Lecture notes on topological insulators

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I. 2D p-WAVE SUPERCONDUCTOR

We now consider spinless p-wave SC in 2D. Two pioneering works on this topic are Read and Green, 2000 and Ivanov, 2001, from which many of the discussions in this Chap are based. *Spinful* p-wave SC in 1D and higher dimensions will be investigated in later chapters.

A. Lattice model

Consider the following lattice model with real Δ_0,

$$\begin{aligned} H &= \sum_{mn}\Big[-t(c^\dagger_{m+1,n}c_{mn}+c^\dagger_{m,n+1}c_{mn})+h.c. \\ &- (\mu-4t)c^\dagger_{mn}c_{mn} \\ &+ \Delta_0 c^\dagger_{m+1,n}c^\dagger_{mn}+i\Delta_0 c^\dagger_{m,n+1}c^\dagger_{mn}+h.c.\Big]. \end{aligned} \tag{1.1}$$

With the Fourier transform,

$$c^\dagger_{mn}=\frac{1}{\sqrt{N}}\sum_k e^{i(k_x m+k_y n)}c^\dagger_{k_xk_y}, \tag{1.2}$$

where N is the total number of lattice sites, one gets ($c_{\vec{k}}$ is simply written as c_k)

$$H=\frac{1}{2}\sum_{\mathbf{k}}(c^\dagger_k\; c_{-k})\mathsf{H}(\mathbf{k})\begin{pmatrix} c_k \\ c^\dagger_{-k}\end{pmatrix}, \tag{1.3}$$

where

$$\begin{aligned} \mathsf{H} &= \begin{pmatrix} \varepsilon(\mathbf{k}) & 2i\Delta_0(\sin k_x+i\sin k_y) \\ -2i\Delta_0(\sin k_x-i\sin k_y) & -\varepsilon(\mathbf{k})\end{pmatrix}, \\ \varepsilon(\mathbf{k}) &= -2t(\cos k_x+\cos k_y)-(\mu-4t). \end{aligned} \tag{1.4}$$

The Hamiltonian matrix $\mathsf{H}(\mathbf{k})$ has the same form as that of the QWZ model in Eq. (**??**). One only needs to identify

$$2t=t_{QWZ},\;\mu=-m,\;\text{and}\;2i\Delta_0=\lambda. \tag{1.5}$$

For example, the QWZ model is gapless at $m=0,-2,-4$. Therefore, here the gap closes at $\mu=0,2,4$.

Choose $t=1/2$, then

$$\begin{aligned} \mathsf{H}(\mathbf{k}) &= \overbrace{(2-\mu-\cos k_x-\cos k_y)}^{\equiv M(\mathbf{k})}\tau_z \\ &- 2\Delta_0(\sin k_x\tau_y+\sin k_y\tau_x). \end{aligned} \tag{1.6}$$

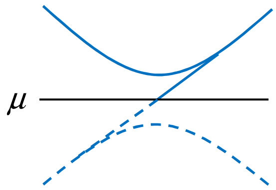

FIG. 1 The energy dispersion of the chiral edge state inside a SC gap.

It has the eigen-energies,

$$E_\pm(\mathbf{k})=\pm\sqrt{M(\mathbf{k})^2+4\Delta_0^2(\sin^2 k_x+\sin^2 k_y)}. \tag{1.7}$$

Based on our understanding of the QWZ model, we know that the system has 3 distinct quantum phases: when $\mu<0$ or $\mu>4$, it is a trivial phase. When $0<\mu<2$, it is a topological SC phase. When $2<\mu<4$, it is another topological SC phase with opposite chirality.

The topological number is characterized by the first Chern number. Given

$$\mathsf{H}(\mathbf{k})=\mathbf{h}(\mathbf{k})\cdot\boldsymbol{\sigma}, \tag{1.8}$$

one has

$$C_1=\frac{1}{4\pi}\int_{BZ}d^2k\frac{1}{h^3}\mathbf{h}\cdot\frac{\partial\mathbf{h}}{\partial k_x}\times\frac{\partial\mathbf{h}}{\partial k_y}. \tag{1.9}$$

However, since the electric charge is not conserved, the topological phases have no quantized Hall conductance.

B. Edge state

For simplicity, we study the edge state in the continuum limit. In the small-k limit, the Hamiltonian matrix reduces to

$$\mathsf{H}(\mathbf{k})=\begin{pmatrix} tk^2-\mu & 2i\Delta_0(k_x+ik_y) \\ -2i\Delta_0(k_x-ik_y) & -tk^2+\mu\end{pmatrix}. \tag{1.10}$$

Note: The second-quantized Hamiltonian is

$$H=\sum_{s=\pm}\varepsilon_k c^\dagger_{ks}c_{ks}+2ik\Delta_0(e^{i\phi_k}c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}-h.c.), \tag{1.11}$$

where $\varepsilon_k=tk^2-\mu, \phi_k=\angle(\mathbf{k},\hat{x})$. This will be referred to in a later chapter.

Assume the chemical potential has a profile similar to $\mu(x)=\tanh x$, then the topological SC occupies the space with $x > 0$. Because of the translation symmetry along y, the eigenstate is of the form $\psi(x)e^{ik_y y}$. We now substitute k_x by $(1/i)(d/dx)$, neglect k^2 terms, and solve for

$$\begin{pmatrix} -\mu & 2i\Delta_0\left(\frac{1}{i}\frac{d}{dx}+ik_y\right) \\ -2i\Delta_0\left(\frac{1}{i}\frac{d}{dx}-ik_y\right) & \mu \end{pmatrix}\psi(x)=\varepsilon_{k_y}\psi(x). \tag{1.12}$$

Again it's easier to make a guess at the edge state. Try

$$\psi(x)=e^{-\frac{1}{2\Delta_0}\int_0^x dx'\mu(x')}\psi_0, \tag{1.13}$$

then we will get

$$\psi_0=\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{1.14}$$

with the eigen-energy $\varepsilon_{k_y}=2\Delta_0 k_y$ (see Fig. 1).

The energy dispersion of the edge state is roughly linear at small k. Furthermore, it is chiral. Therefore, the 2D p-wave SC is sometimes called as the **chiral superconductor**.

The Bogoliubov QP for the edge state is

$$\begin{aligned}\gamma_{k_y} &= \int d^2r\left[u^*(\mathbf{r})\psi(\mathbf{r})+v^*(\mathbf{r})\psi^\dagger(\mathbf{r})\right] \qquad (1.15)\\ &= \int d^2r e^{ik_y y}e^{-\frac{1}{2\Delta_0}\int_0^x dx'\mu(x')}\left[e^{-i\pi/2}\psi+e^{i\pi/2}\psi^\dagger\right],\end{aligned}$$

where we have removed an overall phase $e^{i\pi/2}$. Therefore,

$$\gamma^\dagger_{-k_y}=\gamma_{k_y}. \tag{1.16}$$

When $k_y=0$, $\gamma_0^\dagger=\gamma_0$ and the zero mode is a Majorana mode. However, not being gapped from edge states at higher energy, it can be easily damaged by thermal effect. In the next Sec, we'll see that the Majorana mode inside a vortex is gapped, thus can avoid this problem (to some extent).

C. Vortex and its bound states

In the Ginzberg-Landau (GL) theory of SC, the SC state is described by a macroscopic wave function $\Psi(\mathbf{r})$. This effective theory works near the SC transition, and can be derived from the microscopic BCS theory. In fact, one can show that $\Psi(\mathbf{r})\simeq\Delta(\mathbf{r})$ (e.g., see Fetter and Walecka, 1971), differing only by a multiplicative factor. The current density in the GL theory is given as ($q^*=-2e, m^*=2m$),

$$\begin{aligned}\mathbf{j} &= \frac{q^*}{2m^*}\left[\Psi^*\left(\frac{\hbar}{i}\nabla-q^*\mathbf{A}\right)\Psi+c.c.\right] \qquad (1.17)\\ &= -\frac{e\hbar}{2mi}\left(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*\right)-\frac{2e^2}{m}|\Psi|^2\mathbf{A}. \qquad (1.18)\end{aligned}$$

Therefore, if $\Delta(\mathbf{r})=|\Delta(\mathbf{r})|e^{-i\xi(\mathbf{r})}$, where $\xi(\mathbf{r})$ is a single-valued function, then

$$\mathbf{j}\propto\frac{\hbar}{2e}\nabla\xi-\mathbf{A}. \tag{1.19}$$

The phase of Δ is adjustable via a gauge transformation. For example, if

$$\begin{aligned}\Delta &\to \Delta'=\Delta e^{i\chi}, \qquad (1.20)\\ \text{then}\quad \xi &\to \xi'=\xi-\chi, \qquad (1.21)\\ \text{and}\quad \mathbf{A} &\to \mathbf{A}'=\mathbf{A}-\frac{\hbar}{2e}\nabla\chi. \qquad (1.22)\end{aligned}$$

The current density is gauge invariant, as it should be. Also, you can check that the BdG equation is invariant under the following gauge transformation,

$$\begin{pmatrix} u \\ v \end{pmatrix}\to\begin{pmatrix} u' \\ v' \end{pmatrix}=\begin{pmatrix} e^{i\chi/2}u \\ e^{-i\chi/2}v \end{pmatrix}. \tag{1.23}$$

Far away from a vortex, the circulating current density $\mathbf{j}(\mathbf{r})$ drops to zero, such that for a large loop C,

$$\oint_C d\mathbf{r}\cdot\mathbf{j}=0. \tag{1.24}$$

Therefore,

$$\begin{aligned}\oint_C d\mathbf{r}\cdot\mathbf{A} &= -\frac{\hbar}{2e}[\xi(2\pi)-\xi(0)] \qquad (1.25)\\ &= \frac{h}{2e}n,\quad n\in Z, \qquad (1.26)\end{aligned}$$

in which $\xi(2\pi)-\xi(0)=2\pi n$, since ξ is single-valued. Thus the magnetic flux through a SC vortex needs be quantized in units of $h/2e$. In the case of $n=1$, one can choose $\xi=\theta$, the polar angle.

We now choose $\chi=\xi$ $(=n\theta)$ to remove the SC phase, so that $\Delta'=|\Delta|$. Consequently, after a 2π rotation of θ,

$$\begin{aligned}\begin{pmatrix} u' \\ v' \end{pmatrix} &= \begin{pmatrix} e^{i\xi/2}u \\ e^{-i\xi/2}v \end{pmatrix} \qquad (1.27)\\ &= (-1)^n\begin{pmatrix} u \\ v \end{pmatrix}. \qquad (1.28)\end{aligned}$$

To avoid possible mis-steps, one can add a "branch-cut" emanating from the vortex, so that after circling a vortex (and crossing the branch-cut) once, a phase factor $(-1)^n$ is added.

We now study the bound states inside a vortex. First write the BdG equation in polar coordinate. Recall that

$$\begin{aligned}\frac{\partial}{\partial x} &= \cos\theta\frac{\partial}{\partial r}-\frac{\sin\theta}{r}\frac{\partial}{\partial\theta}, \qquad (1.29)\\ \frac{\partial}{\partial y} &= \sin\theta\frac{\partial}{\partial r}+\frac{\cos\theta}{r}\frac{\partial}{\partial\theta}. \qquad (1.30)\end{aligned}$$

Therefore,

$$\begin{aligned}i(k_x+ik_y) &\to \frac{\partial}{\partial x}+i\frac{\partial}{\partial y} \qquad (1.31)\\ &= e^{i\theta}\left(\frac{\partial}{\partial r}+\frac{i}{r}\frac{\partial}{\partial\theta}\right). \qquad (1.32)\end{aligned}$$

Neglecting k^2 terms, then we have ($\Delta_0(r) \in R$),

$$\begin{pmatrix} -\mu & 2\Delta_0 e^{i\theta}\left(\frac{\partial}{\partial r}+\frac{i}{r}\frac{\partial}{\partial\theta}\right) \\ 2\Delta_0 e^{-i\theta}\left(-\frac{\partial}{\partial r}+\frac{i}{r}\frac{\partial}{\partial\theta}\right) & \mu \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \quad (1.33)$$

One can verify that the following is an zero-energy solution,

$$\begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \underbrace{\frac{i}{\sqrt{r}} e^{-\frac{1}{2}\int_0^r dr' \frac{\mu}{\Delta_0(r')}}}_{\equiv ig(r)} \begin{pmatrix} -e^{i\theta/2} \\ e^{-i\theta/2} \end{pmatrix}. \quad (1.34)$$

The corresponding Bogoliubov QP is,

$$\begin{aligned} \gamma_0 &= \int d^2r \left[u_0^*(\mathbf{r})\psi(\mathbf{r}) + v_0^*(\mathbf{r})\psi^\dagger(\mathbf{r})\right] \quad (1.35) \\ &= \int d^2r \; ig(r)\left[e^{-i\theta/2}\psi(\mathbf{r}) - e^{i\theta/2}\psi^\dagger(\mathbf{r})\right]. \end{aligned}$$

Such a zero-mode bound state is a Majorana mode, $\gamma_0^\dagger = \gamma_0$.

A few remarks: First, for a p-wave SC, near the core of a vortex, $E_n \simeq n\hbar\omega_0$ at low energy, where $\omega_0 \simeq \Delta_0^2/\varepsilon_F \ll \Delta_0$, and n is the angular momentum of the QP (see, e.g., Tewari *et al.*, 2007). However, for a s-wave SC, $E_n \simeq (n+1/2)\hbar\omega_0$ for low-energy bound states (see p. 155 of de Gennes, 1989). The lowest one has energy $\hbar\omega_0/2$, thus there is no zero mode.

Second, candidate host materials for Majorana fermions are: the ruthenate (Sr_2RuO_4), which is a p-wave SC with spin, the A-phase of superfulid He-3, and the fractional quantum Hall phase with filling fraction $\nu = 5/2$ (the Moore-Read state). It is also possible to find them in the hybrid structure of 3D TI+s-wave SC (Fu and Kane, 2008), or 2D Rashba+s-wave SC (Alicea, 2010; Sau *et al.*, 2010).

D. Topological qubit

Like the MF in a Kitaev chain, two MFs (γ_1, γ_2) in the p-wave SC can store one qubit of information:

$$\begin{aligned} f_1 &= \frac{1}{2}(\gamma_1 + i\gamma_2), \quad (1.36) \\ f_1^\dagger &= \frac{1}{2}(\gamma_1 - i\gamma_2), \quad (1.37) \\ \rightarrow \; f_1^\dagger f_1 &= \frac{1 + i\gamma_1\gamma_2}{2} \sim 0, 1. \quad (1.38) \end{aligned}$$

Recall that $-i\gamma_1\gamma_2$ is the fermion parity operator. Such a qubit composed of 2 spatially separated MFs is robust again local decoherence.

In order to understand how to manipulate such qubits, we now consider a system with multiple MFs. For a MF located at $\mathbf{R}_j$, we have (Nayak *et al.*, 2008),

$$\gamma_j = \int d^2r \left[h_j(\mathbf{r})e^{-i\theta_j/2+i\Gamma_j/2}\psi_j + h_j^*(\mathbf{r})e^{i\theta_j/2-i\Gamma_j/2}\psi_j^\dagger\right], \quad (1.39)$$

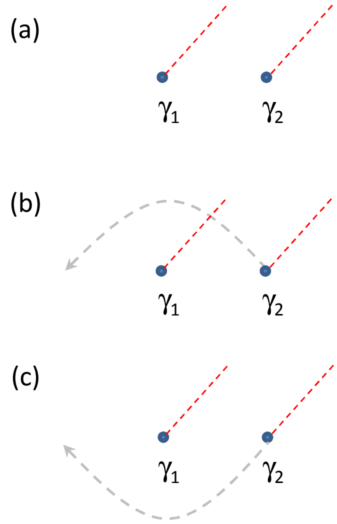

FIG. 2 (a) Attach a branch cut to each vortex. The position of the branch cut is gauge dependent. (b) Exchange the locations of 2 MFs by moving γ_2 counter-clockwise around γ_1. (c) Exchange the locations of 2 MFs by moving γ_2 clockwise around γ_1.

where $h_j(\mathbf{r}) = ig(\mathbf{r} - \mathbf{R}_j)$, and

$$\begin{aligned} \theta_j &= \arg(\mathbf{r} - \mathbf{R}_j), \quad (1.40) \\ \Gamma_j &= \sum_{\ell \neq j} \arg(\mathbf{R}_j - \mathbf{R}_\ell). \quad (1.41) \end{aligned}$$

The phase Γ_j arises because of the anti-periodicity in Eq. (1.28). For example, consider only 2 MFs. If we move γ_2 around γ_1 once, then $\Gamma_2 = \arg(\mathbf{R}_2 - \mathbf{R}_1)$ changes by 2π, and γ_2 changes sign. To register such a change of sign, we add a branch cut to each vortex, as shown in Fig. 2(a).

1. Braiding 2 Majorana fermions

To exchange the locations of 2 MFs, γ_1 and γ_2, we can move γ_2 around γ_1 in 2 ways (see Fig. 2(b),(c)). The results are different, because of the branch cut. In Fig. 2(b), γ_2 crossed the branch cut of γ_1, and we have

$$\begin{aligned} \gamma_1 &\rightarrow \gamma_2, \quad (1.42) \\ \gamma_2 &\rightarrow -\gamma_1. \quad (1.43) \end{aligned}$$

In Fig. 2(c), γ_2 does not cross the branch cut of γ_1, but γ_1 crossed the branch cut of γ_2, and we have

$$\begin{aligned} \gamma_1 &\rightarrow -\gamma_2, \quad (1.44) \\ \gamma_2 &\rightarrow \gamma_1. \quad (1.45) \end{aligned}$$

For clockwise rotation, we can write

$$\gamma_j \rightarrow B_{12}\gamma_j B_{12}^\dagger, \quad (1.46)$$

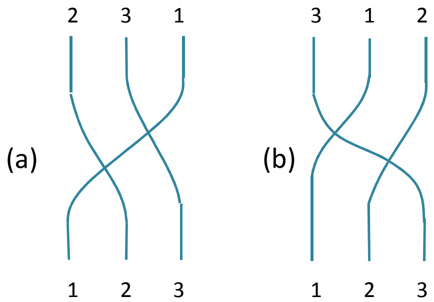

FIG. 3 (a) First exchange γ_1 with γ_2, then exchange γ_2 with γ_3. (b) First exchange γ_2 with γ_3, then exchange γ_3 with γ_1.

where

$$B_{12} = \frac{1}{\sqrt{2}}(1+\gamma_1\gamma_2) \tag{1.47}$$

is called the **braiding operator**.

A full circle is composed of 2 half circles, and

$$B_{12}^2 = \gamma_1\gamma_2. \tag{1.48}$$

It follows that,

$$\gamma_j \to B_{12}^2\gamma_j(B_{12}^\dagger)^2 = -\gamma_j. \tag{1.49}$$

Both MFs change sign since each of them crossed a branch cut once.

Write the states with fermion numbers 0, 1 as $|0\rangle, |1\rangle$, then (see Eq. (1.38))

$$|1\rangle = f_1^\dagger|0\rangle, \tag{1.50}$$

$$\begin{cases} f_1^\dagger f_1|0\rangle = 0, \\ f_1^\dagger f_1|1\rangle = |1\rangle. \end{cases} \tag{1.51}$$

Also,

$$\begin{cases} -i\gamma_1\gamma_2|0\rangle = |0\rangle, \\ -i\gamma_1\gamma_2|1\rangle = -|1\rangle. \end{cases} \tag{1.52}$$

It follows that,

$$B_{12}|0\rangle = \frac{1}{\sqrt{2}}(1+i)|0\rangle = e^{i\pi/4}|0\rangle, \tag{1.53}$$

$$B_{12}|1\rangle = \frac{1}{\sqrt{2}}(1-i)|1\rangle = e^{-i\pi/4}|1\rangle. \tag{1.54}$$

That is, the braiding operator does not switch the states $|0\rangle, |1\rangle$, it only shifts the phases of the states.

2. Braiding 4 Majorana fermions

We now consider a 2-qubit system with 4 MFs,

$$f_1 = \frac{1}{2}(\gamma_1 + i\gamma_2), \tag{1.55}$$

$$f_2 = \frac{1}{2}(\gamma_3 + i\gamma_4). \tag{1.56}$$

The basis of the Hilbert space are $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. For *intra*-fermion braiding, we have, for example,

$$B_{12}|00\rangle = \frac{1}{\sqrt{2}}(1+i)|00\rangle, \tag{1.57}$$

$$B_{34}|00\rangle = \frac{1}{\sqrt{2}}(1+i)|00\rangle. \tag{1.58}$$

For *inter*-fermion braiding, one has, for example,

$$\begin{aligned} B_{23}|00\rangle &= \frac{1}{\sqrt{2}}(1+\gamma_2\gamma_3)|00\rangle \\ &= \frac{1}{\sqrt{2}}(|00\rangle + i|11\rangle). \end{aligned} \tag{1.59}$$

Note that the fermion parity, $n_1 + n_2 \pmod 2$, is not changed by these braidings.

In general, under the basis $(|00\rangle, |01\rangle, |10\rangle, |11\rangle)^T$, these braiding operators can be written as,

$$B_{12} = e^{i\frac{\pi}{4}\sigma_z\otimes 1} = \begin{pmatrix} e^{i\pi/4} & 0 & 0 & 0 \\ 0 & e^{i\pi/4} & 0 & 0 \\ 0 & 0 & e^{-i\pi/4} & 0 \\ 0 & 0 & 0 & e^{-i\pi/4} \end{pmatrix} \tag{1.60}$$

$$B_{34} = e^{1\otimes i\frac{\pi}{4}\sigma_z} = \begin{pmatrix} e^{i\pi/4} & 0 & 0 & 0 \\ 0 & e^{-i\pi/4} & 0 & 0 \\ 0 & 0 & e^{i\pi/4} & 0 \\ 0 & 0 & 0 & e^{-i\pi/4} \end{pmatrix} \tag{1.61}$$

$$B_{23} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & i \\ 0 & 1 & i & 0 \\ 0 & -i & 1 & 0 \\ -i & 0 & 0 & 1 \end{pmatrix}. \tag{1.62}$$

Two braiding operations that act on different fermions would commute,

$$[B_{12}, B_{34}] = 0. \tag{1.63}$$

However,

$$[B_{j-1,j}, B_{j,j+1}] = \gamma_{j-1}\gamma_{j+1}. \tag{1.64}$$

Because the commutator does not vanish, the order of braiding matters, as shown in Fig. 3.

Since the braiding operations do not change the fermion parity. They could only connect $|00\rangle$ and $|11\rangle$ (or $|10\rangle$ and $|01\rangle$) in a 2D Hilbert sub-space. That is, with braiding only, one can only access 1 qubit out of the two-qubit system. Define the new qubit as,

$$|\bar{0}\rangle \equiv |00\rangle, \ |\bar{1}\rangle \equiv |11\rangle, \tag{1.65}$$

then

$$B_{12} = B_{34} = e^{i\frac{\pi}{4}\tau_z}, \tag{1.66}$$

$$B_{23} = e^{i\frac{\pi}{4}\tau_x}. \tag{1.67}$$

They rotate a single qubit by an angle $\pi/2$ around either z-axis or x-axis.

The **universal quantum computation** cannot be achieved by braiding operations alone. It requires logical gates that could change the fermion parity, such as the Controlled NOT gate,

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \tag{1.68}$$

which changes $|10\rangle$ to $|11\rangle$, and $|11\rangle$ to $|10\rangle$.

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