Lecture notes on topological insulators

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CONTENTS

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, the earlier 2-component formulation of the BCS theory needs to be extended to 4 components,

$$\begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\psi}^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}, \tag{1.1}$$

in which $\boldsymbol{\psi}_k \equiv (c_{k\uparrow}, c_{k\downarrow})^T$, and $\boldsymbol{\psi}^\dagger_{-k} \equiv (c^\dagger_{-k\uparrow}, c^\dagger_{-k\downarrow})^T$. I will henceforth call this type-I basis.

Another basis can also be used, which would be called type-II basis,

$$\begin{pmatrix} \boldsymbol{\psi}_k \\ \bar{\boldsymbol{\psi}}^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\downarrow} \\ -c^\dagger_{-k\uparrow} \end{pmatrix}, \tag{1.2}$$

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

$$\begin{pmatrix} \boldsymbol{\psi}_k \\ \bar{\boldsymbol{\psi}}^\dagger_{-k} \end{pmatrix} = \mathsf{S} \begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\psi}^\dagger_{-k} \end{pmatrix}, \quad \mathsf{S} = \begin{pmatrix} 1 & 0 \\ 0 & i\sigma_y \end{pmatrix}, \tag{1.3}$$

and $\mathsf{S}^\dagger \mathsf{S} = \mathsf{S}\mathsf{S}^\dagger = 1$.

Under the type-I basis, we have

$$H = \frac{1}{2}\sum_k (\boldsymbol{\psi}^\dagger_k, \boldsymbol{\psi}_{-k}) \begin{pmatrix} \varepsilon_k & \bar{\Delta}_k \\ \bar{\Delta}^\dagger_k & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\psi}^\dagger_{-k} \end{pmatrix} \tag{1.4}$$

$$= \frac{1}{2}\sum_k (c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} c_{-k\uparrow} c_{-k\downarrow}) \times \begin{pmatrix} \varepsilon_k & 0 & \bar{\Delta}_{11} & \bar{\Delta}_{12} \\ 0 & \varepsilon_k & \bar{\Delta}_{21} & \bar{\Delta}_{22} \\ \bar{\Delta}^*_{11} & \bar{\Delta}^*_{21} & -\varepsilon_{-k} & 0 \\ \bar{\Delta}^*_{12} & \bar{\Delta}^*_{22} & 0 & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}. \tag{1.5}$$

Under the type-II basis, we have

$$H = \frac{1}{2}\sum_k (\boldsymbol{\psi}^\dagger_k, \bar{\boldsymbol{\psi}}_{-k}) \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta^\dagger_k & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi}_k \\ \bar{\boldsymbol{\psi}}^\dagger_{-k} \end{pmatrix} \tag{1.6}$$

$$= \frac{1}{2}\sum_k (c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} c_{-k\downarrow} - c_{-k\uparrow}) \times \begin{pmatrix} \varepsilon_k & 0 & \Delta_{11} & \Delta_{12} \\ 0 & \varepsilon_k & \Delta_{21} & \Delta_{22} \\ \Delta^*_{11} & \Delta^*_{21} & -\varepsilon_{-k} & 0 \\ \Delta^*_{12} & \Delta^*_{22} & 0 & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\downarrow} \\ -c^\dagger_{-k\uparrow} \end{pmatrix}. \tag{1.7}$$

Apparently, the gap functions under different bases are related by $\bar{\Delta}_k = \Delta_k i\sigma_y$.

1. Singlet pairing and triplet pairing

For the type-I basis, the $\bar{\Delta}_k$ block couples the spinor $\boldsymbol{\psi}^\dagger_k$ with the spinor $\boldsymbol{\psi}^\dagger_{-k}$, giving

$$(c^\dagger_{k\uparrow}, c^\dagger_{k\downarrow}) \begin{pmatrix} \bar{\Delta}_{11} & \bar{\Delta}_{12} \\ \bar{\Delta}_{21} & \bar{\Delta}_{22} \end{pmatrix} \begin{pmatrix} c^\dagger_{-k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \tag{1.8}$$

$$= \bar{\Delta}_{11} c^\dagger_{k\uparrow} c^\dagger_{-k\uparrow} + \bar{\Delta}_{12} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \bar{\Delta}_{21} c^\dagger_{k\downarrow} c^\dagger_{-k\uparrow} + \bar{\Delta}_{22} c^\dagger_{k\downarrow} c^\dagger_{-k\downarrow}.$$

The coupling between $\boldsymbol{\psi}_{-k}$ and $\boldsymbol{\psi}_k$ due to the $\bar{\Delta}^\dagger_k$-block can be understood in a similar way.

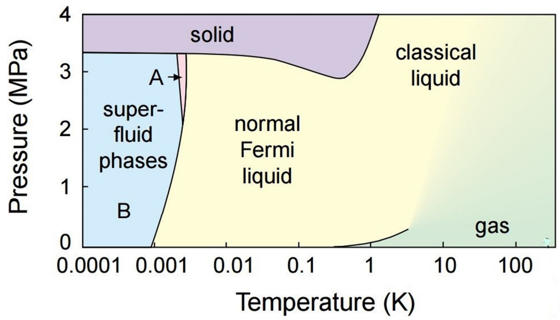

FIG. 1 A-phase and B-phase in the phase diagram of He-3.

With suitable recombinations, we can rewrite these terms as

$$
\begin{aligned}
& d_0(+c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow} - c^\dagger_{k\downarrow}c^\dagger_{-k\uparrow}) \\
+\ & d_x(-c^\dagger_{k\uparrow}c^\dagger_{-k\uparrow} + c^\dagger_{k\downarrow}c^\dagger_{-k\downarrow}) \qquad (1.9) \\
+\ & id_y(+c^\dagger_{k\uparrow}c^\dagger_{-k\uparrow} + c^\dagger_{k\downarrow}c^\dagger_{-k\downarrow}) \qquad (1.10) \\
+\ & d_z(+c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow} + c^\dagger_{k\downarrow}c^\dagger_{-k\uparrow}), \qquad (1.11)
\end{aligned}
$$

in which d_0, d_x, d_y, d_z are linear combinations of $\bar{\Delta}_{11}, \bar{\Delta}_{12}, \bar{\Delta}_{21}, \bar{\Delta}_{22}$.

The d_0-terms describe the s-wave pairing. The orbital part of the Cooper pair is $d_0(\mathbf{k})$, with $d_0(-\mathbf{k}) = d_0(\mathbf{k})$, and the spin part is a spin-singlet,

$$\chi_0 = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \qquad (1.12)$$

The product of the orbital part and the spin part changes sign under particle exchange, as it should be.

The d_x, d_y, d_z terms describe the p-wave pairing. The orbital part of a Cooper pair is antisymmetric, $\mathbf{d}(-\mathbf{k}) = -\mathbf{d}(\mathbf{k})$, similar to that of an atomic p-orbital. Their spin parts are symmetric and form a spin-triplet, (Vollhardt and Wolfle, 1990),

$$
\begin{aligned}
\chi_1 &= \frac{1}{\sqrt{2}}(-|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle), \qquad (1.13) \\
\chi_2 &= \frac{i}{\sqrt{2}}(+|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \qquad (1.14) \\
\chi_3 &= \frac{1}{\sqrt{2}}(+|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle). \qquad (1.15)
\end{aligned}
$$

In terms of d_0 and $d_{x,y,z}$, we have

$$
\begin{aligned}
\bar{\Delta}_k &= \begin{pmatrix} -d_x + id_y & d_0 + d_z \\ -d_0 + d_z & d_x + id_y \end{pmatrix} \qquad (1.16) \\
&= d_0(\mathbf{k})\tilde{\chi}_0 + \mathbf{d}(\mathbf{k}) \cdot \tilde{\boldsymbol{\chi}}, \qquad (1.17)
\end{aligned}
$$

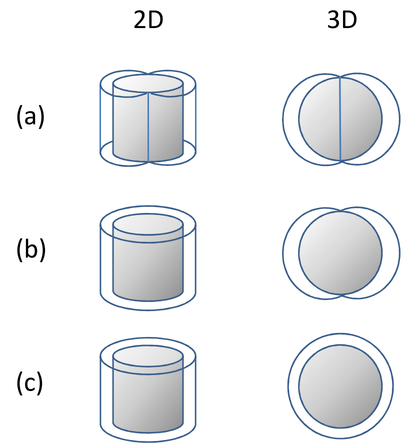

FIG. 2 The energy gap for (a) polar phase with $\mathbf{d} = (k_x, 0, 0)$, (b) A-phase, and (c) B-phase. The polar phase has nodal line in both 2D and 3D. The A-phase is fully gapped in 2D, but has nodal points in 3D. The B-phase is fully gapped in both 2D and 3D. See Mackenzie and Maeno, 2000.

with the matrices (indicated by tilde)

$$
\begin{aligned}
\tilde{\chi}_0 &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_y, \qquad (1.18) \\
\tilde{\chi}_x &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \sigma_x i\sigma_y, \qquad (1.19) \\
\tilde{\chi}_y &= \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} = \sigma_y i\sigma_y, \qquad (1.20) \\
\tilde{\chi}_z &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_z i\sigma_y. \qquad (1.21)
\end{aligned}
$$

That is, when written in terms of Pauli matrices, $\tilde{\chi}_0 = i\sigma_y$, and $\tilde{\boldsymbol{\chi}} = \boldsymbol{\sigma} i\sigma_y$.

Since the gap functions under different bases are related by $\bar{\Delta}_k = \Delta_k i\sigma_y$, it follows that for the type-II basis,

$$\Delta_k = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \qquad (1.22)$$

Under a rotation in spin space, the gap function transforms as (Vollhardt and Wolfle, 1990)

$$\Delta'_k = e^{-\frac{i}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}} \Delta_k e^{\frac{i}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}}. \qquad (1.23)$$

It can be shown that the **order-parameter vector** $\mathbf{d}(\mathbf{k})$ rotates accordingly,

$$\mathbf{d}'(\mathbf{k}) = \mathsf{R}(\boldsymbol{\theta})\mathbf{d}(\mathbf{k}), \qquad (1.24)$$

where $\mathsf{R}(\boldsymbol{\theta})$ is a orthogonal rotation matrix.

Some examples of the order-parameter vector for p-wave pairing are,

$$
\begin{aligned}
\text{polar phase} \quad \mathbf{d}_k &= \Delta_0(0, 0, k_z), \qquad (1.25) \\
\text{ABM phase } (A\text{−phase}) \quad \mathbf{d}_k &= \Delta_0(0, 0, k_x + ik_y), \qquad (1.26) \\
\text{BM phase } (B\text{−phase}) \quad \mathbf{d}_k &= \Delta_0(k_x, k_y, k_z). \qquad (1.27)
\end{aligned}
$$

The spinless 2D p-wave SC in Chap **??** resembles the A-phase,

$$\Delta_k = \Delta_0(k_x + ik_y)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.28)$$

Superfluid helium-3 can have the A-phase and the B-phase (see Fig. 1). The feature of their energy gaps is illustrated in Fig. 2. The A-phase (e.g., the one in spinless p-wave SC) is chiral and breaks TRS, while the B-phase is helical and preserves TRS (see next chap).

For singlet pairing, one has symmetric orbital part $d_0(-\mathbf{k}) = d_0(\mathbf{k}), \mathbf{d}(\mathbf{k}) = 0$; for triplet pairing, one has $d_0(\mathbf{k}) = 0$, and antisymmetric orbital part $\mathbf{d}(-\mathbf{k}) = -\mathbf{d}(\mathbf{k})$. 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, in general

$$\bar{\Delta}(-\mathbf{k}) = -\bar{\Delta}^T(\mathbf{k}), \text{ or } \bar{\Delta}^\dagger(-\mathbf{k}) = -\bar{\Delta}^*(\mathbf{k}) \quad (1.29)$$

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

2. Dirac Hamiltonian

The Dirac Hamiltonian fits in with the formulation above. If we let

$$\varepsilon_k = mc^2; \quad d_0 = 0, \mathbf{d}_k = c\hbar\mathbf{k}, \quad (1.30)$$

then under the type-II basis (see Eq. (1.6)),

$$\begin{aligned} \mathsf{H}(\mathbf{k}) &= \begin{pmatrix} mc^2 & c\hbar\mathbf{k}\cdot\boldsymbol{\sigma} \\ c\hbar\mathbf{k}\cdot\boldsymbol{\sigma} & -mc^2 \end{pmatrix} \\ &= c\hbar\mathbf{k}\cdot\boldsymbol{\alpha} + mc^2\beta, \end{aligned} \quad (1.31)$$

where

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \ \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.32)$$

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

For reference, if one switches to the type-I basis, then in Eq. (1.31),

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} i\sigma_y \\ -i\sigma_y\boldsymbol{\sigma} & 0 \end{pmatrix}, \ \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.33)$$

B. Symmetry of gap function

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

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

$$V = \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}') c^\dagger_{ks_1} c^\dagger_{-k,s_2} c_{-k's_3} c_{k's_4}, \quad (1.34)$$

$$V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}') = \langle \mathbf{k}s_1, -\mathbf{k}s_2|\mathcal{V}| -\mathbf{k}'s_3, \mathbf{k}'s_4\rangle, \quad (1.35)$$

in which the spins need to be summed over, and $\mathcal{V} = \mathcal{V}(\mathbf{r}-\mathbf{r}')$ is the potential energy of two-body interaction. Since the fermion operators anti-commute, one can show that,

$$\begin{aligned} V_{s_2s_1s_3s_4}(-\mathbf{k},\mathbf{k}') &= -V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}'), \quad (1.36) \\ V_{s_1s_2s_4s_3}(\mathbf{k},-\mathbf{k}') &= -V_{s_1s_2s_3s_4}(\mathbf{k}',\mathbf{k}). \quad (1.37) \end{aligned}$$

Also, since V is hermitian, one has

$$V^*_{s_4s_3s_2s_1}(\mathbf{k},\mathbf{k}') = V_{s_1s_2s_3s_4}(\mathbf{k}',\mathbf{k}). \quad (1.38)$$

In the mean-field approximation,

$$\begin{aligned} V_{MF} &= \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}')\langle c^\dagger_{ks_1} c^\dagger_{-k,s_2}\rangle c_{-k's_3} c_{k's_4} \\ &+ \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}') c^\dagger_{ks_1} c^\dagger_{-k,s_2}\langle c_{-k's_3} c_{k's_4}\rangle, \end{aligned} \quad (1.39)$$

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

$$\bar{\Delta}_{ss'}(\mathbf{k}) = \sum_{\mathbf{k}'} V_{ss's_3s_4}\langle c_{-k's_3} c_{k's_4}\rangle. \quad (1.40)$$

Thus,

$$\begin{aligned} V_{MF} &= \frac{1}{2}\sum_{\mathbf{k}} \bar{\Delta}^*_{s's}(\mathbf{k}) c_{-k's} c_{k's'} + \frac{1}{2}\sum_{\mathbf{k}} \bar{\Delta}_{ss'}(\mathbf{k}) c^\dagger_{ks} c^\dagger_{-ks'} \\ &= \frac{1}{2}\sum_k (\boldsymbol{\psi}^\dagger_k, \boldsymbol{\psi}_{-k}) \begin{pmatrix} 0 & \bar{\Delta}_k \\ \bar{\Delta}^\dagger_k & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\psi}^\dagger_{-k} \end{pmatrix} \end{aligned} \quad (1.41)$$

This gives the off-diagonal terms in Eq. (1.4).

With the symmetry in Eq. (1.36), we have

$$\begin{aligned} \bar{\Delta}_{ss'}(-\mathbf{k}) &= \sum_{\mathbf{k}'} V_{ss's_3s_4}(-\mathbf{k},\mathbf{k}')\langle c_{-k's_3} c_{k's_4}\rangle \quad (1.42) \\ &= -\sum_{\mathbf{k}'} V_{s'ss_3s_4}(\mathbf{k},\mathbf{k}')\langle c_{-k's_3} c_{k's_4}\rangle \quad (1.43) \\ &= -\bar{\Delta}_{s's}(\mathbf{k}). \quad (1.44) \end{aligned}$$

This is Eq. (1.29). From this general argument, one can see that Eq. (1.29) is valid for any type of pairing $(s, p, d\cdots)$ and their mixings.

C. Bogoliubov-Valatin transformation

We now solve the eigenenergies 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 that is similar to an unitary matrix,

$$\Delta_k \Delta_k^\dagger = \bar{\Delta}_k \bar{\Delta}_k^\dagger = \alpha_k 1. \tag{1.45}$$

Since

$$\bar{\Delta}_k \bar{\Delta}_k^\dagger = \mathbf{d}_k \cdot \mathbf{d}_k^* + i\mathbf{d}_k \times \mathbf{d}_k^* \cdot \boldsymbol{\sigma}, \tag{1.46}$$

an unitary state has

$$\alpha_k = |\mathbf{d}_k|^2, \ \mathbf{d}_k \times \mathbf{d}_k^* = 0. \tag{1.47}$$

This is so if $\mathbf{d}(\mathbf{k})$ is a real-valued vector, or if (Re $\mathbf{d}_k$)$\times$(Im $\mathbf{d}_k$) $= 0$. The polar phase and the B-phase in Eqs. (1.25) and (1.27) both belong to this class of states. For the A-phase,

$$\mathbf{d}_k = \Delta_0(\hat{\mathbf{e}}_1 + i\hat{\mathbf{e}}_2)\cdot\mathbf{k}\ \hat{\mathbf{z}}, \tag{1.48}$$

in which $\hat{\mathbf{z}}$ is an unit vector in spin space, and it is not an unitary state.

For a unitary states, the spin of a Cooper pair is always perpendicular to its $\mathbf{d}$-vector. For example, for the polar phase, the spin is lying on the $\hat{\mathbf{e}}_1$-$\hat{\mathbf{e}}_2$-plane; for the B-phase, the spin is perpendicular to $\mathbf{k}$.

For a non-unitary state, such as the A-phase with a complex-valued $\mathbf{d}$-vector, the spin would precess around $i\mathbf{d}_k \times \mathbf{d}_k^* \simeq$ (Re $\mathbf{d}_k$) $\times$ (Im $\mathbf{d}_k$). On average the Cooper pairs are spin-polarized along this direction (see Prob. 1). As a result, the time-reversal symmetry is broken, and the excitation spectrum is no longer doubly degenerate (Sigrist and Ueda, 1991).

Recall that in Eq. (1.4), the Hamiltonian matrix is

$$\mathsf{H}(\mathbf{k}) = \begin{pmatrix} \varepsilon_k & \bar{\Delta}_k \\ \bar{\Delta}_k^\dagger & -\varepsilon_k \end{pmatrix}, \tag{1.49}$$

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

$$\mathsf{H}^2(\mathbf{k})\Phi_k = \begin{pmatrix} \varepsilon_k^2 + \bar{\Delta}_k\bar{\Delta}_k^\dagger & 0 \\ 0 & \varepsilon_k^2 + \bar{\Delta}_k^\dagger\bar{\Delta}_k \end{pmatrix}\Phi_k \tag{1.50}$$

$$= E_k^2\Phi_k. \tag{1.51}$$

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

$$E_k^\pm = \pm\sqrt{\varepsilon_k^2 + |\mathbf{d}_k|^2}, \tag{1.52}$$

which are doubly degenerate.

Write

$$\Phi_k = \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix}, \tag{1.53}$$

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

$$\begin{pmatrix} \mathbf{u}_k^{(1)} \\ \mathbf{v}_k^{(1)} \end{pmatrix} = A_k \begin{pmatrix} E_k + \varepsilon_k \\ 0 \\ \bar{\Delta}_{11}^*(\mathbf{k}) \\ \bar{\Delta}_{12}^*(\mathbf{k}) \end{pmatrix}, \tag{1.54}$$

$$\begin{pmatrix} \mathbf{u}_k^{(2)} \\ \mathbf{v}_k^{(2)} \end{pmatrix} = A_k \begin{pmatrix} 0 \\ E_k + \varepsilon_k \\ \bar{\Delta}_{21}^*(\mathbf{k}) \\ \bar{\Delta}_{22}^*(\mathbf{k}) \end{pmatrix}, \tag{1.55}$$

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

$$\begin{pmatrix} \mathbf{u}_k^{(3)} \\ \mathbf{v}_k^{(3)} \end{pmatrix} = A_k \begin{pmatrix} -\bar{\Delta}_{11}(\mathbf{k}) \\ -\bar{\Delta}_{21}(\mathbf{k}) \\ E_k + \varepsilon_k \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{-k}^{(1)*} \\ \mathbf{u}_{-k}^{(1)*} \end{pmatrix}, \tag{1.56}$$

$$\begin{pmatrix} \mathbf{u}_k^{(4)} \\ \mathbf{v}_k^{(4)} \end{pmatrix} = A_k \begin{pmatrix} -\bar{\Delta}_{12}(\mathbf{k}) \\ -\bar{\Delta}_{22}(\mathbf{k}) \\ 0 \\ E_k + \varepsilon_k \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{-k}^{(2)*} \\ \mathbf{u}_{-k}^{(2)*} \end{pmatrix}. \tag{1.57}$$

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

$$\Psi_k = \begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\psi}_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix}. \tag{1.58}$$

The basis that diagonalizes the Hamiltonian is written as,

$$\Gamma_k = \begin{pmatrix} \boldsymbol{\gamma}_k \\ \boldsymbol{\gamma}_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} b_{k\uparrow} \\ b_{k\downarrow} \\ b_{-k\uparrow}^\dagger \\ b_{-k\downarrow}^\dagger \end{pmatrix}. \tag{1.59}$$

They are connected by an unitary transformation,

$$\Psi_k = \mathsf{U}_k\Gamma_k = \begin{pmatrix} \mathsf{u}_k & \mathsf{v}_{-k}^* \\ \mathsf{v}_k & \mathsf{u}_{-k}^* \end{pmatrix}\Gamma_k, \tag{1.60}$$

in which each column of U_k is an eigenvector. For exmple, the elements of 2×2 matrices $\mathsf{u}_k, \mathsf{v}_k$ are,

$$\mathsf{u}_k = \begin{pmatrix} \mathbf{u}_k^{(1)} & \mathbf{u}_k^{(2)} \end{pmatrix} \tag{1.61}$$

$$\mathsf{v}_k = \begin{pmatrix} \mathbf{v}_k^{(1)} & \mathbf{v}_k^{(2)} \end{pmatrix}. \tag{1.62}$$

After the BV transformation, the Hamiltonian is diagonal,

$$\mathsf{H}_D(\mathbf{k}) = \mathsf{U}_k^\dagger\mathsf{H}(\mathbf{k})\mathsf{U}_k, \tag{1.63}$$

and

$$H = \frac{1}{2}\sum_k \Gamma_k^\dagger \mathsf{H}_D(\mathbf{k})\Gamma_k \quad (1.64)$$

$$= \frac{1}{2}\sum_{ks}(E_k^+ b_{ks}^\dagger b_{ks} + E_k^- b_{-ks} b_{-ks}^\dagger) \quad (1.65)$$

$$= \sum_{ks} E_k^+ b_{ks}^\dagger b_{ks} + \text{const.} \quad (1.66)$$

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

$$\bar{\Psi}_k = \begin{pmatrix} \bar{\boldsymbol{\psi}}_k \\ \bar{\boldsymbol{\psi}}_{-k}^\dagger \end{pmatrix} = \mathsf{S}\begin{pmatrix} \boldsymbol{\psi}_k \\ \boldsymbol{\psi}_{-k}^\dagger \end{pmatrix}, \quad (1.67)$$

where S is given in Eq. (1.3). After the transformation,

$$\bar{\Gamma}_k = \begin{pmatrix} \bar{\gamma}_k \\ \bar{\gamma}_{-k}^\dagger \end{pmatrix} = \mathsf{S}\begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix}. \quad (1.68)$$

It follows from Eq. (1.60) that, for the type-II basis,

$$\bar{\Psi}_k = \mathsf{S}\mathsf{U}_k\mathsf{S}^{-1}\bar{\Gamma}_k \quad (1.69)$$

$$= \begin{pmatrix} \mathsf{u}_k & \mathsf{v}_{-k}^*(-i\sigma_y) \\ i\sigma_y\mathsf{v}_k & \sigma_y\mathsf{u}_{-k}^*\sigma_y \end{pmatrix}\bar{\Gamma}_k, \quad (1.70)$$

where $\mathsf{u}_k, \mathsf{v}_k$ are defined in Eqs. (1.61),(1.62).

D. PH and TR symmetries

1. 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. (1.54) to $(\mathbf{u}_k^{(3)}, \mathbf{v}_k^{(3)})^T$ in Eq. (1.56). That is,

$$\begin{pmatrix} \mathbf{u}_k^{(1)} \\ \mathbf{v}_k^{(1)} \end{pmatrix} \to \mathsf{P}\begin{pmatrix} \mathbf{u}_k^{(1)} \\ \mathbf{v}_k^{(1)} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_{-k}^{(3)} \\ \mathbf{v}_{-k}^{(3)} \end{pmatrix}. \quad (1.71)$$

Therefore, for the type-I basis,

$$\mathsf{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K = \tau_x K \otimes 1. \quad (1.72)$$

This applies to the other pair, $(\mathbf{u}_k^{(2)}, \mathbf{v}_k^{(2)})^T$ in Eq. (1.55) maps to $(\mathbf{u}_{-k}^{(4)}, \mathbf{v}_{-k}^{(4)})^T$ in Eq. (1.57) as well. One can check that, $\mathsf{P}^2 = 1$, and

$$\mathsf{P}\mathsf{H}(\mathbf{k})\mathsf{P}^{-1} = -\mathsf{H}(-\mathbf{k}). \quad (1.73)$$

The PH operator for the type-II basis is

$$\mathsf{S}\mathsf{P}\mathsf{S}^{-1} = \begin{pmatrix} 0 & -i\sigma_y \\ i\sigma_y & 0 \end{pmatrix} K = \tau_y \otimes \sigma_y K. \quad (1.74)$$

2. Time-reversal transformation

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

$$\mathsf{T} = 1 \otimes i\sigma_y K = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix} K, \quad (1.75)$$

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

$$\begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} \to \mathsf{T}\begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} = \begin{pmatrix} i\sigma_y\mathbf{u}_k^* \\ i\sigma_y\mathbf{v}_k^* \end{pmatrix} \quad (1.76)$$

The Hamiltonian transforms as,

$$\mathsf{T}\mathsf{H}(\mathbf{k})\mathsf{T}^{-1} = \mathsf{H}(-\mathbf{k}). \quad (1.77)$$

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

$$\Psi_k \to \mathsf{T}\Psi_k, \quad (1.78)$$

one can infer that,

$$\bar{\Psi}_k \to \mathsf{S}\mathsf{T}\mathsf{S}^{-1}\bar{\Psi}_k. \quad (1.79)$$

Therefore, from Eqs. (1.67) and (1.75), the TR operator for the type-II basis is

$$\mathsf{S}\mathsf{T}\mathsf{S}^{-1} = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix} K, \quad (1.80)$$

which is the same as that of the type-I basis.

3. Symmetry transformation of field operator

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

$$\mathsf{P} = \mathsf{U}_P K, \ \ \mathsf{T} = \mathsf{U}_T K, \quad (1.81)$$

where U_P and U_T are unitary operators, and K is complex-conjugate operator. It is known that $\mathsf{P}^2 = -1$ for s-wave SC, $\mathsf{P}^2 = 1$ for p-wave SC, $\mathsf{T}^2 = -1$ for fermions, and

$$\mathsf{P}\mathsf{H}(\mathbf{k})\mathsf{P}^{-1} = -\mathsf{H}(-\mathbf{k}), \quad (1.82)$$

$$\mathsf{T}\mathsf{H}(\mathbf{k})\mathsf{T}^{-1} = \mathsf{H}(-\mathbf{k}). \quad (1.83)$$

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

$$P\psi_\alpha P^{-1} = \sum_\beta (\mathsf{U}_P^*)_{\alpha\beta}\psi_\beta^\dagger, \quad (1.84)$$

$$T\psi_\alpha T^{-1} = \sum_\beta (\mathsf{U}_T)_{\alpha\beta}\psi_\beta. \quad (1.85)$$

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

$$PHP^{-1} = H, \quad (1.86)$$
$$THT^{-1} = H. \quad (1.87)$$

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

E. Real space formulation

Without SC pairing, the real-space Hamiltonian is,

$$h_0 = \sum_s \int d^D r \boldsymbol{\psi}_s^\dagger(\mathbf{r}) \mathsf{h}_0(\mathbf{r}) \boldsymbol{\psi}_s(\mathbf{r}), \quad (1.88)$$
$$\mathsf{h}_0 = \frac{p^2}{2m} + V(\mathbf{r}) + \alpha \boldsymbol{\sigma} \times \mathbf{p} \cdot \mathbf{E} + \cdots - \mu. \quad (1.89)$$

The interaction term is

$$V = \frac{1}{2} \sum_{ss'} \int d^D r d^D r' \mathcal{V}(\mathbf{r} - \mathbf{r}') \psi_s^\dagger(\mathbf{r}) \psi_{s'}^\dagger(\mathbf{r}') \psi_{s'}(\mathbf{r}') \psi_s(\mathbf{r}). \quad (1.90)$$

With the mean-field approximation, one has

$$V_{MF} = \frac{1}{2} \sum_{ss'} \int d^D r d^D r' \bar{\Delta}_{ss'}(\mathbf{r}, \mathbf{r}') \psi_s^\dagger(\mathbf{r}) \psi_{s'}^\dagger(\mathbf{r}') + h.c., \quad (1.91)$$

where

$$\bar{\Delta}_{ss'}(\mathbf{r}, \mathbf{r}') \equiv \mathcal{V}(\mathbf{r} - \mathbf{r}') \langle \psi_{s'}(\mathbf{r}') \psi_s(\mathbf{r}) \rangle. \quad (1.92)$$

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

$$\mathsf{H}_0 = \begin{pmatrix} \mathsf{h}_0(\mathbf{r}) & 0 \\ 0 & -\mathsf{h}_0^*(\mathbf{r}) \end{pmatrix}, \quad (1.93)$$
$$\Delta_{4\times 4}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} 0 & \bar{\Delta}(\mathbf{r}, \mathbf{r}') \\ \bar{\Delta}^\dagger(\mathbf{r}, \mathbf{r}') & 0 \end{pmatrix}, \quad (1.94)$$

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

$$H = \frac{1}{2} \int d^D r d^D r' \Psi^\dagger(\mathbf{r}) [\mathsf{H}_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') + \Delta_{4\times 4}(\mathbf{r}, \mathbf{r}')] \Psi(\mathbf{r}'). \quad (1.95)$$

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

$$\mathsf{H}_0 = \begin{pmatrix} \mathsf{h}_0(\mathbf{r}) & 0 \\ 0 & -\sigma_y \mathsf{h}_0^*(\mathbf{r}) \sigma_y \end{pmatrix}, \quad (1.96)$$
$$\Delta_{4\times 4}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} 0 & \Delta(\mathbf{r}, \mathbf{r}') \\ \Delta^\dagger(\mathbf{r}, \mathbf{r}') & 0 \end{pmatrix}. \quad (1.97)$$

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

$$\begin{pmatrix} \mathbf{v}^*(\mathbf{r}) \\ \mathbf{u}^*(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \mathbf{u}(\mathbf{r}) \\ \mathbf{v}(\mathbf{r}) \end{pmatrix}. \quad (1.98)$$

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

$$\Psi_M(\mathbf{r}) = \begin{pmatrix} \mathbf{u}(\mathbf{r}) \\ \mathbf{u}^*(\mathbf{r}) \end{pmatrix} \quad (1.99)$$

Its time-reversed state is

$$\mathsf{T}\Psi_M(\mathbf{r}) = \begin{pmatrix} i\sigma_y \mathbf{u}^*(\mathbf{r}) \\ i\sigma_y \mathbf{u}(\mathbf{r}) \end{pmatrix}, \quad (1.100)$$

which is an energy eigenstate if the Hamiltonian has TRS.

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

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

$$\Psi_M(\mathbf{r}) = \begin{pmatrix} \mathbf{u}(\mathbf{r}) \\ i\sigma_y \mathbf{u}^*(\mathbf{r}) \end{pmatrix}. \quad (1.101)$$

Its time-reversed state is

$$\mathsf{T}\Psi_M(\mathbf{r}) = \begin{pmatrix} i\sigma_y \mathbf{u}^*(\mathbf{r}) \\ \mathbf{u}(\mathbf{r}) \end{pmatrix}, \quad (1.102)$$

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

Exercise:

1. Show that in a p-wave SC, the expectation value of the spin of a Cooper pair is (Mineev and Samokhin, 1999)

$$\langle \mathbf{S}_k \rangle \equiv \int \frac{d\Omega}{4\pi} \mathrm{tr} \left(\bar{\Delta}_k^\dagger \frac{\hbar}{2} \boldsymbol{\sigma} \bar{\Delta}_k \right) \quad (1.103)$$
$$= i\hbar \int \frac{d\Omega}{4\pi} \mathbf{d}_k \times \mathbf{d}_k^*. \quad (1.104)$$

2. Show that the eigenvectors of the 4×4 Hamiltonian matrix in Eq.(1.49) (with $d_0 = 0$) are Eqs. (1.54),(1.55), (1.56),(1.57). To get the eigenvector in Eq. (1.54), for example, one can choose $\mathbf{u}_k^{(1)} = (1,0)^T$, solve for $\mathbf{v}_k^{(1)}$, then normalize the eigenvector.
3. What are the PH operators for a four-component s-wave SC state in type-I and type-II bases?

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