\uparrow}c^{\dagger}_{j,\downarrow} - c^{\dagger}_{j+1,\downarrow}c^{\dagger}_{j,\uparrow}\right) + h.c.\right)$$

$$\hat{H} = \sum_{k}\left(c^{\dagger}_{k\uparrow}, c^{\dagger}_{k\downarrow}\right)\left[-(t\cos k + \mu)\mathbb{1}_2 + \alpha_R \sin k\cdot\sigma_y\right]\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}\end{pmatrix} + \left(\Delta\cos k\cdot c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow} + h.c.\right)$$

$$H_k = \left(\begin{array}{c|c} \hat{\xi}_k & \hat{\Delta}_k \\ \hline \hat{\Delta}^{\dagger}_k & -\hat{\xi}^T_{-k}\end{array}\right) \text{ for } \Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^{\dagger}_{-k\uparrow} \\ c^{\dagger}_{-k\downarrow}\end{pmatrix} \Rightarrow \hat{\Delta}_k = \left(\begin{array}{c|c} & 2\Delta\cos k \\ \hline & \end{array}\right) \xrightarrow{\text{fermion}} \frac{1}{2}\left(\hat{\Delta}_k - \hat{\Delta}^T_{-k}\right) =$$
$$= \left(\begin{array}{c|c} & \Delta\cos k \\ \hline -\Delta\cos k & \end{array}\right) = \Delta\cos k\,(i\sigma_y)$$

$\hat{\Delta}_k = \Delta\cos k\,(i\sigma_y)$: singlet, k-even, TRS (because $\cos k \in \mathbb{R}$)



would open gap here and set μ there

$$\hat{\xi}_k : |k,\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i\,\mathrm{sgn}(\sin k)\end{pmatrix}$$

T forces also $k\to -k$.

$$T\hat{\Delta}^{\dagger}_k|k,\pm\rangle = i\sigma_2 K\cdot\Delta\cos k\,(i\sigma_2)\,|k,\pm\rangle = -\Delta\cos k\,|-k,\pm\rangle^{*}$$

$$\Rightarrow \delta_{\pm} = \langle k_F^{\pm},\pm|\left(-\Delta\cos k_F^{\pm}\right)|-k_F^{\pm},\pm\rangle^{*} =$$
$$= -\Delta\cos k_F^{\pm}\cdot\frac{1}{2}\left(1 + \mathrm{sgn}(\underbrace{\sin k_F^{\pm}}_{>0,\text{ for } 0<k_F^{\pm}<\pi})\right) = -\Delta\cos k_F^{\pm}$$

$$\nu \equiv (-1)^{\widetilde{CS}_1} = \mathrm{sgn}(\delta_+)\,\mathrm{sgn}(\delta_-) = \mathrm{sgn}(\cos k_F^{+})\cdot\mathrm{sgn}(\cos k_F^{-}).$$

IF $\mu \ll \alpha_R$, $k_F^{\pm} \approx \frac{\pi}{2} \pm q \Rightarrow \nu = -1$ (TOPOLOGICAL)

Precise solution : $\nu = -1$ for $|\mu| < \alpha_R$.

→ Open chain has 2 protected MBS on each endpoint. They form a Kramers pair.

3.B Two dimensions

3.B1 Class D (d=2)

The invariant is the usual first Chern number. For flattened Hamiltonian $Q_{\underline{k}} = 1 - 2P_{\text{filled}}(\underline{k})$:

$$\boxed{Ch_1 = \frac{i}{2\pi}\iint_{BZ} \mathrm{Tr}(\mathcal{F}_{\underline{k}})} \in \boxed{\mathbb{Z}} \qquad ; \ \mathcal{F} = d\mathcal{A} + \mathcal{A}^2$$

$$= -\frac{i}{16\pi}\iint_{BZ} \mathrm{Tr}[Q_{\underline{k}} dQ_{\underline{k}} dQ_{\underline{k}}] \qquad Q_{\underline{k}} = \text{"flattened" } H_{\underline{k}}$$

→ In the case of $[H_{\underline{k}}]_{2\times2}$, $H_{\underline{k}} = \vec{D}_{\underline{k}} \cdot \vec{\sigma}$, and $\boxed{Ch_1 = N_w}$ is the wrapping number of $\vec{D}_{\underline{k}}/|\vec{D}_{\underline{k}}|$ on the sphere of the BZ (torus → sphere).

→ We consider chiral SC's ($p\pm ip$, $d\pm id$) with $C=\pm1,\pm2$ in Excercise, while the defects are considered below.

3.B2 Class DIII (d=2)

The invariant is the first Fu-Kane number, which is expressed through both $\mathcal{F}_{\underline{k}}$ and $\mathcal{A}_{\underline{k}}$ and hence requires a lot of care with gauge choice.

An expression using TRIMs only:

$$\boxed{W = FK_1 = \prod_{K \in TRIM} \frac{\mathrm{Pf}[w_K]}{\sqrt{\det w_K}} = \prod_{K} \frac{\mathrm{Pf}[g_K]}{\sqrt{\det g_K}}}, \quad \begin{cases} \text{"Flattened } H_{\underline{k}}\text{"} = Q_{\underline{k}} = \begin{pmatrix} 0 & g_{\underline{k}} \\ g_{\underline{k}}^{+} & 0 \end{pmatrix} \text{ in} \\ \text{chiral basis.} \\ w_{\underline{k}}^{ab} \equiv \langle \chi_{-\underline{k}}^{(a-)} | T \chi_{\underline{k}}^{(b-)} \rangle : \text{sewing matrix} \end{cases}$$

again requiring to follow a branch of $\sqrt{\ }$.

3.B2.1 Simplification at weak pairing

As in d=1, there is at weak pairing a FS-dependent result:

$$\boxed{N_{2d} = \prod_{s} [\mathrm{sgn}(\delta_s)]^{m_s} = W},$$

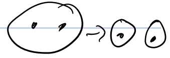
m_s = #TRIM points enclosed by the s-th FS — here, Fermi line. The

$$\delta_s \equiv \langle \underline{k}_F^{(s)}, \alpha_s | T \Delta^{+}_{\underline{k}} | \underline{k}_F^{(s)}, \alpha_s \rangle \in \mathbb{R}$$

does not change sign on the s-th FS as we assumed a gapped SC, hence evaluate it at any $k_F^{(s)} \in$ s-th FS.

→ Odd # of FS enclosing each a TRIM, with $\delta<0$, gives topo SC.

If a FS_s encloses multiple TRIM, it can be reconnected:



3.B2.2 Simplification for triplet pairing

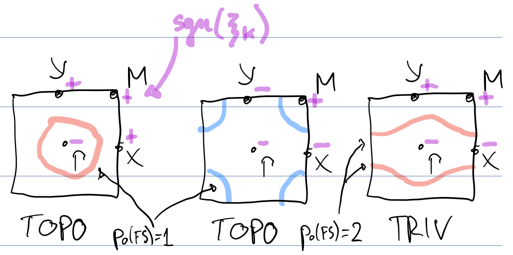
If the normal state $(\xi_{\underline{k}})$ has inversion symmetry (plus the PHS and TRS of DIII), and the pairing is pure triplet, $\phi_{\underline{k}} \equiv 0$, $\vec{d}_{\underline{k}} \neq 0$, then

$$\boxed{\nu_{2d} \equiv \prod_{K \in TRIM} \prod_{i=1}^{r} \operatorname{sgn}(\varepsilon_{K,i}) = W}$$

where the $\varepsilon_{K,i}$ are normal-state energies, i.e., the set of r distinct eigenvalues of $[\xi_K]_{2r\times 2r}$, which are all doubly degenerate due to Kramers.

In case of a single spinful band, $r=1$, we get a FS-related quantity:

$$\boxed{\nu_{2d} \overset{r=1}{=} \prod_{K \in TRIM} \operatorname{sgn}(\xi_K) = (-1)^{P_0(FS)} = W},$$



$P_0(FS)$ = # connected components of the FS.

3.C Three dimensions

In class DIII there is the third winding number:

$$\boxed{\nu_3 = \int_{BZ} \frac{d^3k}{24\pi^2} \varepsilon^{\mu\nu\rho} \mathrm{Tr}\left[(g^{-1}\partial_\mu g)(g^{-1}\partial_\nu g)(g^{-1}\partial_\rho g)\right]} \in \boxed{\mathbb{Z}},$$

; "flattened" $H_{\underline{k}} = \begin{pmatrix} 0 & g_{\underline{k}} \\ g^{+}_{\underline{k}} & 0 \end{pmatrix}$ in chiral basis

In single band case, $r=1$, introduce a 4d vector on sphere S^3: $\hat{\eta}_a = \eta_a / \sqrt{\sum_{b=1}^{4} |\eta_b|^2}$, $a = 1 \dots, 4$; $\eta = (d_x, d_y, d_z, \xi)$, then ν_3 counts the # of wrappings of S^3 as we sweep BZ: $(k_x, k_y, k_z) \in T^3 \simeq S^3$.

For $r=1$ there is a formula (mod 2):

$$\boxed{(-1)^{\nu_3} = \prod_{K \in TRIM} \mathrm{sgn}(\xi_K) = (-1)^{\chi(FS)/2}}, \text{ where } \chi(FS) = \sum_{j=1}^{c} \chi(FS_j) = \sum_{j=1}^{c} 2(1 - g(FS_j)),$$

χ being the Euler characteristic, and g the genus, of connected component $j = 1 \dots c$ of FS.

NOTE: Extensively studied superfluid liquid (not crystal) in DIII ($d=3$) is ^{3}He.

3.D Classes C and CI

When a BdG model has only its PHS and full spin-rotation symmetry ($\Rightarrow$ no SOC), it reduces to blocks for $\psi^{(1)} = \begin{pmatrix} c_\uparrow \\ c^\dagger_\downarrow \end{pmatrix}$ and $\psi^{(2)} = \begin{pmatrix} c_\downarrow \\ c^\dagger_\uparrow \end{pmatrix}$ in which spin rotations impose an effective PHS, $P'^2 = -\mathbb{1}$ (e.g. $P' = \tau_y K$), this is class $\boxed{C}$.

Adding the spinful TRS, which in the block becomes a chirality constraint S', and $P' \cdot S' \equiv T'$ is a new effective TRS with $T'^2 = +\mathbb{1}$ (e.g. $T' = K$). This is class $\boxed{CI}$.

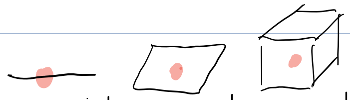
Non-trivial topology is in

① $d=2$ for C, where the invariant is just the Chern number Ch_1 as in class D ($d=2$), but gets doubled because of two copies in spin space

② $d=3$ for CI, where the invariant is just the third winding number ν_3, as in class DIII ($d=2$), but gets doubled due to two spin copies also.

PART 4: BULK-BOUNDARY-DEFECT CORRESPONDENCE

4.A Point defect



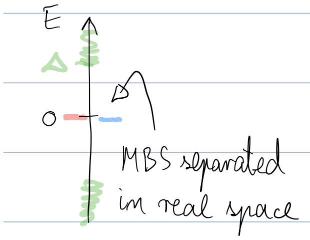
class	T^2	P^2	S^2	$d=1$	2	3
D	0	+1	0	$\mathbb{Z}_2^{\,CS_1}$	$\mathbb{Z}_2^{\,CS_3}$	$\mathbb{Z}_2^{\,CS_5}$
DIII	-1	+1	+1	$\mathbb{Z}_2^{\,\widetilde{CS}_1}$	$\mathbb{Z}_2^{\,\widetilde{CS}_3}$	$\mathbb{Z}_2^{\,\widetilde{CS}_5}$
C	0	-1	0			
CI	+1	-1	+1			

← Majorana Bound State (MBS)

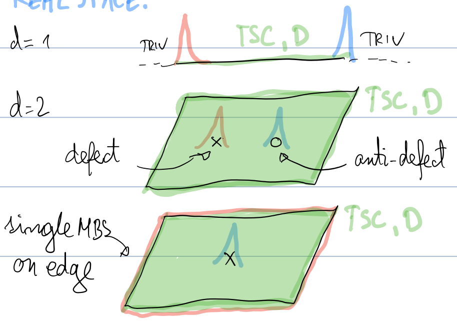
← Kramers pair of MBS

① MBS: class D ($\mathbb{Z}_2$)

ENERGY:

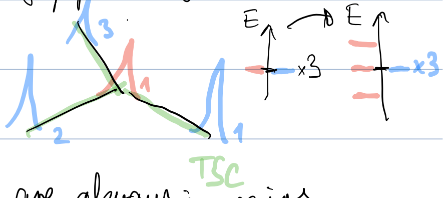


REALSPACE:



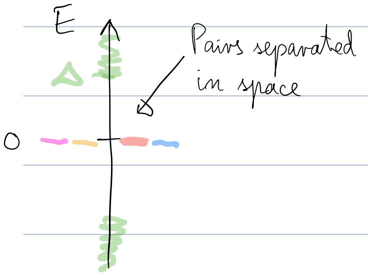
TOPOLOGICAL PROTECTION

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, protection is for 1 MBS. In finite $[H_{\underline{k}}]_{2p\times2p}$ however they are always in pairs.

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

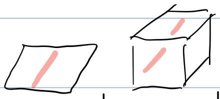


$$\left.\begin{aligned}\lambda_1 &= \sum_a \chi_{1,a}\psi_a \\ \lambda_1' &= \sum_a (T\chi_1)_a\psi_a\end{aligned}\right\}\ \{\lambda_1,\lambda_1'\}=0 \text{ because } \chi_1^\dagger\cdot(T\chi_1)=0, \text{ because } T^2=-1$$

Topology distinguishes odd vs. even # of K. pairs.

If # K.p. = odd, one pair is protected.

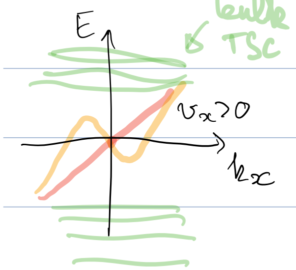
4.B Line defect



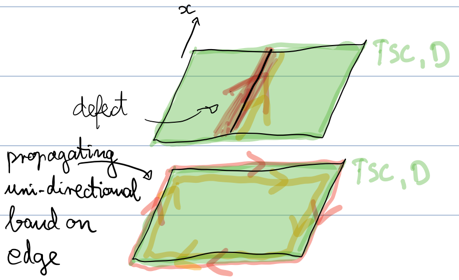
class	T^2	P^2	S^2	d=1	2	3	
D	0	+1	0		$\mathbb{Z}^{C_2}$	$\mathbb{Z}^{C_2}$	← Chiral Majorana Mode (cMM)
DIII	-1	+1	+1		$\mathbb{Z}_2^{FK_2}$	$\mathbb{Z}_2^{FK_2}$	← Helical MM (hMM)
C	0	-1	0		$2\mathbb{Z}^{2C_2}$	$2\mathbb{Z}^{2C_2}$	← Chiral Dirac Mode
CI	+1	-1	+1				

① Chiral MM, class D ($\mathbb{Z}$)

ENERGY:



REALSPACE:



TOPOLOGICAL PROTECTION

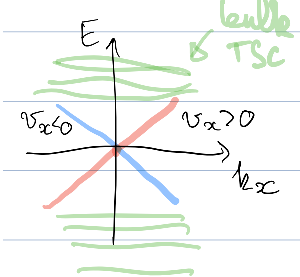
$\mathbb{Z}$ is (# modes. $v_x>0$) − (# modes. $v_x<0$).

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

True Majorana $\lambda^\dagger=\lambda$ only at $k=0$, for the rest of cMM, $\lambda_k^\dagger=\lambda_{-k}$.

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

ENERGY:



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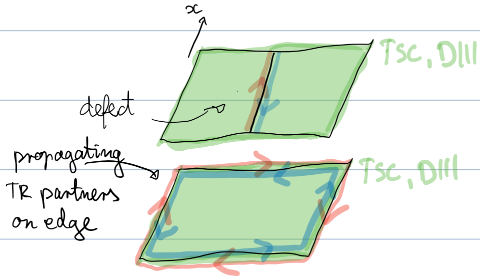


TOPOLOGICAL PROTECTION

Distinguishes odd vs. even pairs ↗↙. The ↙ of one pair can hybridize with ↗ of another pair, so only 1 pair protected.

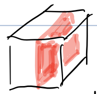
True Majorana's at $k=0$, a Kramers pair. $T\lambda_{k\uparrow}T^{-1}=\lambda_{-k\downarrow}$.

③ Chiral Dirac, class C

Two copies of cMM cannot cannot gap out, but reconstitute a uni-directional normal fermion $c=\lambda_1+i\lambda_2$.

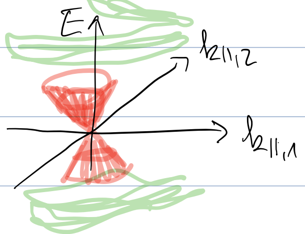
NOTE: Classes C, CI are not good for MBS or MM, they have full spin-rotation symmetry.

4.C Planar defect



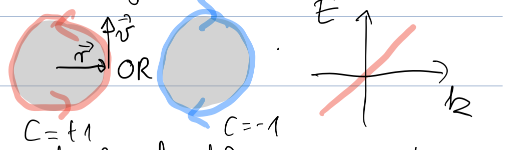
class	T^2	P^2	S^2	d=1	2	3
D	0	+1	0			
DIII	-1	+1	+1			$\mathbb{Z}$ ν_3
C	0	-1	0			
CI	+1	-1	+1			$2\mathbb{Z}$ $2\nu_3$

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



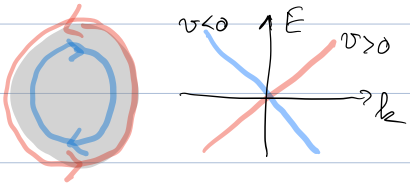
NOTE on language: „CHIRAL" and „HELICAL"

- „Chiral mode" is a 1d band that propagates strictly in one (but not reverse) direction. E.g. quantum Hall edge states.
The chiral partners map into each other by time reversal, or by mirror. So one C state breaks these symmetries.
Uni-directional. The current in the mode carries angular momentum, $\vec{r} \times \vec{v} \sim C$. Inversion is NOT broken ($\vec{r} \to -\vec{r}$, $\vec{v} \to -\vec{v}$). Broken mirror is origin of name.



- „Chiral SC" is a SC state in which a 2-dim IRREP produces a complex combination, e.g. $p_x \pm i p_y$, or $d_{x^2-y^2} \pm i d_{xy}$. It breaks TRS and mirror. A chiral SC is likely to have chiral edge state modes.
- „Chiral symmetry", $S H_{\underline{k}} S^{-1} = -H_{\underline{k}}$, usually realized due to bipartite nature of system, or as P·T. Protected zero mode is eigenstate of S.

- „Helical mode": a pair of time-reversed partner 1-dim modes.
TRS is preserved. In spinfull system, the two modes have opposite spin ($T|\uparrow\rangle = |\downarrow\rangle$).
The locking of movement direction and spin is the origin of name.

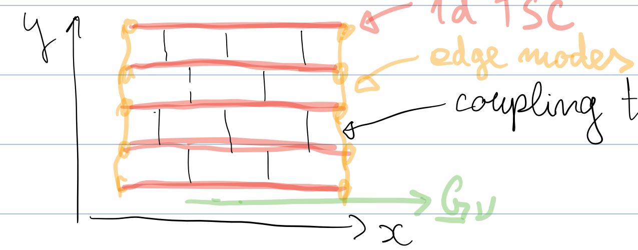


- „Helical basis": eigenbasis of (TR-symmetric) kinetic energy with SOC. Bands have opposite (but k-dependent) spin directions. Concerns bulk system, not edge modes. $c^{\dagger}_{k\sigma} \left(\varepsilon_{\underline{k}} \mathbb{1} + \vec{g}_{\underline{k}} \cdot \vec{\sigma} \right)_{\sigma\sigma'} c_{k\sigma'} \longrightarrow c^{\dagger}_{\underline{k}\pm} \left(\varepsilon_{\underline{k}} \mathbb{1} \pm |\vec{g}_{\underline{k}}| \right) c_{\underline{k}\pm}$

4.D More on MBS

4.D1 Weak topology: MBS in 2d without chiral SC

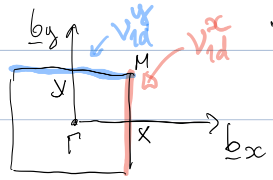
„Weak topology" is understood through layering; e.g. in 2d:



Interlayer coupling may become strong, and system may be trivial regarding its („strong") 2d topological invariant, e.g. $\nu_{2d} = 0$, but still has a directed 1d topology, written as vector:

$$\underline{G}_\nu = \nu_{1d}^x \underline{b}_x + \nu_{1d}^y \underline{b}_y \ , \quad \text{where } \underline{b}_i \text{ are reciprocal vectors, } \underline{a}_i \cdot \underline{b}_j = 2\pi \delta_{ij}$$

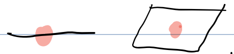
The 1d invariant is calculated on the edge of BZ:



We could have in this example: $(\nu_{1d}^x, \nu_{1d}^y) = (\nu_{1d}, 0)$, so $\underline{G}_\nu = \nu_{1d} \cdot \underline{b}_x$, and there are protected edge modes only on edge orthogonal to $\underline{G}_\nu$, i.e. along $\hat{y}$.

If the ν_{2d} is expressed via TRIMs, e.g. $\nu_{2d} = \prod_{K \in TRIM} \delta_K$, then $\nu_{1d}^x = \delta_X \cdot \delta_M$.

Focus on MBS:

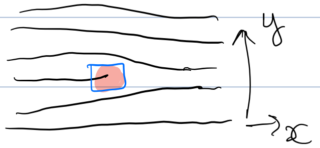


class	T^2 P^2 S^2	d=1	2
D	0 +1 0	$\mathbb{Z}_2$ CS$_1$ $\leftarrow$	$\mathbb{Z}_2$ CS$_3$

In 2d an MBS can occur in chiral $p_x + ip_y$ SC, but is not expected in non-chiral p_x-wave in 2d.

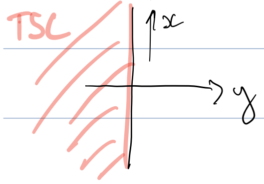
The p_x-wave can have weak topology, because in 1d, p_x-wave in Kitaev wire suffices: we can layer Kitaev chains.

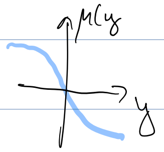
A dislocation defect binds an MBS:
↳ endpoint of Kitaev chain



4.D2 MBS on vortices, and edge states in 2d p+ip SC

① Spinless p+ip edge state (class D, d=2)



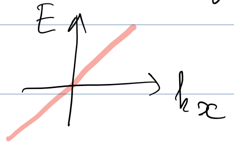


We take $\Delta_{\underline{k}} = \Delta(k_x - ik_y) \to \Delta(k_x - \partial_y)$. Edge at $y=0$ between this p_x-ip_y TSC and a trivial p_x-ip_y SC is achieved by making $\mu(y)<0$ at $y<0$ (like in Kitaev chain $\mu \gtrless 0$ is topo/triv).

We neglect the kinetic energy $\frac{-(\nabla_{\underline{k}})^2}{2m}$, due to slow variation of μ.

$$H^{BdG} = \left(\begin{array}{c|c} -\mu(y) & \Delta(k_x - \partial_y) \\ \hline \Delta(k_x + \partial_y) & \mu(y) \end{array}\right).$$

Solutions localized around $y=0$ are given by



$$\chi_{k_x,y} \sim e^{+\frac{1}{\Delta}\int_0^y dy' \mu(y')} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$ with $\underline{E = \Delta k_x}$, easy to check.

This is a chiral Majorana mode (CMM).

$\boxed{\text{NOTE}}$: For $p_x + ip_y$ pairing, $E = -\Delta k_x$ and $\begin{pmatrix} 1 \\ 1 \end{pmatrix} \to \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

Bogoliubon: $$\gamma_{k_x,y} = e^{\int^y \mu/\Delta}\left(c_{k_x,y} + c^\dagger_{-k_x,y}\right), \text{ while}$$
$$\gamma_{x,y} = e^{\int^y \mu/\Delta}\left(c_{x,y} + c^\dagger_{x,y}\right), \text{ so}$$

$\gamma^\dagger_{k_x,y} = \gamma_{-k_x,y}$: CMM

$\gamma^\dagger_{x,y} = \gamma_{x,y}$: True Majorana, but is local at x,y and <u>NOT</u> an eigenstate

② Spinless p+ip vortex: MBS (class D, d=2)

Consider first a standard s-wave (singlet) uniform SC in 2d, in a rotationally symmetric system, $H^{bulk}_{\underline{k}} = \left(\begin{array}{c|c} \xi_{k,\theta} & \Delta \\ \hline \Delta^* & -\xi^T_{k,\theta+\pi} \end{array}\right)$. It is gapped, and all states have integer angular momentum, $\psi_{k,\theta} \sim e^{im\theta}$, $m \in \mathbb{Z}$, with θ the polar angle.

Contrast to p+ip (triplet) SC: $H^{bulk}_{\underline{k}} = \left(\begin{array}{c|c} \xi_{\underline{k}} & \Delta_0(k_x + ik_y) \\ \hline \Delta_0^*(k_x - ik_y) & -\xi^T_{-\underline{k}} \end{array}\right)$.

Now in real space we note that $-i\partial_x \pm i(-i\partial_y) \sim \hat{L}_\pm$, with $\hat{L}_\pm$ the increasing/decreasing operators for angular momentum $\hat{L}_z$, i.e. $-i(\partial_x \pm i\partial_y)\, e^{im\theta} = \pm i \frac{m}{r} e^{i(m\pm1)\theta}$. Hence the solutions $\chi_{m,m'} = \begin{pmatrix} e^{im\theta} u_m \\ e^{im'\theta} v_m \end{pmatrix}$ of $H\chi_{m,m'} = E_{m,m'}\chi_{m,m'}$ must obey $\begin{cases} m = m'+1 \\ m-1 = m' \end{cases}$, and having the form of Dirac equation, $H_{\underline{k}}$ implies $m = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$, so $\chi_m = e^{il\theta}\begin{pmatrix} e^{i\theta/2} u_l \\ e^{-i\theta/2} v_l \end{pmatrix}$, $l = 0, 1, \ldots$

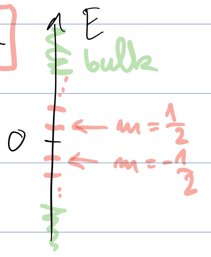
Now we add a SC vortex: $\Delta_{\underline{k}} \to e^{i\theta(\underline{r})}\Delta_{\underline{k}}$, with $\theta(\underline{r})$ the polar angle in real space. Vortex is mapped back to bulk system by a phase transformation $c_{\underline{k}} \to e^{i\frac{\theta(\underline{r})}{2}} c_{\underline{k}} \Rightarrow c^\dagger_{-\underline{k}} \to e^{-i\frac{\theta(\underline{r})}{2}} c^\dagger_{-\underline{k}}$.

In p+ip case, the k_x+ik_y acts on $\theta(\underline{r})$ as $-i\partial_x + i(-i\partial_y)$, but the term generated is even in $\underline{k}$ and vanishes due to fermion constraint.

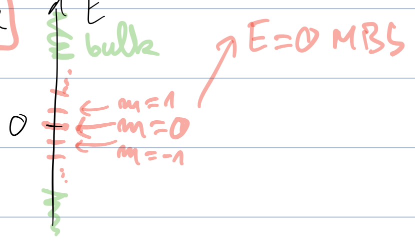
Hence $H^{vortex} = H^{bulk}$, except the $\chi_{\underline{k}}$ now obeys anti-periodic boundary conditions $\chi_{bulk}(\theta=2\pi) = \chi_{bulk}(\theta=0)$, but $\chi_{vor}(\theta=2\pi) = e^{i\frac{2\pi}{2}}\chi_{vor}(\theta=0) = -\chi_{vor}(\theta=0)$. Effectively, we shifted the angular momentum by $\frac{1}{2}$ (with the prefactor $e^{i\frac{\theta}{2}}$) w.r.t. the bulk. Hence, is s-wave vortex $m = \pm\frac{1}{2}, \ldots$, in p+ip, $m = 0, \pm1, \ldots$

The vortex also induces in-gap states bound to vortex (in s-wave, Caroli-Matricon-de Gennes). With m quantum number.

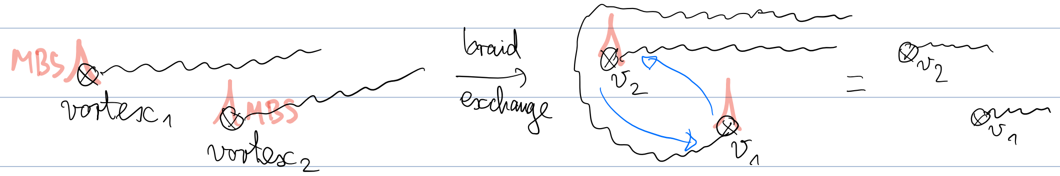
s-wave



p-wave



For p+ip vortex, the anti-PBC acts on all fermions. Hence we can attach a string to vortex, so that a fermion circumventing the vortex and changing sign $\Psi_{\theta=2\pi} = -\Psi_{\theta=0}$, is forced when fermion crosses the string. Also true for MBS in center of vortex if it circumvents another vortex.



Since MBS on v_2 crossed the string of v_1, the exchange is: $\gamma_1 \to -\gamma_2$; $\gamma_2 \to +\gamma_1$, i.e. $U_{ex} = \frac{1}{\sqrt{2}}(1+\gamma_1\gamma_2)$: $U_{ex}\gamma_1 U_{ex}^\dagger = -\gamma_2$, $U_{ex}\gamma_2 U_{ex}^\dagger = \gamma_1$. The $|GS\rangle \to U_{ex}|GS\rangle$:

Non-local operation of braiding changes the ground state (within same parity degenerate subspace) $\Rightarrow$ basis for topological quantum computation.

③ Spinful p+ip vortex: MBS (class D, d=2)

We stay with broken TRS in same class but add spin. Now a vortex means for triplet pairing $\vec{d}_{\underline{k}} \to e^{i\theta(\underline{r})}\vec{d}_{\underline{k}}$, and e.g. $\vec{d}_{\underline{k}} = \Delta_0 \hat{e}_x(k_x + ik_y)$, so

pairing: $\begin{array}{c|c} -d_x+id_y & d_z+\psi \\ \hline d_z-\psi & d_x+id_y \end{array} = \Delta_0 \begin{array}{c|c} -1 & \\ \hline & 1 \end{array} \Rightarrow$ Cooper pairs $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ experience the vortex $\Delta_0 \to \Delta_0 e^{i\theta(\underline{r})}$. Two MBS now have opposite spin, and can be mixed e.g. by SOC (which doesn't change the D class), $H_{mix} = E_{mix}\, i\gamma_\uparrow\gamma_\downarrow$, as we know in class D only one MBS per defect is protected.

However, we can make an MBS in spinful system by adapting the vortex:

Half-Quantum Vortex (flux $\frac{hc}{4e}$): $\Delta_0 \to e^{-i\theta(\underline{r})/2}\Delta_0$; $\hat{d}(\underline{r}) = \cos\frac{\theta}{2}\hat{x} + \sin\frac{\theta}{2}\hat{y}$

since as $\theta: 0 \to 2\pi$, the (-1) of Δ_0 compensates the (-1) of $\hat{d}$.

This $\hat{d}$ gives pairing: $\Delta_0 e^{-i\frac{\theta}{2}}\left(\begin{array}{c|c} -e^{-i\theta/2} & 0 \\ \hline 0 & e^{i\theta/2} \end{array}\right) = \Delta_0 \begin{array}{c|c} -e^{-i\theta} & \\ \hline & 1 \end{array}$, so $\begin{cases} c_\uparrow^\dagger \Delta_0 e^{-i\theta}(\partial_x + i\partial_y) c_\uparrow^\dagger \leftarrow \text{vortex \& } \boxed{\text{MBS}} \text{ as above} \\ c_\downarrow^\dagger \Delta_0 (\partial_x + i\partial_y) c_\downarrow^\dagger \leftarrow \text{gapped SC} \end{cases}$

PART 5: EXPERIMENTAL SIGNATURES OF TSC

① Zero-bias conductance peak in STS/tunnel junction

(1a) MBS:

Isolated MBS should give LDOS at zero energy. It also modifies Andreev reflection, affecting point-contact spectra.

- Quantization

$$\left.\frac{dI}{dV}\right|_{V=0} = \begin{cases} 2\frac{e^2}{h} & (\text{MBS}) \\ 4\frac{e^2}{h} & (\text{Kramers MBS}) \end{cases}$$

If two MBS coupled, the peak diminishes.

Measurements: hard to find good plateau of quantization, e.g as function of magnetic field B. Trivial Andreev bound states give same signature.

- Spin-polarized STM, for spin texture of MBS (due to SOC): hard

(1b) Chiral or helical MM:

Peak much broader as function of bias voltage V.

(1c) Majorana surface mode (MSM)

Subtle due to non-trivial dependence of tunneling on incident angle. Can produce a peak or dip at zero bias. Sensitive to details of dispersion of MSM, e.g. anisotropy, flatness, sensitive to tunneling

② Quantized thermal Hall conductivity

In DIII, $d=3$, need to gap by proximitized s-wave the helical MSM $\rightarrow \kappa_{yx}/T = \pi^2 k_B/12h$

③ Thermal conductivity and spin current

MM don't carry charge. ⇒ heat (Cooper pairs do not carry, phonons suppressed $\sim T^3$).

In helical MM or MSM, heat current also is a spin current.

④ Anomalous Josephson effect

MM (edge) or MSM (surface) on interface makes it anomalous, periodic in 4π not 2π. Hard to find due to „quasiparticles poisoning".

⑤ Transport through wire

Thermal conductance is affected by MBS at wire ends, has a quantized peak at the transition, but same signature in chiral systems with zero modes.

Andreev bound states in wire due to inhomogeneity of magnetic field are also near zero energy and poison signal.

- Time-Reversal Transformation (TRT) or Symmetry (TRS)

TRT: $\begin{pmatrix}\mathcal{T}c_{\alpha\uparrow}\mathcal{T}^{1}\\ \mathcal{T}c_{\alpha\downarrow}\mathcal{T}^{-1}\end{pmatrix} = \begin{pmatrix}c_{\alpha\downarrow}\\ -c_{\alpha\uparrow}\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}c_{\alpha\uparrow}\\ c_{\alpha\downarrow}\end{pmatrix}$ and $\mathcal{T}$ anti-unitary.

so $\mathcal{T}(z\,c_{\alpha\sigma})\mathcal{T}^{-1} = z^*(i\sigma_2)_{\sigma\sigma'}\,c_{\alpha\sigma'}$, for any $z \in \mathbb{C}$, α = real space basis index

$\Rightarrow \mathcal{T}\Psi_{\underline{k}}\mathcal{T}^{-1} = \mathbb{1}_r \otimes (i\sigma_2)\Psi_{-\underline{k}}$ (due to $e^{i\underline{k}\cdot\underline{R}}$)

TRS: $\mathcal{T}\hat{H}\mathcal{T}^{-1} \equiv \hat{H} \Rightarrow \sum_{\underline{k}}\frac{1}{2}\left(\Psi^\dagger_{-\underline{k}}(i\sigma_2)^\dagger\right)H^*_{\underline{k}}\left(i\sigma_2\Psi_{-\underline{k}}\right) \equiv \hat{H} \Rightarrow \boxed{\sigma_2 H^*_{-\underline{k}}\sigma_2 \equiv H_{\underline{k}}}$

At BdG level, $\underline{T \equiv i\sigma_2 K}$, with K = complex conjugation in real-space basis,

$T^2 = (i\sigma_2 K)(i\sigma_2 K) = -\sigma_2^2 = -\mathbb{1}$, so $T^{-1} = -T$, and

$\underline{T H_{\underline{k}} T^{-1} = \sigma_2 H^*_{-\underline{k}}\sigma_2 \equiv H_{\underline{k}}}$ (spinful TRS, $T^2 = -\mathbb{1}$).

For pairing, $H^{ab}_{\underline{k}} \xrightarrow{TRT} \sigma_2 H^{ab*}_{-\underline{k}}\sigma_2 \Rightarrow \Delta_{\underline{k}ab} \xrightarrow{TRT} \sigma_2 \Delta^*_{-\underline{k}ab}\sigma_2$

$\Delta_{\underline{k}} \xrightarrow{TRT} \sigma_2\left[\left(\hat{\phi}^*_{-\underline{k}}\mathbb{1}_2 + \hat{\vec{d}}^*_{-\underline{k}}\cdot\vec{\sigma}^*\right)(i\sigma_2)^*\right]\sigma_2$, so

$\begin{cases}\hat{\phi}_{\underline{k}} \xrightarrow{TRT} \hat{\phi}^*_{-\underline{k}}\\ \hat{\vec{d}}_{\underline{k}} \xrightarrow{TRT} -\hat{\vec{d}}^*_{-\underline{k}}\end{cases}$, so TRS $\Rightarrow \begin{cases}\hat{\phi}_{\underline{k}} = \hat{\phi}^*_{-\underline{k}}\\ \hat{\vec{d}}_{\underline{k}} = -\hat{\vec{d}}^*_{-\underline{k}}\end{cases}$ | for $r \equiv 1$ $\begin{cases}\phi_{\underline{k}} = \phi^*_{-\underline{k}}\\ \vec{d}_{\underline{k}} = -\vec{d}^*_{-\underline{k}}\end{cases}$,

with fermionic constraint, $\underline{\text{TRS}} \Rightarrow \underline{\begin{cases}\hat{\phi}_{\underline{k}} = \hat{\phi}^\dagger_{\underline{k}}\\ \hat{\vec{d}}_{\underline{k}} = \hat{\vec{d}}^\dagger_{\underline{k}}\end{cases}}$ | for $r \equiv 1$ $\underline{\begin{cases}\phi_{\underline{k}} \in \mathbb{R}\\ \vec{d}_{\underline{k}} \in \mathbb{R}\end{cases}}$