1.5. Topological superconductors in 1D: The Majorana chain

1.5.1. Preliminaries: Particle-hole symmetry and mean-field superconductors

* **Particle-hole symmetry (PHS) $\mathcal{C}_U$:**

$$\mathcal{C}_U\, i\, \mathcal{C}^{-1} = +i \quad \text{and} \quad \mathcal{C}_U c_i \mathcal{C}_U^{-1} = \sum_j U_{ij}^{*\dagger} c_j^\dagger$$

$$[\hat{H}, \mathcal{C}_U] = 0 \iff U H^* U^\dagger \overset{!}{=} -H \iff \{H, \overbrace{UK}^{C_U}\} = 0$$

→ Unitary symmetry on MB Hamiltonian, antiunitary pseudosymmetry on SP Hamiltonian

* **BCS-theory of superconductivity**

1. BCS Hamiltonian:

pairing potential

$$\hat{H}_{BCS} = \sum_{\vec{k}\sigma} (\varepsilon_{\vec{k}} - \mu)\, c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + \sum_{\vec{k},\vec{k}'} V_{\vec{k}\vec{k}'}\, c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow}$$

2. Mean-field theory:

$$c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow} = \underbrace{\overset{\langle c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow}\rangle}{X_{k'}}}_{\text{Mean}} + \underbrace{\left(c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow} - X_{k'} \right)}_{\text{Small fluctuations } \delta X_{\vec{k}'}}$$

Cooper pair condensation: $X_{\vec{k}'} \neq 0$ and $\delta X_{\vec{k}'}$ small

$\rightarrow$ Drop terms of order $\mathcal{O}(\delta X_{\vec{k}'}^2)$:

$$\hat{H}_{BCS}^{mf} = \sum_{\vec{k},\sigma} (\varepsilon_{\vec{k}} - \mu)\, c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} + \sum_{\vec{k}} \Big(\Delta_{\vec{k}} \underbrace{c_{\vec{k}\uparrow}^{\dagger} c_{-\vec{k}\downarrow}^{\dagger}}_{\text{Quadratic pairing terms}} + \Delta_{\vec{k}}^{*} c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \Big)$$

With order parameter

$$\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} X_{\vec{k}'} \in \mathbb{C}$$

s-wave superconductor:

$c_{-k\downarrow} c_{k\uparrow}$

1.5.2. The Majorana chain

1. A 1D superconductor of spinless fermions c_i (p-wave superconductor)

$$\boxed{\hat{H}_{MC} = -\sum_{i=1}^{L'}\left(\underbrace{w}_{\in\mathbb{R}\text{ tunneling amplitude}}\, c_i^\dagger c_{i+1} - \Delta\, c_i c_{i+1} + h.c.\right) - \sum_{i=1}^{L}\underbrace{\mu}_{\in\mathbb{R}\text{ chemical potential}}\left(c_i^\dagger c_i - \frac{1}{2}\right)}$$

$\Delta = e^{i\theta}|\Delta| \in \mathbb{C}$ superconducting gap parameter (θ phase of the condensate)

$L' = L$ (PBC)

$L' = L-1$ (OBC)

Gauge transformation: $\quad c_i = e^{-i\frac{\theta}{2}} c_i' \quad \Rightarrow \quad \Delta = |\Delta|$ real

Note:

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2. & PBC → Fourier transform:

$$\hat{H}_{MC} = -\sum_{k \in BZ}' \Big[\underbrace{(2w \cos(k)}_{-\varepsilon_k} + \mu) \tilde{c}_k^\dagger \tilde{c}_k + \underbrace{i\Delta \sin(k)}_{\Delta_k} \tilde{c}_k \tilde{c}_{-k} - i\Delta \sin(k) \tilde{c}_{-k}^\dagger \tilde{c}_k^\dagger \Big]$$

3. Bogoliubov - de Gennes Hamiltonian:

$$(2w \cos k + \mu) \tilde{c}_k^\dagger \tilde{c}_k \to \frac{1}{2}\Big[(2w \cos k + \mu) \tilde{c}_k^\dagger \tilde{c}_k + (2w \cos k + \mu) \tilde{c}_{-k}^\dagger \tilde{c}_{-k} \Big]$$

$$\rightarrow \quad \hat{H}_{MC} = -\frac{1}{2} \sum_{k \in BZ}' \Big[(2w \cos k + \mu)\, \tilde{c}_k^\dagger \tilde{c}_k + (2w \cos k + \mu)\, \tilde{c}_{-k}^\dagger \tilde{c}_{-k}$$
$$+ i 2\Delta \sin(k)\, \tilde{c}_k \hat{c}_{-k} - 2i\Delta \sin(k)\, \tilde{c}_{-k} \hat{c}_k^\dagger \Big]$$

$\rightarrow$ *Nambu spinors:*

$$\vec{\psi}_k = \begin{pmatrix} \tilde{c}_k \\ \tilde{c}_{-k}^\dagger \end{pmatrix}$$

$\rightarrow$

$$\hat{H}_{MC} = \frac{1}{2} \sum_{k \in BZ} \underbrace{\begin{pmatrix} \tilde{c}_k^\dagger & \tilde{c}_{-k} \end{pmatrix}}_{\vec{\psi}_k^\dagger} \underbrace{\begin{pmatrix} -2w \cos k - \mu & -2\Delta i \sin k \\ 2\Delta i \sin k & 2w \cos k + \mu \end{pmatrix}}_{H_{BdG}(k)} \underbrace{\begin{pmatrix} \hat{c}_k \\ \tilde{c}_{-k}^\dagger \end{pmatrix}}_{\vec{\psi}_k}$$

with BdG Hamiltonian

$$H_{BdG}(k) = \vec{d}(k) \cdot \vec{\sigma} \qquad \vec{d}(k) = \begin{pmatrix} 0 \\ 2\Delta \sin(k) \\ -2w \cos(k) - \mu \end{pmatrix}$$

4. Bogoliubov transformation:

$$U_k H_{BdG}(k) U_k^\dagger = \begin{pmatrix} E(k) & 0 \\ 0 & -E(k) \end{pmatrix}$$

U_k: unitary rotation in Nambu space

$$\rightarrow \quad \tilde{\Psi}_k = \begin{pmatrix} \tilde{c}_k \\ \tilde{c}^\dagger_{-k} \end{pmatrix} := U_k \Psi_k = \begin{pmatrix} u_k \tilde{c}_k + v_k \tilde{c}^\dagger_{-k} \\ v^*_{-k} \tilde{c}_k + u^*_{-k} \tilde{c}^\dagger_{-k} \end{pmatrix}$$

$|u_k|^2 + |v_k|^2 = 1$, $\quad v_{-k} = v_k$, $\quad u_{-k} = -u_k$

5. Spectrum:

$$E(k) = |\vec{d}(k)| = \sqrt{(2w\cos(k) + \mu)^2 + 4\Delta^2 \sin^2(k)}$$

Note:

$$\hat{H}_{MC} = \frac{1}{2}\sum_k \left(\tilde{a}_k^\dagger \; \tilde{a}_{-k}\right) \begin{pmatrix} E(k) & 0 \\ 0 & -E(k) \end{pmatrix} \begin{pmatrix} \tilde{a}_k \\ \tilde{a}_{-k}^\dagger \end{pmatrix}$$

$$= \frac{1}{2}\sum_k \left[E(k)\,\tilde{a}_k^\dagger \tilde{a}_k - E(k)\,\underbrace{\tilde{a}_{-k}\tilde{a}_{-k}^\dagger}_{-\tilde{a}_{-k}^\dagger \tilde{a}_{-k} + 1} \right]$$

$$= \sum_k E(k)\,\tilde{a}_k^\dagger \tilde{a}_k + \text{const.}$$

$$E(k) = |\vec{d}(k)| = \sqrt{(2w\cos(k)+\mu)^2 + 4\Delta^2\sin^2(k)}$$

6. Phase diagram: Let $\Delta \neq 0$ $\rightarrow$ $E(k) = 0$ only possible at $k = 0, \pi$

$\rightarrow$ $E(0/\pi) = |\pm 2w + \mu| \overset{!}{=} 0$ $\Rightarrow$ $2|w| = |\mu|$

$\rightarrow$ Two phases:

$$\boxed{\text{Phase A: } 2|w| > |\mu| \quad \text{and} \quad \text{Phase B: } 2|w| < |\mu|}$$

7. Ground state $|\Omega\rangle$ with

$$\tilde{a}_k |\Omega\rangle \overset{!}{=} 0 \qquad \forall_{k \in BZ}$$

→ Unique BCS ground state:

$$|\Omega\rangle \propto \prod_{k:\, \tilde{a}_k|0\rangle \neq 0} \tilde{a}_k |0\rangle$$

$\omega = \Delta$
$\mu = 0$

$$\propto \prod_{k \in (-\pi, \pi)} \tilde{a}_k |0\rangle = \tilde{a}_0 \prod_{k \in (0, \pi]} \left(u_k + v_k \tilde{c}_k^\dagger \tilde{c}_{-k}^\dagger \right) |0\rangle$$

1.5.3. Symmetries and topological indices

1. Time-reversal symmetry

a) W.l.o.g. Δ real $\rightarrow$ $\mathcal{T} = \mathcal{K}$ TRS: $[\hat{H}_{MC}, \mathcal{T}] = 0$

$\xrightarrow{6}$

$$\mathbb{1} \cdot H^*_{BdG}(k) \cdot \mathbb{1} = H_{BdG}(-k)$$

$\rightarrow$ $\tilde{T} = \mathbb{1} K$: TRS with $\tilde{T}^2 = +\mathbb{1}$

$\rightarrow$ $\boxed{\text{Symmetry class AI}}$

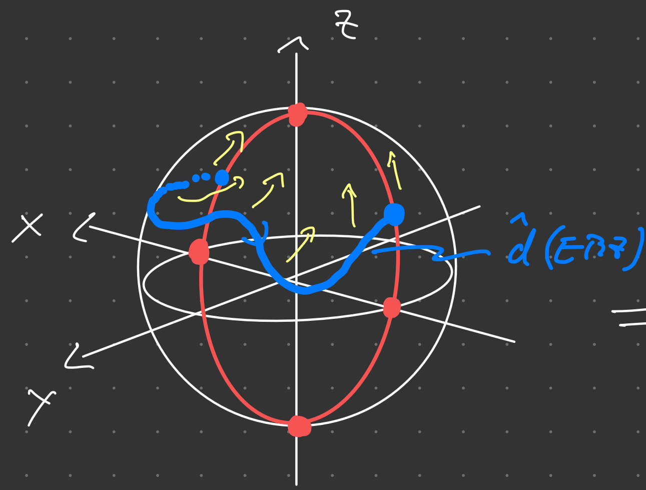
b) Constraints:

$$\boxed{\begin{aligned} d_x(-k) &= d_x(k) \\ d_y(-k) &= -d_y(k) \\ d_z(-k) &= d_z(k) \end{aligned}}$$

$\rightarrow$ $\vec{d}(k)$ on EBZ $[0, \pi]$ determines $H_{BdG}(k)$ completely

c) $\forall$ $k \in \{0, \pi\}$ TRIM $\rightarrow$ $d_y(k) = 0$

$\rightarrow$ Image $\hat{d}(EBZ)$ $(\hat{d} = \vec{d}/|\vec{d}|)$ on S^2 must start & end on great circle:



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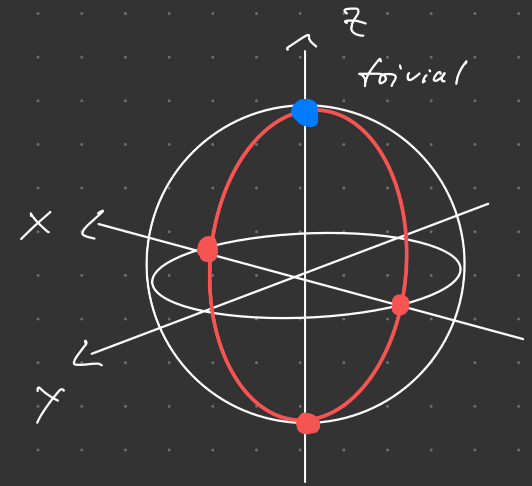


$\rightarrow$ All paths (= gapped & symmetric Hamiltonians) can be continuously contracted

$\rightarrow$ No topological phases

d) $\boxed{\text{In 1D, systems of class AI do not allow for TPs.}}$

e) Conclusion for MC: TRS alone cannot make the MC topological.

2. Particle-Hole "Symmetry":

a)

$$\sigma^x H^*_{BdG}(k)\,\sigma^x = -H_{BdG}(-k)$$

$\rightarrow$ $\tilde{C} = \sigma^x K$: PHS with $\tilde{C}^2 = +\mathbb{1}$

$\rightarrow$ $\boxed{\text{Symmetry class D}}$

Real space:

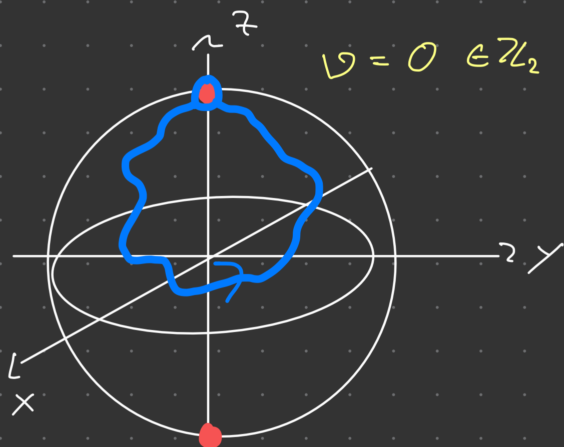
$U H^*_{BdG} U^\dagger = -H$

b) Constraints:

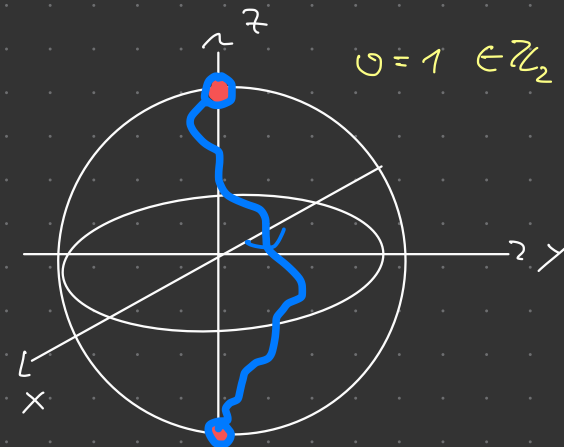
$$\boxed{\begin{aligned} d_x(-k) &= -d_x(k) \\ d_y(-k) &= -d_y(k) \\ d_z(-k) &= d_z(k) \end{aligned}}$$

c) $\nexists$ a TRIM $\rightarrow$ $d_x(k) = d_y(k) \overset{!}{=} 0$

$\rightarrow$ Image $\hat{d}$ (EBZ) on S^2 must start & end on north or south pole:



$\neq$



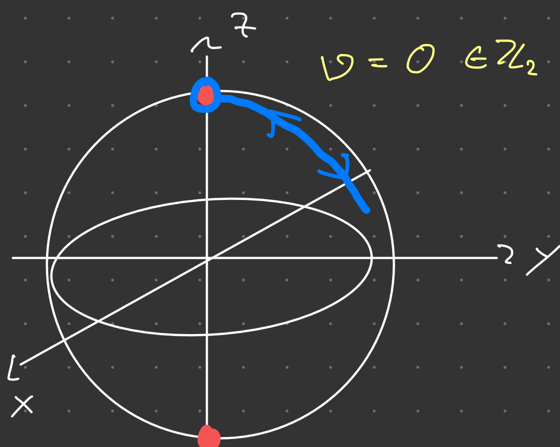
$\rightarrow$ Two topological distinct classes of paths

$\rightarrow$ One topological phase possible $\rightarrow$ $\mathbb{Z}_2$ - index

d) $\boxed{\text{In 1D, systems of class D allow for a single TP labeled by a } \mathbb{Z}_2\text{-index.}}$

e) Conclusion for MC:

$$\vec{d}(k) = \begin{pmatrix} 0 \\ 2\Delta \sin(k) \\ -2\omega \cos(k) - \mu \end{pmatrix}$$



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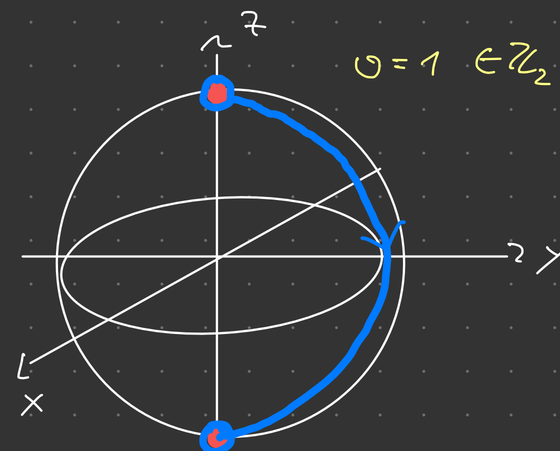


trivial phase

Phase B $\quad 2|\omega| < |\mu|$

topological phase

Phase A: $\quad 2|\omega| > |\mu|$

3. PHS & TRS:

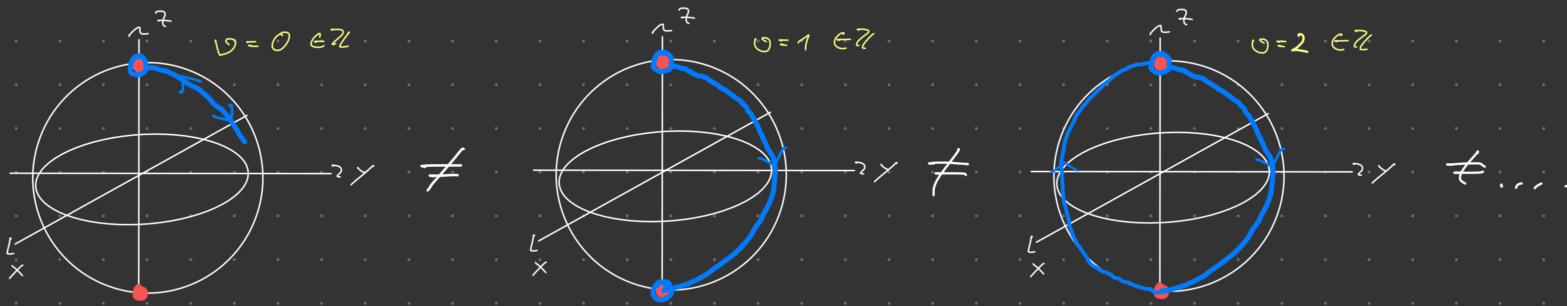
a) TRS with $\tilde{T}^2 = +\mathbb{1}$ and PHS with $\tilde{C}^2 = +\mathbb{1}$

$\rightarrow$ $\boxed{\text{Symmetry class BDI}}$

b) Constraints:

$$\boxed{\begin{aligned} d_x(-k) &= 0 \\ d_y(-k) &= -d_y(k) \\ d_z(-k) &= d_z(k) \end{aligned}}$$

c) Image $\hat{d}\,(\in \mathbb{R}^3)$ on S^2 is constrained to the great circle with $d_x = 0$ and must start & end either on north or south pole:



→ Infinitely many topologically distinct classes of paths

→ —"— topological phases → $\mathbb{Z}$ - index

d) $\boxed{\text{In 1D, systems of class BDI allow for many TPs labeled by a } \mathbb{Z}\text{ - index}}$

e) Conclusions for MC: Only important for multiple MC!

f) PHS: $U_C H^* U_C^\dagger = -H$

TRS: $U_T H^* U_T^\dagger = +H$

$\rightarrow U_S := U_T \cdot U_C^*$

$\rightarrow \quad U_S H U_S^\dagger = -H \quad \rightarrow$ Sublattice symmetry (SLS)

1.5.4 Majorana fermions

1. $\exists$ Set of fermion operator $\{c_i\}$ and define Majorana operators

$$\boxed{\gamma_{2i-1} = c_i + c_i^\dagger \quad \text{and} \quad \gamma_{2i} = i(c_i^\dagger - c_i)}$$

2. $\rightarrow$ Properties:

$$\boxed{\gamma_n^\dagger = \gamma_n \quad \text{and} \quad \{\gamma_n, \gamma_m\} = 2\delta_{nm}}$$

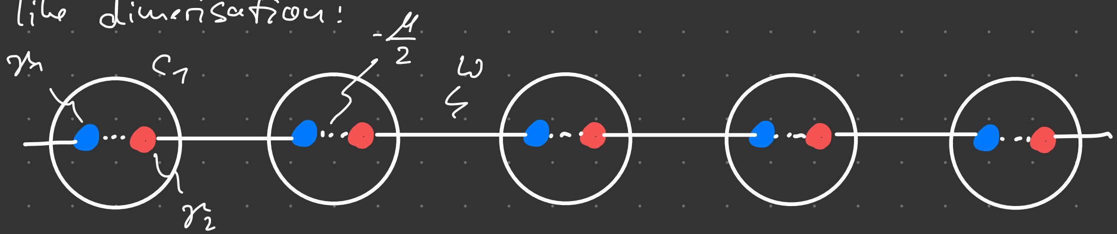
3.
$$\boxed{c_i = \frac{\gamma_{2i-1} + i\gamma_{2i}}{2} \quad , \quad c_i^{\dagger} = \frac{\gamma_{2i-1} - i\gamma_{2i}}{2}}$$

4.
$$\hat{H}_{MC} \hat{=} \frac{i}{2} \sum_{i=1}^{L'} (\Delta + \omega)\, \gamma_{2i}\gamma_{2i+1} + (\Delta - \omega)\, \gamma_{2i-1}\gamma_{2i+2}$$
$$- \frac{i}{2} \sum_{i=1}^{L} \mu\, \gamma_{2i-1}\gamma_{2i}$$

5. Let $\Delta = \omega \longrightarrow$

$$\boxed{\hat{H}_{MC} \hat{=} -\frac{i}{2} \sum_{i=1}^{L} \mu\, \gamma_{2i-1}\gamma_{2i} + i \sum_{i=1}^{L'} \omega\, \gamma_{2i}\gamma_{2i+1}}$$

$\rightarrow$ SSH-like dimerisation:



6. Comparison to SSH chain:

$$\frac{|\mu|}{2} = |\omega| \left\{ \begin{array}{c|c} \text{Majorana} & \text{SSH} \\ \hline -\frac{\mu}{2} & t \\ \omega & \omega \end{array} \right\} |t| = |\omega|$$

1.5.5 Edge modes

1. Trivial phase (Phase B): $\omega = \Delta = 0$ and $\mu > 0 \longrightarrow$

$$\hat{H}_{MC} = -\frac{\mu}{2} \sum_{i=1}^{L} i(\gamma_{2i-1} \gamma_{2i}) = -\mu \sum_{i=1}^{L} \left(c_i^\dagger c_i - \frac{1}{2} \right)$$

$\rightarrow$ Unique ground state

2. <u>Topological phase (Phase A)</u>: Let $\omega = \Delta > 0$ and $\mu = 0$ $\rightarrow$

$$\hat{H}_{MC} = \omega \sum_{i=1}^{L' = L-1} i(\gamma_{2i}\gamma_{2i+1})$$

$\rightarrow$ Unique ground state for PBC <u>but</u> 2-fold degenerate ground space for OBC

a) New fermion modes $(i = 1, \dots, L-1)$

$$a_i := \frac{1}{2}(\gamma_{2i} + i\gamma_{2i+1}) \quad \text{and} \quad a_i^\dagger = \frac{1}{2}(\gamma_{2i} - i\gamma_{2i+1})$$

$\overset{\text{ö}}{\rightarrow}$

$$\hat{H}_{MC} = 2\omega \sum_{i=1}^{L-1} \left(a_i^\dagger a_i - \frac{1}{2} \right)$$

b) One fermion mode missing:

$$e = \frac{1}{2}(\gamma_{2L} + i\gamma_1) \quad \text{and} \quad e^\dagger = \frac{1}{2}(\gamma_{2L} - i\gamma_1)$$

$\rightarrow$ One fermionic edge mode

$\rightarrow \quad e \overset{\circledcirc}{=} \frac{i}{2}\left(c_L^{+} - c_L + c_1^{+} + c_1\right)$ $\rightarrow$ delocalized edge mode

c) Ground states for OBC:

$$|\Omega_u\rangle \text{ GS of } \hat{H}_M \Leftrightarrow a_i |\Omega_u\rangle \overset{!}{=} 0 \quad \forall i = 1, \dots, L-1$$

$[\hat{H}_{MC}, e] = 0 \rightarrow$ Two ground states:

$$e^{+}e\,|\Omega_0\rangle = 0\,|\Omega_0\rangle, \qquad e^{+}e\,|\Omega_1\rangle = 1\,|\Omega_1\rangle$$

with $\quad |\Omega_1\rangle = e^{+}|\Omega_0\rangle$

Note:

* $\hat{H}_{MC} + e^{\dagger} e \longrightarrow$ not local !

$\gamma_1 e = -e^{\dagger} \gamma_1$

* Check $|\Omega_1\rangle = \gamma_1 |\Omega_0\rangle \longrightarrow \langle \Omega_1 | \gamma_1 | \Omega_0 \rangle \neq 0$

local ! $\quad \gamma_1^{\dagger} = \gamma_1$

$\longrightarrow \hat{H}_{MC} + \gamma_1$

$[P, \gamma_1] \neq 0$

$$P = (-1)^{\hat{N}}$$

$\gamma_1 \rightarrow \sigma^x$

$\gamma_{2L} \rightarrow \sigma^z$