

§1. Many-particle quantum mechanics

* Second quantization: fermions

- Algebra

$$\hat{f}, \hat{f}^+ \quad \{\hat{f}, \hat{f}^+\} = 1$$

$$\hat{f}^2 = (\hat{f}^+)^2 = 0$$

anticommutator:

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

Hilbert space: $|0\rangle$ ($\hat{f}|0\rangle = 0$)

 $|1\rangle = \hat{f}^+|0\rangle$

$|n\rangle, n=0,1$

$$\begin{cases} \langle n | n' \rangle = \delta_{nn'} \\ \sum_{n=0,1} |n\rangle \langle n| = \hat{1} \end{cases}$$

orthonormal & complete basis

particle-number operator: $\hat{n} = \hat{f}^+ \hat{f}$

$$\hat{n} |n\rangle = n |n\rangle$$

fermion-parity operator: $\hat{P} = (-1)^{\hat{n}}$

$$\hat{P} |n\rangle = (-1)^n |n\rangle$$

- Many fermions

$$\hat{f}_j, \hat{f}_j^+ \quad j=1, 2, \dots, N$$

$$\left\{ \begin{array}{l} \{\hat{f}_j, \hat{f}_l\} = \{\hat{f}_j^+, \hat{f}_l^+\} = 0 \\ \{\hat{f}_j, \hat{f}_l^+\} = \delta_{jl} \end{array} \right.$$

$n_j = 0, 1 \quad \forall j$

$$|n_1, n_2, \dots, n_N\rangle = (\hat{f}_1^+)^{n_1} (\hat{f}_2^+)^{n_2} \dots (\hat{f}_N^+)^{n_N} |0\rangle$$

orthonormal & complete basis!

annihilated by all \hat{f}_j ,

particle-number operator: $\hat{n} = \sum_{j=1}^N \hat{n}_j$

$$\hat{f}_j^\dagger |0\rangle = 0 \quad \forall j$$

fermion-parity operator: $\hat{P} = (-1)^\hat{n} = (-1) \sum_{j=1}^N \hat{n}_j$

- Quadratic Hamiltonians of fermions → "pairing"

$$\hat{H} = \sum_{j,l=1}^N t_{jl} \hat{f}_j^+ \hat{f}_l + \sum_{j,l=1}^N (\Delta_{jl} \hat{f}_j \hat{f}_l + \Delta_{jl}^* \hat{f}_l^+ \hat{f}_j^+)$$

(known as Bogoliubov-de Gennes Hamiltonian, relevant for superconductors)
Eigenstates & energies?

Case 1: no pairing ($\Delta_{jl} = 0 \quad \forall j, l$)

$$\hat{H} = \sum_{j,l=1}^N t_{jl} \hat{f}_j^+ \hat{f}_l \quad t_{jl} = t_{lj}^*$$

$[\hat{H}, \hat{n}] = 0$ particle number conserved $\Rightarrow U(1)$ symmetry

Unitary transformation on fermionic modes:

(identical to bosonic case)

$$\hat{d}_p = \sum_{j=1}^N U_{pj} \hat{c}_j$$

$$\hat{d} = U \hat{c}$$

$$\hat{d}_p^+ = \sum_{j=1}^N \hat{c}_j^+ (U^+)_j p$$

$$\hat{d}^+ = \hat{c}^+ U^+$$

$\nwarrow N \times N$ unitary matrix

$$\Rightarrow \begin{cases} \{\hat{d}_p, \hat{d}_q\} = \{\hat{d}_p^+, \hat{d}_q^+\} = 0 \\ \{\hat{d}_p, \hat{d}_q^+\} = \delta_{pq} \end{cases} \quad p, q = 1, \dots, N$$

Unitary transformation preserves fermionic commutation relations.

$$\hat{H} = \sum_{j,l=1}^N t_{jl} \hat{f}_j^+ \hat{f}_l$$

$$\begin{aligned} &= \hat{f}^+ T \hat{f} \\ &= \underbrace{\hat{f}^+}_{\hat{d}^+} \underbrace{U^+}_{\hat{d}} \underbrace{U T U^+}_{\hat{f}} \underbrace{U f}_{\hat{d}} \end{aligned}$$

choose U such that

$$U T U^+ = \begin{pmatrix} \varepsilon_1 & & & \\ & \varepsilon_2 & & \\ & & \ddots & \\ & & & \varepsilon_N \end{pmatrix}$$

$$\Rightarrow \hat{H} = \hat{d}^+ \begin{pmatrix} \varepsilon_1 & & & \\ & \varepsilon_2 & & \\ & & \ddots & \\ & & & \varepsilon_N \end{pmatrix} \hat{d} = \sum_{p=1}^N \varepsilon_p \hat{d}_p^+ \hat{d}_p$$

$$\hat{n}_p = \hat{d}_p^+ \hat{d}_p, \quad [\hat{n}_p, \hat{n}_q] = 0$$

Eigenstates: Fermi sea

$$|n_1, n_2, \dots, n_N\rangle_d = (\hat{d}_1^+)^{n_1} (\hat{d}_2^+)^{n_2} \cdots (\hat{d}_N^+)^{n_N} |0\rangle_d$$

$$\hat{H} |n_1, \dots, n_N\rangle_d = \left(\sum_{p=1}^N \varepsilon_p n_p \right) |n_1, \dots, n_N\rangle_d$$

\downarrow identical to $|0\rangle_f$

Case 2: Presence of pairing

$$[\hat{H}, \hat{P}] = 0$$

Solution: Bogoliubov transformation

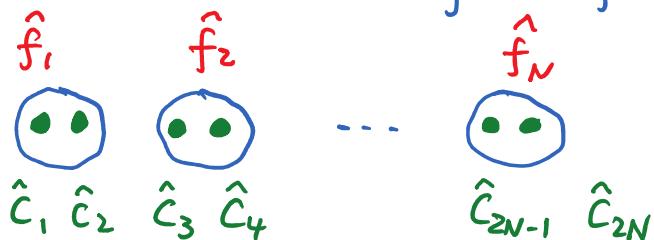
fermion parity conserved
 \downarrow
 \mathbb{Z}_2 symmetry

Below we use an alternative approach with Majorana fermions.

— Majorana fermions

$$\hat{f}_j, \hat{f}_j^+ \Rightarrow \begin{cases} \hat{c}_{2j-1} = \hat{f}_j + \hat{f}_j^+ \\ \hat{c}_{2j} = -i(\hat{f}_j - \hat{f}_j^+) \end{cases}$$

N fermions $\Rightarrow 2N$ Majorana fermions



$$\begin{aligned} \hat{c}_{2j-1}^+ &= \hat{c}_{2j-1} \\ \hat{c}_{2j}^+ &= \hat{c}_{2j} \end{aligned}$$

"real" fermions

(\hat{f}_j, \hat{f}_j^+ : "complex" fermions)

$$\text{Algebra: } \hat{c}_{2j-1}^2 = (\hat{f}_j + \hat{f}_j^+)(\hat{f}_j + \hat{f}_j^+)$$

$$= \hat{f}_j \hat{f}_j^+ + \hat{f}_j^+ \hat{f}_j = \{\hat{f}_j, \hat{f}_j^+\} = 1$$

$$\hat{c}_{2j}^2 = -(\hat{f}_j - \hat{f}_j^+)(\hat{f}_j - \hat{f}_j^+) = 1$$

$$\{\hat{c}_{2j-1}, \hat{c}_{2j}\} = -i\{\hat{f}_j + \hat{f}_j^+, \hat{f}_j - \hat{f}_j^+\} = -i(-1 + 1) = 0$$

Generally, $\{c_j, c_l\} = 2\delta_{jl} \rightarrow$ Clifford algebra

which transformations preserve commutation relations of Majoranas?

$$\hat{C}_P = \sum_{j=1}^{2N} O_{Pj} \hat{C}_j$$

$$\hat{C} = O \hat{C}$$

$\downarrow 2N \times 2N \text{ matrix}$

$$\begin{pmatrix} \hat{C}_1 \\ \hat{C}_2 \\ \vdots \\ \hat{C}_{2N} \end{pmatrix} = O \begin{pmatrix} \hat{C}_1 \\ \hat{C}_2 \\ \vdots \\ \hat{C}_{2N} \end{pmatrix}$$

Orthogonal transformations ! $O^T O = O O^T = I$

$$\begin{aligned} \{\hat{C}_P, \hat{C}_Q\} &= \left\{ \sum_{j=1}^{2N} O_{Pj} \hat{C}_j, \sum_{l=1}^{2N} O_{Ql} \hat{C}_l \right\} \\ &= \sum_{j,l=1}^{2N} O_{Pj} O_{Ql} \underbrace{\{\hat{C}_j, \hat{C}_l\}}_{= 2\delta_{jl}} \\ &= 2 \sum_{j=1}^{2N} O_{Pj} O_{Qj} \\ &= 2 \underbrace{(O O^T)}_{= I}_{pq} \\ &= 2 \delta_{pq} \end{aligned}$$

Remark: Unitary transformations of "complex" fermions

form a subset of orthogonal transformations of Majorana fermions.

Mathematically, $U(N) \in O(2N)$

Quadratic Hamiltonians of complex fermions



Quadratic Hamiltonians of Majorana fermions

$$\left\{ \begin{array}{l} \hat{f}_j = \frac{1}{2} (\hat{c}_{2j-1} + i\hat{c}_{2j}) \\ \hat{f}_j^+ = \frac{1}{2} (\hat{c}_{2j-1} - i\hat{c}_{2j}) \end{array} \right.$$

examples: $\hat{f}_j^+ \hat{f}_\ell + \hat{f}_\ell^+ \hat{f}_j = \frac{1}{4} (\underbrace{\hat{c}_{2j-1} - i\hat{c}_{2j}}_{(j \neq \ell)})(\underbrace{\hat{c}_{2\ell-1} + i\hat{c}_{2\ell}}_{(j \neq \ell)}) + \frac{1}{4} (\underbrace{\hat{c}_{2\ell-1} - i\hat{c}_{2\ell}}_{(j \neq \ell)})(\underbrace{\hat{c}_{2j-1} + i\hat{c}_{2j}}_{(j \neq \ell)}) = \frac{i}{2} (\hat{c}_{2j-1} \hat{c}_{2\ell} - \hat{c}_{2j} \hat{c}_{2\ell-1})$

$$\begin{aligned} \hat{f}_j^+ \hat{f}_\ell + \hat{f}_\ell^+ \hat{f}_j &= \frac{1}{4} (\underbrace{\hat{c}_{2j-1} + i\hat{c}_{2j}}_{(j \neq \ell)})(\underbrace{\hat{c}_{2\ell-1} + i\hat{c}_{2\ell}}_{(j \neq \ell)}) \\ &\quad + \frac{1}{4} (\underbrace{\hat{c}_{2\ell-1} - i\hat{c}_{2\ell}}_{(j \neq \ell)})(\underbrace{\hat{c}_{2j-1} - i\hat{c}_{2j}}_{(j \neq \ell)}) \\ &= \frac{i}{2} (\hat{c}_{2j-1} \hat{c}_{2\ell} + \hat{c}_{2j} \hat{c}_{2\ell-1}) \end{aligned}$$

$$\begin{aligned} \hat{f}_j^+ \hat{f}_j &= \frac{1}{4} (\hat{c}_{2j-1} - i\hat{c}_{2j})(\hat{c}_{2j-1} + i\hat{c}_{2j}) \\ &= \frac{1}{2} (1 + i\hat{c}_{2j-1} \hat{c}_{2j}) \end{aligned}$$

General quadratic Hamiltonian of fermions:

$$\begin{aligned} \hat{H} &= \frac{i}{4} \sum_{j,\ell=1}^{2N} A_{j\ell} \hat{c}_j \hat{c}_\ell \\ &= \frac{i}{4} \hat{c}^\top A \hat{c} \end{aligned}$$

real antisymmetric matrix

Diagonalization:

$$\hat{H} = \frac{i}{4} \hat{C}^T A \hat{C} = \frac{i}{4} \underbrace{\hat{C}^T}_{\parallel \hat{C}^T} O^T D A D^T O \underbrace{\hat{C}}_{\parallel \hat{C}} \rightarrow \text{Majorana modes}$$

choose orthogonal matrix O such that

$$DAD^T = \begin{pmatrix} 0 & \varepsilon_1 & & \\ -\varepsilon_1 & 0 & & \\ & & 0 & \varepsilon_2 \\ & & -\varepsilon_2 & 0 \\ & & & \ddots \\ & & & 0 & \varepsilon_N \\ & & & -\varepsilon_N & 0 \end{pmatrix}_{2N \times 2N}$$

$\varepsilon_i \geq 0 \quad \forall i$

(always possible when A is real antisymmetric matrix)

$$\begin{aligned}
 \hat{H} &= \frac{i}{4} \sum_{p=1}^N (\hat{\tilde{C}}_{2p-1} \quad \hat{\tilde{C}}_{2p}) \begin{pmatrix} 0 & \epsilon_p \\ -\epsilon_p & 0 \end{pmatrix} \begin{pmatrix} \hat{\tilde{C}}_{2p-1} \\ \hat{\tilde{C}}_{2p} \end{pmatrix} \\
 &= \frac{i}{2} \sum_{p=1}^N \epsilon_p \underbrace{\hat{\tilde{C}}_{2p-1} \quad \hat{\tilde{C}}_{2p}}_{\text{new complex fermionic modes.}} \\
 &= \sum_{p=1}^N \epsilon_p (\hat{d}_p^\dagger \hat{d}_p - \frac{1}{2})
 \end{aligned}$$

Eigenstates :

$$|\vec{n}_1, \vec{n}_2, \dots, \vec{n}_N\rangle_d = (\hat{d}_1^+)^{n_1} (\hat{d}_2^+)^{n_2} \cdots (\hat{d}_N^+)^{n_N} |\vec{0}\rangle_d$$

not necessarily identical to $|\vec{0}\rangle_f$!

Think about how this "d"-fermion basis is related to the original "f"-fermion basis!

Example : Kitaev's Majorana chain

Ref.: A. Kitaev, cond-mat/0010440

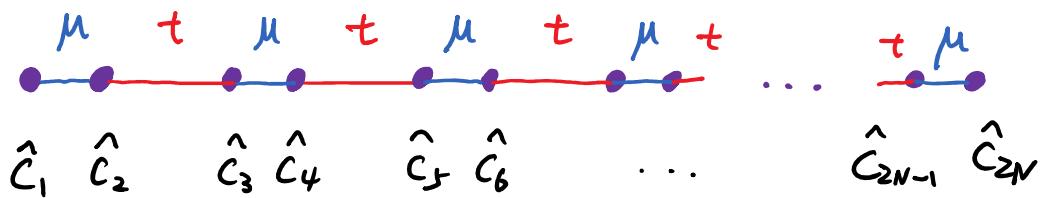
$$\hat{H} = \sum_{j=1}^{N-1} \left[-t (\hat{f}_j^\dagger \hat{f}_{j+1} + \hat{f}_{j+1}^\dagger \hat{f}_j) + t (\hat{f}_j^\dagger \hat{f}_{j+1}^\dagger + \hat{f}_{j+1}^\dagger \hat{f}_j^\dagger) \right] - \mu \sum_{j=1}^N (2\hat{f}_j^\dagger \hat{f}_j - 1)$$

without loss of generality,
consider $t \geq 0, \mu \geq 0$.

Open boundary condition (OBC)

Use Majorana representation (see Page ⑥)

$$\hat{H} = \sum_{j=1}^{N-1} it \hat{c}_{2j}^\dagger \hat{c}_{2j+1} - \sum_{j=1}^N i\mu \hat{c}_{2j-1}^\dagger \hat{c}_{2j}$$



Competition between "t"-term and "μ" term!

Special cases :

1) $\mu = 0$: $\hat{H} = \sum_{j=1}^{N-1} it \hat{c}_{2j}^\dagger \hat{c}_{2j+1}$

\hat{c}_1 and \hat{c}_{2N} decoupled from \hat{H}

Majorana zero-energy modes !

New fermionic modes:

$$\hat{d}_1 = \frac{1}{2}(\hat{c}_2 + i\hat{c}_3)$$

$$\hat{d}_2 = \frac{1}{2}(\hat{c}_4 + i\hat{c}_5)$$

⋮

$$\hat{d}_{N-1} = \frac{1}{2}(\hat{c}_{2N-2} + i\hat{c}_{2N-1})$$

$\hat{d} = \frac{1}{2}(\hat{c}_1 + i\hat{c}_{2N}) \Rightarrow$ highly nonlocal fermion
formed by Majorana edge modes

$$\Rightarrow \hat{H} = \sum_{p=1}^{N-1} 2t (\hat{d}_p^\dagger \hat{d}_p - \frac{1}{2})$$

Ground states: $|G_{S_1}\rangle = |\alpha\rangle_d$
 $|G_{S_2}\rangle = d^+ |\alpha\rangle_d \Rightarrow$ topological degeneracy

Excited states are separated by a gap $\Delta = 2t$.

Majorana zero-energy modes:

Potentially useful for quantum information processing
(memory, computing ...)

Advantage: information encoded in a highly nonlocal fashion
and protected topologically (supposed to be
robust against noise)

Questions: Where can we find Majorana zero modes?

How can we detect and manipulate them?

active research direction ...

$$2) \quad t=0: \quad \hat{H} = - \sum_{j=1}^N i\mu \hat{c}_{2j-1} \hat{c}_{2j}$$

$$= -\mu \sum_{j=1}^N (2\hat{f}_j^\dagger \hat{f}_j - 1)$$

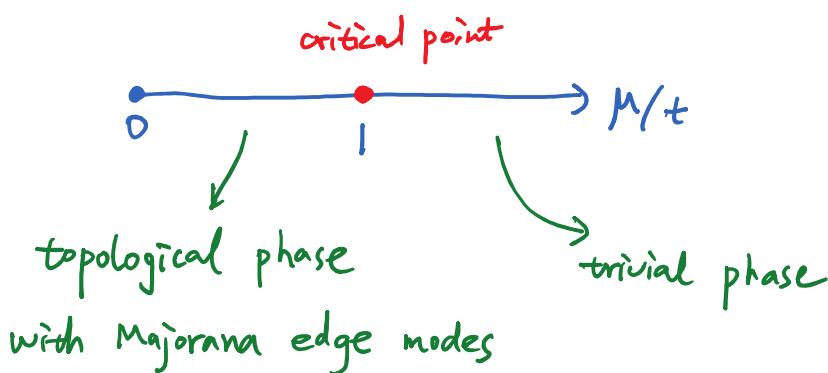
No Majorana zero-energy edge modes.

Ground state:

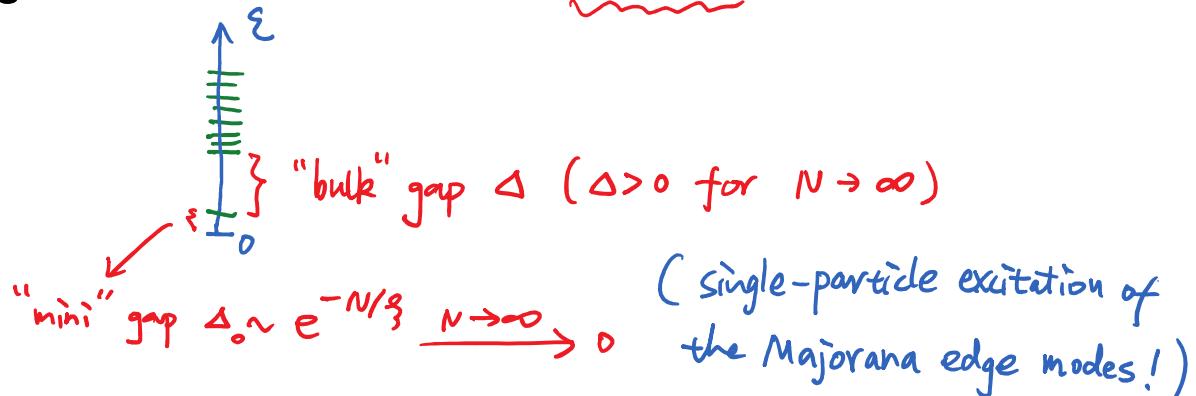
$$|GS\rangle = \hat{f}_1^\dagger \hat{f}_2^\dagger \cdots \hat{f}_N^\dagger |0\rangle_f$$

trivially gapped, no degeneracy!

Phase diagram of the Kitaev's Majorana chain:



Single-particle energies in the topological phase:



Exercise: calculate the single-particle energies for $\mu/t = \frac{1}{2}$ and determine the form of the Majorana edge modes.
 (You may need to increase N to see "mini"-gap $\Delta_0 \rightarrow 0$)