Lecture notes on topological insulators

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CONTENTS

I. TOPOLOGICAL SUPERCONDUCTOR WITH TIME-REVERSAL SYMMETRY

After establishing the 4-component formulation, we now discuss spinful p-wave SC with TRS. That is, a system with $P^2 = 1, T^2 = -1$

A. PH and TR Symmetries of the Hamiltonian matrix

1. PH symmetry

Under the type-I basis, the PH operator is $\mathsf{P} = \tau_x K \otimes 1$ (see previous Chap). We write a general 4×4 Hamiltonian matrix as,

$$\mathsf{H}_k = \begin{pmatrix} \mathsf{h}_k & \mathsf{g}_k \\ \mathsf{g}_k^\dagger & \mathsf{h}'_k \end{pmatrix}. \tag{1.1}$$

Then $\mathsf{P}\mathsf{H}_k\mathsf{P}^{-1} = -\mathsf{H}_{-k}$ gives

$$\begin{pmatrix} \mathsf{h}'^*_k & \mathsf{g}_k^\dagger \\ \mathsf{g}_k^* & \mathsf{h}_k^* \end{pmatrix} = \begin{pmatrix} -\mathsf{h}_{-k} & -\mathsf{g}_{-k} \\ -\mathsf{g}_{-k}^\dagger & -\mathsf{h}'_{-k} \end{pmatrix}. \tag{1.2}$$

Therefore,

$$\begin{aligned} \mathsf{h}'_k &= -\mathsf{h}^*_{-k}, & (1.3)\\ \mathsf{g}_k^T &= -\mathsf{g}_{-k}. & (1.4) \end{aligned}$$

For the Hamiltonian matrix in Eq. (??), $\mathsf{g}_k = \bar{\Delta}_k$, and Eq. (1.4) is merely a restatement of Eq. (??), $\bar{\Delta}^\dagger(\mathbf{k}) = -\bar{\Delta}^*(-\mathbf{k})$. The Hamiltonian matrix with PHS is thus of the form,

$$\mathsf{H}_k = \begin{pmatrix} \mathsf{h}_k & \mathsf{g}_k \\ \mathsf{g}_k^\dagger & -\mathsf{h}^*_{-k} \end{pmatrix}. \tag{1.5}$$

For type-II basis, $\mathsf{P} = \tau_y \otimes \sigma_y K$, and it gives the following constraints,

$$\begin{aligned} \mathsf{h}'_k &= -\sigma_y \mathsf{h}^*_{-k}\sigma_y, & (1.6)\\ \mathsf{g}_k^T &= \sigma_y \mathsf{g}_{-k}\sigma_y. & (1.7) \end{aligned}$$

The Hamiltonian matrix with PHS is thus of the form,

$$\mathsf{H}_k = \begin{pmatrix} \mathsf{h}_k & \mathsf{g}_k \\ \mathsf{g}_k^\dagger & -\sigma_y\mathsf{h}^*_{-k}\sigma_y \end{pmatrix}. \tag{1.8}$$

2. TR symmetry

For both types of bases, the TR operator for p-wave SC is $\mathsf{T} = 1 \otimes i\sigma_y K$ (see previous Chap). Then $\mathsf{T}\mathsf{H}_k\mathsf{T}^{-1} = \mathsf{H}_{-k}$ gives

$$\begin{pmatrix} \sigma_y \mathsf{h}_k^* \sigma_y & \sigma_y \mathsf{g}_k^* \sigma_y \\ \sigma_y \mathsf{g}_k^T \sigma_y & \sigma_y \mathsf{h}'^*_k \sigma_y \end{pmatrix} = \begin{pmatrix} \mathsf{h}_{-k} & \mathsf{g}_{-k} \\ \mathsf{g}_{-k}^\dagger & \mathsf{h}'_{-k} \end{pmatrix}. \tag{1.9}$$

Therefore,

$$\begin{aligned} \sigma_y \mathsf{h}_k^* \sigma_y &= \mathsf{h}_{-k}, \text{ (same for } \mathsf{h}') & (1.10)\\ \sigma_y \mathsf{g}_k^* \sigma_y &= \mathsf{g}_{-k}. & (1.11) \end{aligned}$$

B. Chiral symmetry

The product of the PH operator and the TR operator is called the **chiral symmetry operator** S,

$$\mathsf{S} = \mathsf{P}\mathsf{T}, \tag{1.12}$$

which is an unitary operator. Its square, S^2, can be ± 1, depending on the signs of P^2 and T^2. But we usually only take $\mathsf{S}^2 = 1$, after redefining the phase of S (for $\mathsf{S}^2 = -1$, redefine $\mathsf{S} = \pm i\mathsf{P}\mathsf{T}$). Note that similar phase shift would not change the signs of P^2, T^2.

If a system has both PHS and TRS, then

$$\mathsf{S}\mathsf{H}_k\mathsf{S}^{-1} = \mathsf{P}\mathsf{T}\mathsf{H}_k\mathsf{T}^{-1}\mathsf{P}^{-1} = -\mathsf{H}_k. \tag{1.13}$$

That is, S is an unitary operator that *anti-commutes* with the Hamiltonian. In general, any unitary operator that anti-commutes with the Hamiltonian qualifies as a chiral symmetry operator, and the system is said to have the chiral symmetry. Note that a system cannot have chiral symmetry if PH or TR symmetry is broken. However, when neither of the PH nor TR symmetry exists, a system can still have chiral symmetry.

If H_k has chiral symmetry, then its eigenvalues would come in pairs with opposite signs:

$$\begin{aligned} \mathsf{H}_k\Phi_{nk} &= \varepsilon_{nk}\Phi_{nk}, & (1.14)\\ \rightarrow \quad \mathsf{H}_k(\mathsf{S}\Phi_{nk}) &= -\varepsilon_{nk}(\mathsf{S}\Phi_{nk}). & (1.15)\end{aligned}$$

This implies that the order N of the H matrix is even. Under the basis that block-diagonalizes S, a Hamiltonian with chiral symmetry has the standard form (see Prob. 1),

$$\mathsf{H}_k = \begin{pmatrix} 0 & \mathsf{f}_k \\ \mathsf{f}_k^\dagger & 0 \end{pmatrix}. \quad (1.16)$$

The tight-binding Hamiltonian of a bipartite lattice with only nearest-neighbor couplings (sublattice-A couples with sublattice-B) can always be put in this form (if the on-site energies are all the same). Because we can assign the upper half of the basis to sublattice-A, and the lower half to sublattice-B. As a result, there must exist an unitary matrix S that anti-commutes with H. That is, such a bipartite lattice has the chiral symmetry. A specific example that has this symmetry would be the 1D Su-Schrieffer-Heeger model (in its original form).

Suppose the eigenstates of H are $(\boldsymbol{\psi}_n, \boldsymbol{\phi}_n)^T, n = 1, \cdots, N$, then

$$\begin{pmatrix} 0 & \mathsf{f} \\ \mathsf{f}^\dagger & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{\psi}_n^\pm \\ \boldsymbol{\phi}_n^\pm \end{pmatrix} = \pm\varepsilon_n \begin{pmatrix} \boldsymbol{\psi}_n^\pm \\ \boldsymbol{\phi}_n^\pm \end{pmatrix}, \varepsilon_n \geq 0. \quad (1.17)$$

Both $\boldsymbol{\psi}_n$ and $\boldsymbol{\phi}_n$ are assumed to be normalized, $\boldsymbol{\psi}_n^\dagger\boldsymbol{\psi}_n = \boldsymbol{\phi}_n^\dagger\boldsymbol{\phi}_n = 1$. Then the normalized eigenstates are (for $\varepsilon_n \neq 0$),

$$|\Psi_n^\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \boldsymbol{\psi}_n^\pm \\ \boldsymbol{\phi}_n^\pm \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \boldsymbol{\psi}_n \\ \pm\frac{\mathsf{f}^\dagger}{\varepsilon_n}\boldsymbol{\psi}_n \end{pmatrix}. \quad (1.18)$$

Also, for either sign of the eigenvalues,

$$\begin{aligned} \mathsf{f}\,\mathsf{f}^\dagger\boldsymbol{\psi}_n &= \varepsilon_n^2\boldsymbol{\psi}_n, & (1.19)\\ \mathsf{f}^\dagger\mathsf{f}\,\boldsymbol{\phi}_n &= \varepsilon_n^2\boldsymbol{\phi}_n. & (1.20)\end{aligned}$$

As an example, consider the 4×4 Hamiltonian in Eq. (1.1) with both PHS and TRS ($P^2 = 1, T^2 = -1$). Under the type-I basis,

$$\begin{aligned} \mathsf{S} \equiv -i\mathsf{P}\mathsf{T} &= \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} & (1.21)\\ &= \mathsf{U}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\mathsf{U}^{-1}, & (1.22)\end{aligned}$$

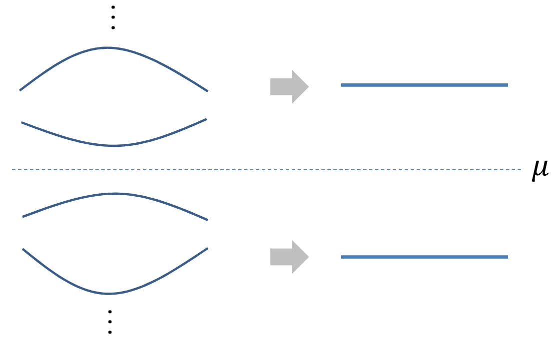

FIG. 1 The energy gap between filled states and empty states remains open during the spectral flattening.

where

$$\mathsf{U} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & \sigma_y \\ \sigma_y & -1 \end{pmatrix}. \quad (1.23)$$

With both PHS and TRS, one can show that (type-I basis),

$$\mathsf{U}\mathsf{H}_k\mathsf{U}^{-1} = \begin{pmatrix} 0 & \mathsf{h}_k\sigma_y - \mathsf{g}_k \\ \sigma_y\mathsf{h}_k - \mathsf{g}_k^\dagger & 0 \end{pmatrix}. \quad (1.24)$$

That is,

$$\mathsf{f}_k = \mathsf{h}_k\sigma_y - \mathsf{g}_k. \quad (1.25)$$

After the chiral rotation U, the PH operator and the TR operator become,

$$\begin{aligned} \mathsf{U}\mathsf{P}\mathsf{U}^{-1} &= \begin{pmatrix} 0 & -K \\ -K & 0 \end{pmatrix} = -\sigma_x K \otimes 1, & (1.26)\\ \mathsf{U}\mathsf{T}\mathsf{U}^{-1} &= \begin{pmatrix} 0 & -iK \\ iK & 0 \end{pmatrix} = \sigma_y K \otimes 1. & (1.27)\end{aligned}$$

For the Hamiltonian with the general form in Eq. (1.1), Eqs. (1.3) and (1.4) remain valid, while Eqs. (1.10) and (1.11) become

$$\begin{aligned} \mathsf{h}_k^* &= \mathsf{h}_{-k}, & (1.28)\\ \mathsf{g}_k^T &= -\mathsf{g}_{-k}. & (1.29)\end{aligned}$$

Specifically, for the Hamiltonian in Eq. (1.16), $\mathsf{h}_k = 0, \mathsf{g}_k = \mathsf{f}_k$, so that

$$\mathsf{f}_k^T = -\mathsf{f}_{-k}. \quad (1.30)$$

C. Topology of system with chiral symmetry

We first discuss systems with only chiral symmetry (class AIII). Other symmetry would impose further constraint on the Hamiltonian matrix, which would also be discussed.

1. Spectral flattening

If we are only interested in topological property, then the trick of **spectral flattening** can be employed to simplify a problem (see Fig. 1). That is, all the valence bands collapse to one flat band, similarly for the conduction bands,

$$\pm\varepsilon_{nk} \to \pm 1. \tag{1.31}$$

The energy hap between filled bands and empty bands remain open during the continuous deformation, so that the topology of the system is not changed.

The operators of projection onto two flat bands are defined as,

$$\begin{aligned} \mathsf{P}_k^{\pm} &= \sum_{n=1}^{N} |\Psi_n^{\pm}\rangle\langle\Psi_n^{\pm}| &(1.32)\\ &= \frac{1}{2}\sum_{n=1}^{N} \begin{pmatrix} \boldsymbol{\psi}_n^{\pm} \\ \boldsymbol{\phi}_n^{\pm} \end{pmatrix} \left(\boldsymbol{\psi}_n^{\pm\dagger}, \boldsymbol{\phi}_n^{\pm\dagger}\right). &(1.33) \end{aligned}$$

The *flattened* Hamiltonian $\mathsf{H}_k \to \mathsf{Q}_k$ can be written as,

$$\begin{aligned} \mathsf{Q}_k &= \sum_{n=1}^{N} \left(|\Psi_n^{+}\rangle\langle\Psi_n^{+}| - |\Psi_n^{-}\rangle\langle\Psi_n^{-}|\right) &(1.34)\\ &= 1 - 2\mathsf{P}_k^{-} &(1.35)\\ &= \sum_{n=1}^{N} \begin{pmatrix} 0 & \boldsymbol{\psi}_n\boldsymbol{\psi}_n^{\dagger}\frac{\mathsf{f}}{\varepsilon_n} \\ \frac{\mathsf{f}^{\dagger}}{\varepsilon_n}\boldsymbol{\psi}_n\boldsymbol{\psi}_n^{\dagger} & 0 \end{pmatrix} &(1.36)\\ &= \begin{pmatrix} 0 & \mathsf{q}_k \\ \mathsf{q}_k^{\dagger} & 0 \end{pmatrix}, &(1.37) \end{aligned}$$

with

$$\mathsf{q}_k = \sum_{n=1}^{N} \boldsymbol{\psi}_{nk}\boldsymbol{\psi}_{nk}^{\dagger}\frac{\mathsf{f}_k}{\varepsilon_{nk}}. \tag{1.38}$$

The eigenstates of Q_k with eigenvalues ±1 now become (see Eq. (1.18)),

$$|\Phi_{nk}^{\pm}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \boldsymbol{\eta}_n \\ \pm\mathsf{q}_k^{\dagger}\boldsymbol{\eta}_n \end{pmatrix}, \text{ where } (\boldsymbol{\eta}_n)_a = \delta_{na};\ a = 1,\cdots,N. \tag{1.39}$$

2. Singular-value decomposition

With the **singular-value decomposition** (SVD), which applies to *any* complex-valued matrix, the off-diagonal blocks f_k can be decomposed as,

$$\mathsf{f}_k = \mathsf{u}_k^{\dagger}\mathsf{d}_k\mathsf{v}_k, \tag{1.40}$$

where d_k is diagonal with (non-negative) real elements, and u_k, v_k are unitary. It follows that,

$$\begin{aligned} \mathsf{H}_k &= \begin{pmatrix} 0 & \mathsf{u}_k^{\dagger}\mathsf{d}_k\mathsf{v}_k \\ \mathsf{v}_k^{\dagger}\mathsf{d}_k\mathsf{u}_k & 0 \end{pmatrix} &(1.41)\\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} \mathsf{u}_k^{\dagger} & \mathsf{u}_k^{\dagger} \\ \mathsf{v}_k^{\dagger} & -\mathsf{v}_k^{\dagger} \end{pmatrix}\begin{pmatrix} \mathsf{d}_k & 0 \\ 0 & -\mathsf{d}_k \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} \mathsf{u}_k & \mathsf{v}_k \\ \mathsf{u}_k & -\mathsf{v}_k \end{pmatrix}. \end{aligned}$$

The $N\times N$ diagonal matrix is flanked by unitary matrices. Therefore, the eigenvalues of H_k are the eigenvalues of d_k (positive) and $-\mathsf{d}_k$ (negative). After spectral flattening, $\pm\mathsf{d}_k \to \pm1$, and

$$\mathsf{q}_k = \mathsf{u}_k^{\dagger}\mathsf{v}_k \ \in U(N). \tag{1.42}$$

The topology of the chiral system can be characterized by the winding number of the mapping $\mathbf{k}(\in BZ) \to \mathsf{q}_k$.

3. Topology

If the BZ (a torus) can be replaced by a sphere S^D, that is, the effect of the lattice can be ignored, then we can rely on the homotopy theory to find out the winding number. For example, it is known that (Actor, 1979),

$$\begin{aligned} \pi_1(U(N)) &= Z \text{ for } N \geq 1 &(1.43)\\ \pi_2(U(N)) &= 0 \text{ for } N \geq 1 &(1.44)\\ (\text{In fact, } \pi_2(G) &= 0 \text{ for any Lie group } G)\\ \pi_3(U(1)) = 0, \pi_3(U(N)) &= Z \text{ for } N \geq 2. &(1.45) \end{aligned}$$

In general, for a large enough N, the result is "stabilized" (i.e., independent of N),

$$\pi_{2d}(\mathsf{U}) = 0,\ \pi_{2d+1}(\mathsf{U}) = Z. \tag{1.46}$$

Therefore, we expect a chiral system in *even* dimension to be topologically trivial. In *odd* dimension, the topology is characterized by the winding number,

$$\begin{aligned} \nu_{2d+1} &= N_d\int_{BZ} d^{2d+1}k\ \epsilon_{ab\cdots}\mathrm{tr}\left(\mathsf{q}^{\dagger}\partial_a\mathsf{q}\mathsf{q}^{\dagger}\partial_b\mathsf{q}\cdots\right)\\ &= N_d\int_{BZ}\mathrm{tr}\left(\mathsf{q}^{\dagger}d\mathsf{q}\right)^{2d+1}, &(1.47)\\ N_d &= -\frac{d!}{(2d+1)!(2\pi i)^{d+1}}. &(1.48) \end{aligned}$$

The second integral is written in differential form.

For example,

$$\begin{aligned} \nu_1 &= \frac{i}{2\pi}\int_{BZ} dk\mathrm{tr}\left(\mathsf{q}^{\dagger}\partial_k\mathsf{q}\right) &(1.49)\\ &= \frac{1}{2\pi i}\int_{BZ} dk\partial_k \ln\det\mathsf{q}_k, &(1.50) \end{aligned}$$

and

$$\nu_3 = \frac{1}{24\pi^2}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{q}^{\dagger}\partial_a\mathsf{q}\mathsf{q}^{\dagger}\partial_b\mathsf{q}\mathsf{q}^{\dagger}\partial_c\mathsf{q}\right). \tag{1.51}$$

For more details, see the Supp material of Schnyder and Ryu, 2011. Condensed matter systems with only chiral symmetry are rare in real world, however.

4. Additional symmetry

If in addition to chiral symmetry, the system has PHS and TRS, $\mathsf{P}^2 = 1, \mathsf{T}^2 = -1$ (class DIII), then from either of the symmetries, we get $\mathsf{f}_k^T = -\mathsf{f}_{-k}$ (Eq. (1.30)), or $\mathsf{q}_k^T = -\mathsf{q}_{-k}$. As a result, the winding number could be zero, instead of Z, in some odd dimensions. This is proved as follows (Ryu *et al.*, 2010). First,

$$\mathrm{tr}\left[\mathsf{q}^\dagger(\mathbf{k})\frac{\partial \mathsf{q}(\mathbf{k})}{\partial k_a}\ \mathsf{q}^\dagger(\mathbf{k})\frac{\partial}{\partial k_b}\mathsf{q}(\mathbf{k})\cdots\right] \tag{1.52}$$

$$= \mathrm{tr}\left[\mathsf{q}^*(-\mathbf{k})\frac{\partial \mathsf{q}^T(-\mathbf{k})}{\partial k_a}\ \mathsf{q}^*(-\mathbf{k})\frac{\partial}{\partial k_b}\mathsf{q}^T(-\mathbf{k})\cdots\right] \tag{1.53}$$

$$= \mathrm{tr}\left[\mathsf{q}^\dagger(-\mathbf{k})\frac{\partial \mathsf{q}(-\mathbf{k})}{\partial(-k_a)}\ \mathsf{q}^\dagger(-\mathbf{k})\frac{\partial}{\partial(-k_b)}\mathsf{q}(-\mathbf{k})\cdots\right]^*, \tag{1.54}$$

where we have used $\mathsf{q}^\dagger\partial_a\mathsf{q} = -(\partial_a\mathsf{q}^\dagger)\mathsf{q}$ in the last equation. It follows that,

$$\nu_{2d+1} = (-1)^{d+1}\nu^*_{2d+1}, \tag{1.55}$$

in which $(-1)^{d+1}$ comes from the imaginary number i in N_d. As a result, $\nu_{2d+1} = 0$ when $2d+1 = 1, 5, 9\cdots$.

Even though the winding number for class-DIII materials in dimension $D = 1, 2$ is zero, other topological characterization other than the winding number is possible. At a TRIM Λ, q_Λ is anti-symmetric, $\mathsf{q}_\Lambda^T = -\mathsf{q}_\Lambda$ (see Eq. 1.29). This reminds us of the sewing matrix of a topological insulator in Chap **??**. In fact, for a p-wave SC with TRS ($\mathsf{T}^2 = -1$), one can write down a similar Z_2 topological number (for $D = 1, 2$), as shown below. For $D = 3$, the topological number is given by the one in Eq. (1.51).

Following Schnyder and Ryu, 2011, define the sewing matrix,

$$w_{mn}(\mathbf{k}) = \langle\Phi_m^+(-\mathbf{k})|\mathsf{T}\Phi_n^+(\mathbf{k})\rangle, \tag{1.56}$$

in which (Eq. (1.27))

$$\mathsf{T} = \mathsf{U}(1\otimes i\sigma_y K)\mathsf{U}^{-1} = \sigma_y K\otimes 1. \tag{1.57}$$

As a result,

$$\begin{aligned} w_{mn}(\mathbf{k}) &= \frac{1}{2}(\boldsymbol{\eta}_m^\dagger, \boldsymbol{\eta}_m^\dagger\mathsf{q}_{-k})(\sigma_y K\otimes 1)\begin{pmatrix}\boldsymbol{\eta}_n\\ \mathsf{q}_k^\dagger\boldsymbol{\eta}_n\end{pmatrix}\\ &= q_{mn}^T(\mathbf{k})/i. \end{aligned} \tag{1.58}$$

Note that $m, n = 1, \cdots N$, and N is an even integer.

Analogous to the topological insulator, one can define a Kane-Mele index ν (see **??**),

$$(-1)^\nu = \prod_a \frac{\mathrm{Pf}\ [\mathsf{w}(\Lambda_a)]}{\sqrt{\det[\mathsf{w}(\Lambda_a)]}} \tag{1.59}$$

$$= \prod_a \frac{\mathrm{Pf}\ [\mathsf{q}^T(\Lambda_a)/i]}{\sqrt{\det[\mathsf{q}^T(\Lambda_a)/i]}} = \pm 1. \tag{1.60}$$

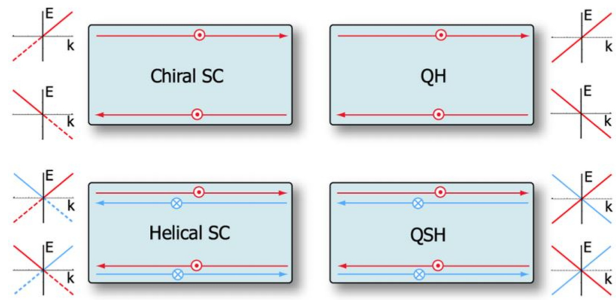

FIG. 2 Chiral superconductor, helical superconductor, and their edge states. Quantum Hall system and quantum spin Hall system and their edge states are also plotted for comparison. The figure is from Qi *et al.*, 2009.

D. 1D and 2D system

Recall that the QWZ model of QAHE breaks TRS and has chiral edge state. The BHZ model for QSHE, which consists of a QWZ model and its time-reversal partner, has TRS and helical edge state. Similarly, the spinless p-wave superconductors in previous chapters have chiral edge state and no TRS. Here we construct a SC with TRS from a pair of time-reversal conjugated p-wave superconductors (Fig. 2).

1. 1D and 2D model

In the Kitaev model of 1D p-wave SC, we have the Hamiltonian (see Eq. (**??**)),

$$\mathsf{h}(\mathbf{k}) = \begin{pmatrix} -t\cos k - \mu & i\Delta_0\sin k\\ -i\Delta_0\sin k & t\cos k + \mu\end{pmatrix}, \tag{1.61}$$

with the basis $(c_k, c_{-k}^\dagger)^T$. According to the recipe mentioned above, one can extend the basis to $(c_{k\uparrow}, c_{-k\uparrow}^\dagger, c_{k\downarrow}, c_{-k\downarrow}^\dagger)^T$, and construct a TRS SC with the Hamiltonian,

$$\begin{aligned} \mathsf{H}_0 &= \begin{pmatrix} \varepsilon_k & i\Delta_0\sin k & 0 & 0\\ -i\Delta_0\sin k & -\varepsilon_k & 0 & 0\\ 0 & 0 & \varepsilon_k & i\Delta_0\sin k\\ 0 & 0 & -i\Delta_0\sin k & -\varepsilon_k\end{pmatrix}\\ &= \varepsilon_k\ 1\otimes\tau_z - \Delta_0\sin k\ 1\otimes\tau_y, \end{aligned} \tag{1.62}$$

where $\varepsilon_k = -t\cos k - \mu$.

If the basis $(c_{k\uparrow}, c_{k\downarrow}, c_{-k\uparrow}^\dagger, c_{-k\downarrow}^\dagger)^T$ is used, then one first switches the 2nd and the 3rd rows, then switches the 2nd and the 3rd columns of the Hamiltonian matrix (i.e. switch the order of the product between $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$). Furthermore, one can add a spin-orbit (SO) coupling with strength α (Liu *et al.*, 2014), such that

$$\begin{aligned}\mathsf{H} &= \begin{pmatrix} \varepsilon_k & -i\alpha\sin k & i\Delta_0\sin k & 0 \\ i\alpha\sin k & \varepsilon_k & 0 & i\Delta_0\sin k \\ -i\Delta_0\sin k & 0 & -\varepsilon_k & i\alpha\sin k \\ 0 & -i\Delta_0\sin k & -i\alpha\sin k & -\varepsilon_k \end{pmatrix}, \\ &= \varepsilon_k\tau_z\otimes 1 - \Delta_0\sin k\ \tau_y\otimes 1 + \alpha\sin k\ \tau_z\otimes\sigma_y. \quad (1.63)\end{aligned}$$

It can be verified that such a Hamiltonian does have both PHS and TRS.

The 1D model above can be generalized to 2D as follows (Liu *et al.*, 2014),

$$\begin{aligned}\mathsf{H} &= \varepsilon_k\tau_z + \alpha\sin k_x\ \tau_z\otimes\sigma_y - \alpha\sin k_y\ \sigma_x \\ &- \Delta_0\sin k_x\ \tau_y + \Delta_0\sin k_y\ \tau_x\otimes\sigma_z, \quad (1.64)\end{aligned}$$

where $\varepsilon_k = -t(\cos k_x + \cos k_y) - \mu$. This corresponds to $\mathbf{d} = \Delta_0(-\sin k_y, \sin k_x, 0)$ (see Eq. (**??**)). Also, it can be shown that such a Hamiltonian does have both PHS and TRS. It reduces to the 1D model by setting $k_y = 0$.

Some remarks: Note that the normal-state Hamiltonian is of the form,

$$\mathsf{h}_k = \varepsilon_k + \boldsymbol{\ell}_{so}(\mathbf{k})\cdot\boldsymbol{\sigma}, \quad (1.65)$$

where $\boldsymbol{\ell}_{so}(\mathbf{k}) = \alpha(-\sin k_y, \sin k_x, 0)$, which is chosen to be parallel to $\mathbf{d}(\mathbf{k})$. If $\boldsymbol{\ell}$ is not parallel to $\mathbf{d}$, then the SO coupling may break the Cooper pairs (Schnyder and Ryu, 2011). The SC model here only has p-wave pairing. We have ignored possible s-wave pairing that could be induced by the SO coupling (more information in Sec I.E).

Noncentrosymmetric superconductors, such as the heavy-fermion material $CePt_3Si$, has intrinsic SO coupling. In reality, the energy scale of the SO coupling could be larger than the SC gap. See Yip, 2014 for more details.

2. Topological number

One can identify the blocks h_k and g_k defined in Eq. (1.1) as,

$$\begin{aligned}\mathsf{h}_k &= \varepsilon_k + \alpha\sin k_x\ \sigma_y - \alpha\sin k_y\ \sigma_x, \quad (1.66)\\ \mathsf{g}_k &= i\Delta_0\sin k_x + \Delta_0\sin k_y\ \sigma_z. \quad (1.67)\end{aligned}$$

It can be verified that Eqs. (1.3),(1.4),(1.10), and (1.11) are all satisfied. Also,

$$\begin{aligned}\mathsf{f}_k &= \mathsf{h}_k\sigma_y - \mathsf{g}_k \quad (1.68)\\ &= \varepsilon_k\sigma_y + (\alpha - i\Delta_0)\sin k_x - i(\alpha - i\Delta_0)\sin k_y\ \sigma_z.\end{aligned}$$

It follows that,

$$\begin{aligned}\mathsf{f}_k\mathsf{f}_k^\dagger &= \varepsilon_k^2 + (\alpha^2+\Delta_0^2)\left(\sin^2 k_x + \sin^2 k_y\right) \quad (1.69)\\ &- 2\alpha\varepsilon_k\begin{pmatrix} 0 & \sin k_y + i\sin k_x \\ \sin k_y - i\sin k_x & 0\end{pmatrix},\end{aligned}$$

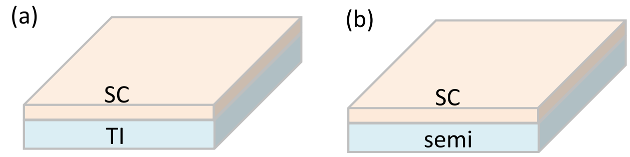

FIG. 3 Hybrid structure of (a) a superconductor and a topological insulator, (b) a superconductor and a semiconductor with SO coupling.

which has the eigenvalues,

$$\begin{aligned}\lambda_\pm(=\varepsilon_{k\pm}^2) &= \varepsilon_k^2 + (\alpha^2+\Delta_0^2)\left(\sin^2 k_x + \sin^2 k_y\right)\\ &\pm 2\alpha\varepsilon_k\sqrt{\sin^2 k_x + \sin^2 k_y}. \quad (1.70)\end{aligned}$$

The corresponding eigenvectors are,

$$\boldsymbol{\psi}_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm\frac{-\sin k_y + i\sin k_x}{\sqrt{\sin^2 k_x+\sin^2 k_y}}\end{pmatrix}. \quad (1.71)$$

Note that at TRIM, there are removable singularities and the eigenvectors remain finite. From these, we can get the flattened off-diagonal part q_Λ, and determine the Z_2 topological number ν.

It is left as an exercise (Prob. 2) to show that in 1D, $|\mu| < t$ is a topological phase with $\nu = 1$, while $|\mu| > t$ is a trivial phase with $\nu = 0$ (Liu *et al.*, 2014). The 2D case can also be dealt with in a similarly way.

E. Hybrid structure

P-wave superconductors are rare in nature. However, it is possible to have effective p-wave pairing using hybrid structures that combines s-wave SC with materials with SO coupling. This comes with two types: SC/TI, and SC/semi (see Fig. 3). They can be described within the same framework.

For the first type, there is a layer of SC on top of a TI. Because of the **proximity effect** (that is, the Cooper pairs would leak to the TI), the 2D surface-state electrons of TI would feel both the spin-momentum locking (see Chap **??**) and the superconductor pairing. Because of the spin-momentum locking, s-wave pairing could turn into effective p-wave pairing (Fu and Kane, 2008).

The TI can be replaced by a semiconductor with Rashba (or other type of) SO coupling (Alicea, 2010; Sau *et al.*, 2010). One difference between this setup with the one above is that, for the Rashba system, the chemical potential would inevitably cut through two Fermi surfaces (see Fig. 4).

First, we consider a general situation where a SC can have both s-wave and p-wave pairings (Santos *et al.*, 2010). Under the type-II basis, $\Psi_k = (c_{k\uparrow}, c_{k\downarrow}, c^\dagger_{-k\downarrow},$

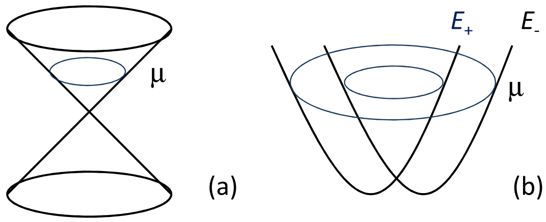

FIG. 4 The energy levels of (a) the surface electrons of topological insulator, (b) 2D electrons with Rashba SO coupling.

$-c^\dagger_{-k\uparrow})^T$, the Hamiltonian matrix is (see Eq. (1.8))

$$\mathsf{H}_k = \begin{pmatrix} \mathsf{h}_k & \Delta_k \\ \Delta_k^\dagger & -\sigma_y \mathsf{h}^T_{-k}\sigma_y \end{pmatrix}, \tag{1.72}$$

in which

$$\begin{aligned} \mathsf{h}_k &= \varepsilon^0_k - \mu + \boldsymbol{\ell}_k \cdot \boldsymbol{\sigma}, &(1.73)\\ \Delta_k &= d^0_k + \mathbf{d}_k \cdot \boldsymbol{\sigma}. &(1.74) \end{aligned}$$

For the surface electrons of TI, $\varepsilon^0_k = 0$ near a Dirac point; for Rashba electron, $\varepsilon^0_k = \hbar^2 k^2/2m^*$. The z-component of $\boldsymbol{\ell}_k$ is zero if TRS is not broken, while the other two components depend on actual materials used. We assume $\boldsymbol{\ell}_k \parallel \mathbf{d}_k$ for simplicity (Eq. (1.65) and below).

This two blocks can be written as

$$\begin{aligned} \mathsf{h}_k &= \begin{pmatrix} \varepsilon^0_k - \mu & \ell_k e^{-i\varphi_k} \\ \ell_k e^{i\varphi_k} & \varepsilon^0_k - \mu \end{pmatrix}, &(1.75)\\ \Delta_k &= \begin{pmatrix} \Delta_{ks} & \Delta_{kt} e^{-i\varphi_k} \\ \Delta_{kt} e^{i\varphi_k} & \Delta_{ks} \end{pmatrix}, &(1.76) \end{aligned}$$

where

$$e^{i\varphi_k} = \frac{\ell_{kx} + i\ell_{ky}}{\ell_k},\ \ \ell_k \equiv |\boldsymbol{\ell}_k| \neq 0. \tag{1.77}$$

The eigenvalues and eigenvectors of h_k are,

$$\begin{aligned} \varepsilon_{k\pm} &= \varepsilon^0_k - \mu \pm |\boldsymbol{\ell}_k|, &(1.78)\\ \boldsymbol{\psi}_{k\pm} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{i\varphi_k} \end{pmatrix}. &(1.79) \end{aligned}$$

In terms of second quantization,

$$\begin{pmatrix} c_{k+} \\ c_{k-} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & +e^{-i\varphi_k} \\ 1 & -e^{-i\varphi_k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix}, \tag{1.80}$$

or

$$\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ e^{i\varphi_k} & -e^{i\varphi_k} \end{pmatrix} \begin{pmatrix} c_{k+} \\ c_{k-} \end{pmatrix}, \tag{1.81}$$

$$\begin{pmatrix} c^\dagger_{-k\downarrow} \\ -c^\dagger_{-k\uparrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ e^{i\varphi_k} & -e^{i\varphi_k} \end{pmatrix} \begin{pmatrix} -e^{-i\varphi_k} c^\dagger_{-k+} \\ e^{-i\varphi_k} c^\dagger_{-k-} \end{pmatrix}. \tag{1.82}$$

Note that $\boldsymbol{\ell}_{-k} = -\boldsymbol{\ell}_k$, and $e^{i\varphi_{-k}} = -e^{i\varphi_k}$. Therefore, under time reversal, one has

$$\begin{aligned} \mathsf{T}\boldsymbol{\psi}_{k\uparrow} &= \boldsymbol{\psi}_{-k\downarrow}, &(1.83)\\ \mathsf{T}\boldsymbol{\psi}_{k\downarrow} &= -\boldsymbol{\psi}_{-k\uparrow}. &(1.84) \end{aligned}$$

It follows that

$$\mathsf{T}\boldsymbol{\psi}_{k\pm} = \pm e^{-i\varphi_{-k}} \boldsymbol{\psi}_{-k\pm}. \tag{1.85}$$

Note that the TR transformation does not flip the $\pm$-branch.

The Cooper pairs consist of TR-conjugate electrons, and

$$\Delta_{k\lambda} \sim \langle c_{-k\lambda} c_{k\lambda} \rangle,\ \lambda = \pm. \tag{1.86}$$

Define a new basis $\tilde{\Psi}_k = (c_{k+}, c_{k-}, e^{-i\varphi_{-k}} c^\dagger_{-k+}, -e^{-i\varphi_{-k}} c^\dagger_{-k-})^T$, which is related to the old one by an unitary transformation,

$$\Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\downarrow} \\ -c^\dagger_{-k\uparrow} \end{pmatrix} = \mathsf{U} \begin{pmatrix} c_{k+} \\ c_{k-} \\ e^{-i\varphi_{-k}} c^\dagger_{-k+} \\ -e^{-i\varphi_{-k}} c^\dagger_{-k-} \end{pmatrix} = \mathsf{U}\tilde{\Psi}_k. \tag{1.87}$$

Under the new basis,

$$\begin{aligned} H &= \sum_{\mathbf{k}} \Psi^\dagger_k \begin{pmatrix} \mathsf{h}_k & \Delta_k \\ \Delta^\dagger_k & -\sigma_y \mathsf{h}^T_{-k} \sigma_y \end{pmatrix} \Psi_k &(1.88)\\ &= \sum_{\mathbf{k}} \tilde{\Psi}^\dagger_k \begin{pmatrix} \tilde{\mathsf{h}}_k & \tilde{\Delta}_k \\ \tilde{\Delta}^\dagger_k & -\tilde{\mathsf{h}}^T_{-k} \end{pmatrix} \tilde{\Psi}_k, &(1.89) \end{aligned}$$

where

$$\begin{aligned} \tilde{\mathsf{h}}_k &= \begin{pmatrix} \varepsilon_{k+} & 0 \\ 0 & \varepsilon_{k-} \end{pmatrix}, &(1.90)\\ \tilde{\Delta}_k &= \begin{pmatrix} \Delta_{k+} & 0 \\ 0 & \Delta_{k-} \end{pmatrix}, &(1.91) \end{aligned}$$

and

$$\Delta_{k\pm} = d^0_k \pm |\mathbf{d}_k| = \Delta_{ks} \pm \Delta_{kt}. \tag{1.92}$$

Both blocks are diagonalized simultaneously since $\mathbf{d}_k \parallel \boldsymbol{\ell}_k$, see Eq. (1.65) and below.

After the diagonalization,

$$H = \sum_{k\lambda} \left[\varepsilon_{k\lambda} c^\dagger_{k\lambda} c_{k\lambda} + \lambda (e^{i\varphi_{-k}} \Delta_{k\lambda} c_{-k\lambda} c_{k\lambda} + h.c.) \right]. \tag{1.93}$$

It consists of decoupled subsystems with $\lambda = \pm$, and each subsystem resembles a spinless p-wave SC in Eq. (**??**).

Finally, the eigenvalues of the 4×4 Hamiltonian matrix are,

$$E_{k\lambda} = \pm\sqrt{\varepsilon^2_{k\lambda} + \Delta^2_{k\lambda}}. \tag{1.94}$$

If one of Δ_{ks}, Δ_{kt} is zero, then $|\Delta_{k+}| = |\Delta_{k-}|$, and the excitation spectrum is two-fold degenerate. The degeneracy is lifted if both are non-zero. Furthermore, particle-hole symmetry requires

$$\begin{aligned} \Delta_{-ks} &= \Delta_{ks},\ \Delta_{-kt} = \Delta_{kt} && (1.95)\\ \text{or}\ \ \Delta_{-k\lambda} &= \Delta_{k\lambda}. && (1.96)\end{aligned}$$

Time reversal symmetry requires

$$\begin{aligned} \Delta_{-ks} &= \Delta^*_{ks},\ \Delta_{-kt} = \Delta^*_{kt} && (1.97)\\ \text{or}\ \ \Delta_{-k\lambda} &= \Delta^*_{k\lambda}. && (1.98)\end{aligned}$$

Now, we turn off the p-wave pairing. That is, we start with a s-wave SC in the hybrid structure. Then we have $\mathbf{d}_k = 0$, $\boldsymbol{\ell}_k \neq 0$, $\Delta_{k+} = \Delta_{k-}$, and

$$H = \sum_{k\lambda} \left[\varepsilon_{k\lambda} c^\dagger_{k\lambda} c_{k\lambda} + \lambda(e^{i\varphi_{-k}} \Delta_{ks} c_{-k\lambda} c_{k\lambda} + h.c.)\right]. \quad (1.99)$$

The angular dependence of the effective gap function, $e^{i\varphi_{-k}}\Delta_{ks}$, arises from spin-momentum locking due to SO coupling. This coupling forces the electron spins within Cooper pairs to lock with their momenta, resulting in a p-wave-like gap function.

Finally, in the SC/TI structure or the SC/semi structure, TRS must be broken to achieve non-degenerate Majorana fermions (see related discussion in previous Chap). This means that to obtain stable Majorana fermions, the degeneracy between TR-conjugated Majorana fermions needs to be lifted by magnetic field or magnetic material.

Since 2012, intense experimental efforts have focused on implementing the hybrid-structure design. Unfortunately, numerous false signals of the Majorana mode have emerged due to various spurious physical processes near zero energy. For a critical review of research on this topic and relevant references, see Das Sarma, 2023.

Exercise:

1. Suppose matrix S is unitary, with $\mathsf{S}^2 = 1$, and anti-commutes with H. Any basis state $\boldsymbol{\psi}_i$ $(i = 1, \cdots, 2N)$ can be decomposed as,

$$\begin{aligned} \boldsymbol{\psi}_i &= \frac{1}{2}(1+\mathsf{S})\boldsymbol{\psi}_i + \frac{1}{2}(1-\mathsf{S})\boldsymbol{\psi}_i && (1.100)\\ &\equiv \boldsymbol{\psi}_{i+} + \boldsymbol{\psi}_{i-}. && (1.101)\end{aligned}$$

Show that under the new basis,

$$\{\boldsymbol{\psi}_{1+}, \cdots, \boldsymbol{\psi}_{N+}; \boldsymbol{\psi}_{N+1,-}, \cdots, \boldsymbol{\psi}_{2N,-}\} \quad (1.102)$$

the two $N \times N$ off-diagonal blocks of S are zero, while the two $N \times N$ diagonal blocks of H are zero.

2. Given the 1D Hamiltonian in Eq. (1.63), evaluate its Kane-Mele topological number using Eq. (1.60). Show that (assume $t > 0$),

$$(-1)^\nu = \text{sgn}(\mu + t)\text{sgn}(\mu - t). \quad (1.103)$$

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