

# Lecture notes on topological insulators

Ming-Che Chang

Department of Physics, National Taiwan Normal University, Taipei, Taiwan

(Dated: May 26, 2017)

## I. SUPERCONDUCTOR PAIRING WITH SPIN

In either the  $s$ -wave superconductor or the spinless  $p$ -wave superconductor, the electron spin does not play an explicit role. We now consider superconducting phases in which the spin degree of freedom does play a role.

### A. 4-component Nambu formulation

To fully accommodate the particle/hole and spin-up/down degrees of freedom, we choose the basis,

$$\begin{pmatrix} \psi_k \\ \bar{\psi}_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix}, \quad (1.1)$$

in which  $\psi_k \equiv (c_{k\uparrow}, c_{k\downarrow})^T$ , and the  $T$  in  $(\psi_{-k}^\dagger)^T$  is omitted. I will henceforth call this as the type-I basis.

Another type of basis is also used, which I will call it as the type-II basis,

$$\begin{pmatrix} \psi_k \\ \bar{\psi}_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\downarrow}^\dagger \\ -c_{-k\uparrow}^\dagger \end{pmatrix}, \quad (1.2)$$

where  $\bar{\psi}_{-k}^\dagger = i\sigma_y \psi_{-k}^\dagger = (c_{-k\downarrow}^\dagger, -c_{-k\uparrow}^\dagger)^T$ . It is connected with the type-I basis via an unitary transformation,

$$\begin{pmatrix} \psi_k \\ \bar{\psi}_{-k}^\dagger \end{pmatrix} = S \begin{pmatrix} \psi_k \\ \psi_{-k}^\dagger \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i\sigma_y \end{pmatrix}, \quad (1.3)$$

and  $S^\dagger S = S S^\dagger = 1$ .

The earlier 2-component formulation of the BCS theory can be extended to 4-component. Under the type-II basis, we have

$$H = \frac{1}{2} \sum_k (\psi_k^\dagger, \bar{\psi}_{-k}) \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta_k^\dagger & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} \psi_k \\ \bar{\psi}_{-k}^\dagger \end{pmatrix} \quad (1.4)$$

$$= \frac{1}{2} \sum_k (c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger c_{-k\downarrow} - c_{-k\uparrow}) \times \begin{pmatrix} \varepsilon_k & 0 & \Delta_{11} & \Delta_{12} \\ 0 & \varepsilon_k & \Delta_{21} & \Delta_{22} \\ \Delta_{11}^* & \Delta_{21}^* & -\varepsilon_{-k} & 0 \\ \Delta_{12}^* & \Delta_{22}^* & 0 & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\downarrow}^\dagger \\ -c_{-k\uparrow}^\dagger \end{pmatrix} \quad (1.5)$$

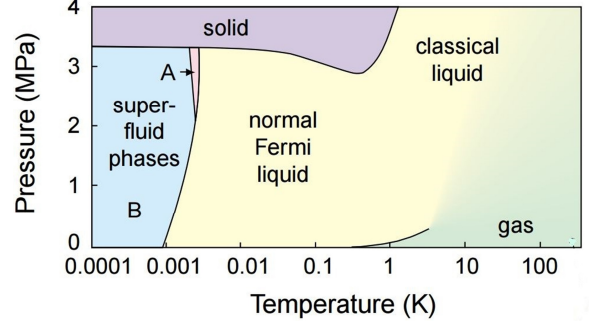


FIG. 1 A-phase and B-phase in the phase diagram of He-3.

Note that for the  $s$ -wave SC (Chap ??),

$$\Delta_k = \Delta_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.6)$$

For the spinless  $p$ -wave SC considered so far, for example, the 2D  $p$ -wave SC in Chap ??,

$$\Delta_k = 2\Delta_0(k_x + ik_y) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.7)$$

In the two cases above, there is no coupling between (1,3) components and (2,4) components. In fact, the (2,4) components of the states are redundant. You can verify that they just duplicate the physics described by the (1,3) components.

In general, the gap function can be expanded as,

$$\Delta_k = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (1.8)$$

where  $\mathbf{d}_k$  is sometimes called as the **order-parameter vector**. For example, one can have ( $d_0 = 0$ ),

$$\text{polar phase } \mathbf{d}_k = \Delta_0(0, 0, k_z), \quad (1.9)$$

$$\text{ABM phase (A-phase) } \mathbf{d}_k = \Delta_0(0, 0, k_x + ik_y) \quad (1.10)$$

$$\text{BM phase (B-phase) } \mathbf{d}_k = \Delta_0(k_x, k_y, k_z). \quad (1.11)$$

The A-phase and the B-phase can be found in He-3 (see Fig. 1). The structures of these energy gaps are illustrated in Fig. 2. One can see Chap 3 of [Vollhardt and Wolfe, 1990](#) for more details. The A-phase is chiral and breaks TRS, while the B-phase is helical and preserves TRS (see next chap).

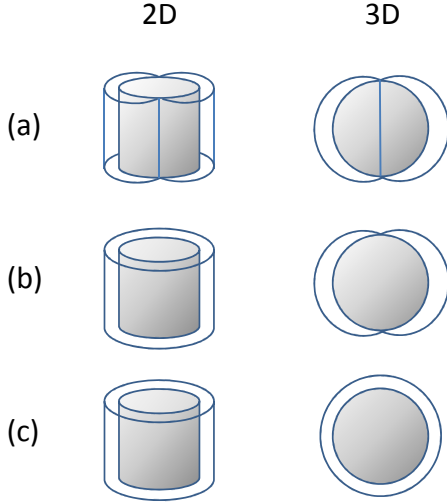


FIG. 2 The energy gap for (a) polar phase with  $\mathbf{d} = (k_x, 0, 0)$ , (b) A-phase, and (c) B-phase. The polar phase has nodal line in both 2D and 3D. The A-phase is fully gapped in 2D, but has nodal points in 3D. The B-phase is fully gapped in both 2D and 3D. See [Mackenzie and Maeno, 2000](#).

Using the type-I basis, we have

$$\begin{aligned}
 H &= \frac{1}{2} \sum_k (\psi_k^\dagger, \psi_{-k}) \begin{pmatrix} \varepsilon_k & \bar{\Delta}_k \\ \bar{\Delta}_k^\dagger & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} \psi_k \\ \psi_{-k}^\dagger \end{pmatrix} \quad (1.12) \\
 &= \frac{1}{2} \sum_k (c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger c_{-k\uparrow} c_{-k\downarrow}) \\
 &\quad \times \begin{pmatrix} \varepsilon_k & 0 & \bar{\Delta}_{11} & \bar{\Delta}_{12} \\ 0 & \varepsilon_k & \bar{\Delta}_{21} & \bar{\Delta}_{22} \\ \bar{\Delta}_{11}^* & \bar{\Delta}_{21}^* & -\varepsilon_{-k} & 0 \\ \bar{\Delta}_{12}^* & \bar{\Delta}_{22}^* & 0 & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix}, \quad (1.13)
 \end{aligned}$$

where  $\bar{\Delta} = \Delta i\sigma_y$ , or

$$\bar{\Delta} = \begin{pmatrix} d_0 + d_z & d_x - id_y \\ d_x + id_y & d_0 - d_z \end{pmatrix} i\sigma_y \quad (1.14)$$

$$= \begin{pmatrix} -d_x + id_y & d_0 + d_z \\ -d_0 + d_z & d_x + id_y \end{pmatrix}. \quad (1.15)$$

For singlet pairing, one has  $d_0(-\mathbf{k}) = d_0(\mathbf{k})$ ,  $\mathbf{d}(-\mathbf{k}) = 0$ ; for triplet pairing,  $d_0(\mathbf{k}) = 0$ ,  $\mathbf{d}(-\mathbf{k}) = -\mathbf{d}(\mathbf{k})$ . That is, for singlet pairing,  $\bar{\Delta}(-\mathbf{k}) = \bar{\Delta}(\mathbf{k})$ ; for triplet pairing,  $\bar{\Delta}(-\mathbf{k}) = -\bar{\Delta}(\mathbf{k})$ . Therefore,

$$\bar{\Delta}(-\mathbf{k}) = -\bar{\Delta}^T(\mathbf{k}), \text{ or } \bar{\Delta}^\dagger(-\mathbf{k}) = -\bar{\Delta}^*(\mathbf{k}) \quad (1.16)$$

for *both* types of pairing. Note that this is not true for  $\Delta(\mathbf{k})$ .

### 1. Dirac Hamiltonian

If we let

$$\varepsilon_k = mc^2; \quad d_0 = 0, \quad \mathbf{d}_k = c\hbar\mathbf{k}, \quad (1.17)$$

then under type-I basis (see Eq. (1.4)),

$$H(\mathbf{k}) = \begin{pmatrix} mc^2 & c\hbar\mathbf{k} \cdot \boldsymbol{\sigma} \\ c\hbar\mathbf{k} \cdot \boldsymbol{\sigma} & -mc^2 \end{pmatrix} \quad (1.18)$$

$$= c\hbar\mathbf{k} \cdot \boldsymbol{\alpha} + mc^2\beta, \quad (1.19)$$

where

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.20)$$

This is the Dirac Hamiltonian in momentum space (and in the Dirac representation), which is similar to that of the BM phase of He-3.

For reference, if one switches to type-II basis, then in Eq. (1.19),

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} i\sigma_y \\ -i\sigma_y \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.21)$$

### 2. Symmetry of gap function

Here we offer more details about the gap function and its symmetries ([Sigrist and Ueda, 1991](#)). This part can be skipped, if you are not familiar with the language of second quantization.

Using second quantization, the interaction between Cooper pairs is described as,

$$V = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{s_1 s_2 s_3 s_4}(\mathbf{k}, \mathbf{k}') c_{k s_1}^\dagger c_{-k, s_2}^\dagger c_{-k' s_3} c_{k' s_4}, \quad (1.22)$$

$$V_{s_1 s_2 s_3 s_4}(\mathbf{k}, \mathbf{k}') = \langle \mathbf{k} s_1, -\mathbf{k} s_2 | \mathcal{V} | -\mathbf{k}' s_3, \mathbf{k}' s_4 \rangle, \quad (1.23)$$

where  $\mathcal{V} = \mathcal{V}(\mathbf{r} - \mathbf{r}')$  is the potential energy of two-body interaction. Since the fermion operators anti-commute, one can show that,

$$V_{s_2 s_1 s_3 s_4}(-\mathbf{k}, \mathbf{k}') = -V_{s_1 s_2 s_3 s_4}(\mathbf{k}, \mathbf{k}'), \quad (1.24)$$

$$V_{s_1 s_2 s_4 s_3}(\mathbf{k}, -\mathbf{k}') = -V_{s_1 s_2 s_3 s_4}(\mathbf{k}', \mathbf{k}). \quad (1.25)$$

Also, since  $V$  is hermitian, one has

$$V_{s_4 s_3 s_2 s_1}^*(\mathbf{k}, \mathbf{k}') = V_{s_1 s_2 s_3 s_4}(\mathbf{k}', \mathbf{k}). \quad (1.26)$$

In the mean-field approximation,

$$\begin{aligned}
 V_{MF} &= \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{s_1 s_2 s_3 s_4}(\mathbf{k}, \mathbf{k}') \langle c_{k s_1}^\dagger c_{-k, s_2}^\dagger \rangle c_{-k' s_3} c_{k' s_4} \\
 &\quad + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{s_1 s_2 s_3 s_4}(\mathbf{k}, \mathbf{k}') c_{k s_1}^\dagger c_{-k, s_2}^\dagger \langle c_{-k' s_3} c_{k' s_4} \rangle, \quad (1.27)
 \end{aligned}$$

where  $\langle \dots \rangle$  is a quantum statistical average over many-body states. The gap function is defined as,

$$\bar{\Delta}_{s s'}(\mathbf{k}) = \sum_{\mathbf{k}'} V_{s s' s_3 s_4} \langle c_{-k' s_3} c_{k' s_4} \rangle. \quad (1.28)$$

Thus,

$$V_{MF} = \frac{1}{2} \sum_{\mathbf{k}} \bar{\Delta}_{s's}^*(\mathbf{k}) c_{-k's} c_{k's'} + \frac{1}{2} \sum_{\mathbf{k}} \bar{\Delta}_{ss'}(\mathbf{k}) c_{ks}^\dagger c_{-ks'}^\dagger. \quad (1.29)$$

These are the off-diagonal terms in Eq. (1.12).

Using the symmetry in Eq. (1.24), we have

$$\bar{\Delta}_{ss'}(-\mathbf{k}) = \sum_{\mathbf{k}'} V_{ss's_3s_4}(-\mathbf{k}, \mathbf{k}') \langle c_{-k's_3} c_{k's_4} \rangle \quad (1.30)$$

$$= - \sum_{\mathbf{k}'} V_{s's_3s_4}(\mathbf{k}, \mathbf{k}') \langle c_{-k's_3} c_{k's_4} \rangle \quad (1.31)$$

$$= -\bar{\Delta}_{s's}(\mathbf{k}). \quad (1.32)$$

This is Eq. (1.16). From this general argument, one can see that Eq. (1.16) is valid for any type of pairing ( $s, p, d \dots$ ) and their mixings.

## B. Bogoliubov-Valatin transformation

We now solve the eigen-energies and eigenstates of the 4-component Hamiltonian. For the singlet case,  $\mathbf{d}_k = 0$ , and it's basically just two copies of the 2-component  $s$ -wave BdG equations discussed earlier. Therefore, we focus only on the triplet case ( $d_0 = 0$ ). Furthermore, we consider only the **unitary state**. That is (for both type-I and type-II basis), the state with a gap function whose square is proportional to an unitary matrix,

$$\Delta_k \Delta_k^\dagger = \bar{\Delta}_k \bar{\Delta}_k^\dagger = \alpha_k 1. \quad (1.33)$$

Since

$$\bar{\Delta}_k \bar{\Delta}_k^\dagger = \mathbf{d}_k \cdot \mathbf{d}_k^* + i \mathbf{d}_k \times \mathbf{d}_k^* \cdot \boldsymbol{\sigma}, \quad (1.34)$$

an unitary state has

$$\alpha_k = |\mathbf{d}_k|^2, \quad \mathbf{d}_k \times \mathbf{d}_k^* = 0. \quad (1.35)$$

This is so if, and only if,  $\mathbf{d}(\mathbf{k}) = f(\mathbf{k}) \hat{\mathbf{n}}(\mathbf{k})$ , where  $\hat{\mathbf{n}}$  is a real vector. The SC phases in Eqs. (1.9), (1.10), (1.11) all belong to this class of states.

Note: For a non-unitary state, distributions of spin-up and spin-down electrons are not everywhere balanced in momentum space, and time-reversal symmetry is broken. Also, the excitation spectrum is no longer doubly degenerate (Sigrist and Ueda, 1991).

Recall that in Eq. 1.12, the matrix Hamiltonian is

$$\mathbf{H}(\mathbf{k}) = \begin{pmatrix} \varepsilon_k & \bar{\Delta}_k \\ \bar{\Delta}_k^\dagger & -\varepsilon_k \end{pmatrix}, \quad (1.36)$$

If  $\mathbf{H}(\mathbf{k})\Phi_k = E_k\Phi_k$ , then

$$\mathbf{H}^2(\mathbf{k})\Phi_k = \begin{pmatrix} \varepsilon_k^2 + \bar{\Delta}_k \bar{\Delta}_k^\dagger & 0 \\ 0 & \varepsilon_k^2 + \bar{\Delta}_k^\dagger \bar{\Delta}_k \end{pmatrix} \Phi_k \quad (1.37)$$

$$= E_k^2 \Phi_k. \quad (1.38)$$

For the unitary state,  $\bar{\Delta}_k \bar{\Delta}_k^\dagger = \bar{\Delta}_k^\dagger \bar{\Delta}_k = |\mathbf{d}_k|^2$ . Therefore, the eigen-energies can be easily solved,

$$E_k^\pm = \pm \sqrt{\varepsilon_k^2 + |\mathbf{d}_k|^2}, \quad (1.39)$$

which are doubly degenerate (see Fig. 2) for the gap structures.

Write

$$\Phi_k = \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix}, \quad (1.40)$$

where  $\mathbf{u}_k, \mathbf{v}_k$  are 2-component column vectors. Then, for positive eigen-energy  $E_k^+$ , one has the eigenvectors (Nomura, 2013; Sigrist and Ueda, 1991),

$$\begin{pmatrix} \mathbf{u}_k^{(1)} \\ \mathbf{v}_k^{(1)} \end{pmatrix} = A_k \begin{pmatrix} E_k + \varepsilon_k \\ 0 \\ \bar{\Delta}_{11}^*(\mathbf{k}) \\ \bar{\Delta}_{12}^*(\mathbf{k}) \end{pmatrix}, \quad (1.41)$$

$$\begin{pmatrix} \mathbf{u}_k^{(2)} \\ \mathbf{v}_k^{(2)} \end{pmatrix} = A_k \begin{pmatrix} 0 \\ E_k + \varepsilon_k \\ \bar{\Delta}_{21}^*(\mathbf{k}) \\ \bar{\Delta}_{22}^*(\mathbf{k}) \end{pmatrix}, \quad (1.42)$$

where  $A_k = [2E_k(E_k + \varepsilon_k)]^{-1/2}$ . For negative eigen-energy  $E_k^-$ , one has

$$\begin{pmatrix} \mathbf{u}_k^{(3)} \\ \mathbf{v}_k^{(3)} \end{pmatrix} = A_k \begin{pmatrix} -\bar{\Delta}_{11}(\mathbf{k}) \\ -\bar{\Delta}_{21}(\mathbf{k}) \\ E_k + \varepsilon_k \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{-k}^{(1)*} \\ \mathbf{u}_{-k}^{(1)*} \end{pmatrix}, \quad (1.43)$$

$$\begin{pmatrix} \mathbf{u}_k^{(4)} \\ \mathbf{v}_k^{(4)} \end{pmatrix} = A_k \begin{pmatrix} -\bar{\Delta}_{12}(\mathbf{k}) \\ -\bar{\Delta}_{22}(\mathbf{k}) \\ 0 \\ E_k + \varepsilon_k \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{-k}^{(2)*} \\ \mathbf{u}_{-k}^{(2)*} \end{pmatrix}. \quad (1.44)$$

Before the Bogoliubov-Valatin (BV) transformation, the basis is,

$$\Psi_k = \begin{pmatrix} \psi_k \\ \psi_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix}. \quad (1.45)$$

The basis that diagonalizes the Hamiltonian is written as,

$$\Gamma_k = \begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} b_{k\uparrow} \\ b_{k\downarrow} \\ b_{-k\uparrow}^\dagger \\ b_{-k\downarrow}^\dagger \end{pmatrix}. \quad (1.46)$$

They are connected by an unitary transformation,

$$\Psi_k = \mathbf{U}_k \Gamma_k = \begin{pmatrix} \mathbf{u}_k & \mathbf{v}_{-k}^* \\ \mathbf{v}_k & \mathbf{u}_{-k}^* \end{pmatrix} \Gamma_k, \quad (1.47)$$

in which each column is an eigenvector. For example, the elements of  $2 \times 2$  matrices  $\mathbf{u}_k, \mathbf{v}_k$  are,

$$\mathbf{u}_k = \begin{pmatrix} \mathbf{u}_k^{(1)} & \mathbf{u}_k^{(2)} \end{pmatrix} \quad (1.48)$$

$$\mathbf{v}_k = \begin{pmatrix} \mathbf{v}_k^{(1)} & \mathbf{v}_k^{(2)} \end{pmatrix}. \quad (1.49)$$

After the BV transformation, the Hamiltonian is diagonal,

$$\mathbf{H}_D(\mathbf{k}) = \mathbf{U}_k^\dagger \mathbf{H}(\mathbf{k}) \mathbf{U}_k, \quad (1.50)$$

and

$$H = \frac{1}{2} \sum_k \Gamma_k^\dagger \mathbf{H}_D(\mathbf{k}) \Gamma_k \quad (1.51)$$

$$= \frac{1}{2} \sum_{ks} (E_k^+ b_{ks}^\dagger b_{ks} + E_k^- b_{-ks} b_{-ks}^\dagger) \quad (1.52)$$

$$= \sum_{ks} E_k^+ b_{ks}^\dagger b_{ks} + \text{const.} \quad (1.53)$$

The BV transformation matrix for type-II basis can be found as follows: Before the transformation,

$$\bar{\Psi}_k = \begin{pmatrix} \psi_k \\ \psi_{-k}^\dagger \end{pmatrix} = \mathbf{S} \begin{pmatrix} \psi_k \\ \psi_{-k}^\dagger \end{pmatrix}, \quad (1.54)$$

where  $\mathbf{S}$  is given in Eq. (1.3). After the transformation,

$$\bar{\Gamma}_k = \begin{pmatrix} \gamma_k \\ \bar{\gamma}_{-k}^\dagger \end{pmatrix} = \mathbf{S} \begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix}. \quad (1.55)$$

It follows from Eq. (1.47) that, for type-II basis,

$$\bar{\Psi}_k = \mathbf{S} \mathbf{U}_k \mathbf{S}^{-1} \bar{\Gamma}_k \quad (1.56)$$

$$= \begin{pmatrix} \mathbf{u}_k & \mathbf{v}_{-k}^* (-i\sigma_y) \\ i\sigma_y \mathbf{v}_k & \sigma_y \mathbf{u}_{-k}^* \sigma_y \end{pmatrix} \bar{\Gamma}_k, \quad (1.57)$$

where  $\mathbf{u}_k, \mathbf{v}_k$  are defined in Eqs. (1.48), (1.49).

### C. Real space formulation

Without SC pairing, the real-space Hamiltonian is,

$$h_0 = \sum_s \int d^D r \psi_s^\dagger(\mathbf{r}) h_0(\mathbf{r}) \psi_s(\mathbf{r}), \quad (1.58)$$

$$h_0 = \frac{p^2}{2m} + V(\mathbf{r}) + \alpha \boldsymbol{\sigma} \times \mathbf{p} \cdot \mathbf{E} + \dots - \mu \quad (1.59)$$

The interaction term is

$$V = \frac{1}{2} \sum_{ss'} \int d^D r d^D r' \mathcal{V}(\mathbf{r} - \mathbf{r}') \psi_s^\dagger(\mathbf{r}) \psi_{s'}^\dagger(\mathbf{r}') \psi_{s'}(\mathbf{r}') \psi_s(\mathbf{r}). \quad (1.60)$$

With the mean-field approximation, one has

$$V_{MF} = \frac{1}{2} \sum_{ss'} \Delta_{ss'}(\mathbf{r}, \mathbf{r}') \psi_s^\dagger(\mathbf{r}) \psi_{s'}^\dagger(\mathbf{r}') + h.c., \quad (1.61)$$

where

$$\Delta_{ss'}(\mathbf{r}, \mathbf{r}') \equiv \mathcal{V}(\mathbf{r} - \mathbf{r}') \langle \psi_{s'}(\mathbf{r}') \psi_s(\mathbf{r}) \rangle. \quad (1.62)$$

Therefore, under type-I basis (Chamon *et al.*, 2010),  $\Psi(\mathbf{r}) = (\psi_\uparrow, \psi_\downarrow, \psi_\uparrow^\dagger, \psi_\downarrow^\dagger)^T$ ,

$$\mathbf{H}_0 = \begin{pmatrix} h_0(\mathbf{r}) & 0 \\ 0 & -h_0^*(\mathbf{r}) \end{pmatrix}, \quad (1.63)$$

$$\Delta_{4 \times 4}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} 0 & \bar{\Delta}(\mathbf{r}, \mathbf{r}') \\ \bar{\Delta}^\dagger(\mathbf{r}, \mathbf{r}') & 0 \end{pmatrix}, \quad (1.64)$$

where  $\bar{\Delta} = \Delta i\sigma_y$ , and the full Hamiltonian is

$$H = \frac{1}{2} \int d^D r d^D r' \Psi^\dagger(\mathbf{r}) [\mathbf{H}_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') + \Delta_{4 \times 4}(\mathbf{r}, \mathbf{r}')] \Psi(\mathbf{r}'). \quad (1.65)$$

Under type-II basis (Leijnse and Flensberg, 2012),  $\Psi(\mathbf{r}) = (\psi_\uparrow, \psi_\downarrow, \psi_\uparrow^\dagger, -\psi_\downarrow^\dagger)^T$ , and

$$\mathbf{H}_0 = \begin{pmatrix} h_0(\mathbf{r}) & 0 \\ 0 & -\sigma_y h_0^*(\mathbf{r}) \sigma_y \end{pmatrix}, \quad (1.66)$$

$$\Delta_{4 \times 4}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} 0 & \Delta(\mathbf{r}, \mathbf{r}') \\ \Delta^\dagger(\mathbf{r}, \mathbf{r}') & 0 \end{pmatrix}. \quad (1.67)$$

### D. TR and PH symmetries

#### 1. Time-reversal transformation

For type-I basis, the TR operator for  $p$ -wave SC is (Bernevig and Hughes, 2013)

$$\mathbf{T} = 1 \otimes i\sigma_y K = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix} K, \quad (1.68)$$

in which  $i\sigma_y K$  operates in the spin subspace, and  $\mathbf{T}^2 = -1$ . The state transforms as,

$$\begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} \rightarrow \mathbf{T} \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} = \begin{pmatrix} i\sigma_y \mathbf{u}_k^* \\ i\sigma_y \mathbf{v}_k^* \end{pmatrix} \quad (1.69)$$

The Hamiltonian transforms as,

$$\mathbf{T} \mathbf{H}(\mathbf{k}) \mathbf{T}^{-1} = \mathbf{H}(-\mathbf{k}). \quad (1.70)$$

What about the TR operator for type-II basis? From the relation  $\bar{\Psi}_k = \mathbf{S} \Psi_k$ , and

$$\Psi_k \rightarrow \mathbf{T} \Psi_k, \quad (1.71)$$

one can infer that,

$$\bar{\Psi}_k \rightarrow \mathbf{S} \mathbf{T} \mathbf{S}^{-1} \bar{\Psi}_k. \quad (1.72)$$

Therefore, from Eqs. (1.54) and (1.68), the TR operator for type-II basis is

$$\mathbf{S} \mathbf{T} \mathbf{S}^{-1} = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix} K, \quad (1.73)$$

the same as that of type-I basis.

## 2. Particle-hole transformation

We will focus on the PH transformation of  $p$ -wave state. A PH operator maps a positive energy state to a negative energy state. For example, it maps  $(\mathbf{u}_k^{(1)}, \mathbf{v}_k^{(1)})^T$  in Eq. (1.41) to  $(\mathbf{u}_k^{(3)}, \mathbf{v}_k^{(3)})^T$  in Eq. (1.43). That is,

$$\begin{pmatrix} \mathbf{u}_k^{(1)} \\ \mathbf{v}_k^{(1)} \end{pmatrix} \rightarrow \mathbf{P} \begin{pmatrix} \mathbf{u}_k^{(1)} \\ \mathbf{v}_k^{(1)} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_{-k}^{(3)} \\ \mathbf{v}_{-k}^{(3)} \end{pmatrix}. \quad (1.74)$$

Therefore, for type-I basis,

$$\mathbf{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K = \tau_x K \otimes 1. \quad (1.75)$$

This applies to the other pair,  $(\mathbf{u}_k^{(2)}, \mathbf{v}_k^{(2)})^T$  in Eq. (1.42) maps to  $(\mathbf{u}_{-k}^{(4)}, \mathbf{v}_{-k}^{(4)})^T$  in Eq. (1.44) as well. One can check that,  $\mathbf{P}^2 = 1$ , and

$$\mathbf{P}\mathbf{H}(\mathbf{k})\mathbf{P}^{-1} = -\mathbf{H}(-\mathbf{k}). \quad (1.76)$$

The PH operator for type-II basis is

$$\mathbf{S}\mathbf{P}\mathbf{S}^{-1} = \begin{pmatrix} 0 & -i\sigma_y \\ i\sigma_y & 0 \end{pmatrix} K = \tau_y \otimes \sigma_y K. \quad (1.77)$$

A Majorana fermion state satisfies  $\mathbf{P}\Psi = \Psi$ . That is, for type-I basis, in real-space,

$$\begin{pmatrix} \mathbf{v}^*(\mathbf{r}) \\ \mathbf{u}^*(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \mathbf{u}(\mathbf{r}) \\ \mathbf{v}(\mathbf{r}) \end{pmatrix}. \quad (1.78)$$

Thus, a Majorana fermion state requires only half of the degrees of freedom,

$$\Psi_M(\mathbf{r}) = \begin{pmatrix} \mathbf{u}(\mathbf{r}) \\ \mathbf{u}^*(\mathbf{r}) \end{pmatrix} \quad (1.79)$$

Its time-reversed state is

$$\mathbf{T}\Psi_M(\mathbf{r}) = \begin{pmatrix} i\sigma_y \mathbf{u}^*(\mathbf{r}) \\ i\sigma_y \mathbf{u}(\mathbf{r}) \end{pmatrix}, \quad (1.80)$$

which is an energy eigenstate if the Hamiltonian has TRS.

Since  $|\mathbf{T}\Psi_M(\mathbf{r})|^2 = |\Psi_M(\mathbf{r})|^2 = 2\mathbf{u}^\dagger \cdot \mathbf{u}$ ,  $\Psi_M$  and  $\mathbf{T}\Psi_M$  have the same probability distribution in space. Therefore, to have an isolated MF not overlapped by its TR partner, TRS needs be broken (Leijnse and Flensberg, 2012).

For reference, for type-II basis, a Majorana state is

$$\Psi_M(\mathbf{r}) = \begin{pmatrix} \mathbf{u}(\mathbf{r}) \\ i\sigma_y \mathbf{u}^*(\mathbf{r}) \end{pmatrix}. \quad (1.81)$$

Its time-reversed state is

$$\mathbf{T}\Psi_M(\mathbf{r}) = \begin{pmatrix} i\sigma_y \mathbf{u}^*(\mathbf{r}) \\ \mathbf{u}(\mathbf{r}) \end{pmatrix}, \quad (1.82)$$

which again has the same spatial distribution as  $\Psi_M(\mathbf{r})$ .

## 3. Symmetry transformation of field operator

The TR operator and the PH operator mentioned so far operate in the single-particle Hilbert space. They are anti-unitary operators,

$$\mathbf{T} = \mathbf{U}_T K, \quad \mathbf{P} = \mathbf{U}_P K, \quad (1.83)$$

where  $\mathbf{U}_T$  and  $\mathbf{U}_P$  are unitary operators. It is known that  $\mathbf{T}^2 = -1$  for fermions,  $\mathbf{P}^2 = -1$  for  $s$ -wave SC,  $\mathbf{P}^2 = 1$  for  $p$ -wave SC, and

$$\mathbf{T}\mathbf{H}(\mathbf{k})\mathbf{T}^{-1} = \mathbf{H}(-\mathbf{k}), \quad (1.84)$$

$$\mathbf{P}\mathbf{H}(\mathbf{k})\mathbf{P}^{-1} = -\mathbf{H}(-\mathbf{k}). \quad (1.85)$$

We now introduce the TR and PH operators,  $T$  and  $P$ , for field operators  $\psi_\alpha(\mathbf{r})$ . They are required to operate in the following way (Ryu *et al.*, 2010),

$$T\psi_\alpha T^{-1} = \sum_\beta (\mathbf{U}_T)_{\alpha\beta} \psi_\beta, \quad (1.86)$$

$$P\psi_\alpha P^{-1} = \sum_\beta (\mathbf{U}_P^*)_{\alpha\beta} \psi_\beta^\dagger. \quad (1.87)$$

While the TR operator  $T$  remains anti-unitary, the PH operator  $P$  now becomes unitary (while the chiral operator becomes anti-unitary)! If a system has TRS and PHS, then

$$THT^{-1} = H, \quad (1.88)$$

$$PHP^{-1} = H. \quad (1.89)$$

Both operators *commute* with the Hamiltonian. Also,  $T^2 = \pm 1$ ,  $P^2 = \pm 1$ , depending on the symmetries. For more details, see p.6 of Ryu *et al.*, 2010.

### Exercise:

1. Show that the eigenvectors of the  $4 \times 4$  Hamiltonian matrix in Eq.(1.36) (with  $d_0 = 0$ ) are Eqs. (1.41),(1.42), (1.43),(1.44). To get the eigenvector in Eq. (1.41), for example, one can choose  $\mathbf{u}_k^{(1)} = (1, 0)^T$ , solve for  $\mathbf{v}_k^{(1)}$ , then normalize the eigenvector.

## References

- Bernevig, B. A., and T. L. Hughes, 2013, *Topological Insulators and Topological Superconductors* (Princeton University Press).
- Chamon, C., R. Jackiw, Y. Nishida, S.-Y. Pi, and L. Santos, 2010, Phys. Rev. B **81**, 224515.
- Leijnse, M., and K. Flensberg, 2012, Semiconductor Science and Technology **27**(12), 124003.
- Mackenzie, A., and Y. Maeno, 2000, Physica B: Condensed Matter **280**(14), 148.
- Nomura, K., 2013, Fundamental theory of topological insulator, unpublished, written in Japanese.
- Ryu, S., A. P. Schnyder, A. Furusaki, and A. W. W. Ludwig, 2010, New Journal of Physics **12**(6), 065010.
- Sigrist, M., and K. Ueda, 1991, Rev. Mod. Phys. **63**, 239.
- Vollhardt, D., and P. Wolfe, 1990, *The superfluid phases of Helium 3* (Taylor and Francis).