Lecture notes on topological insulators

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Contents

I. 1D p-WAVE SUPERCONDUCTOR

Here we study p-wave SC in 1D with non-trivial topology. Material with p-wave SC is rare (an example is strontium ruthenate, Sr_2RuO_4), but as we will see in later chapters, effective p-wave pairing can be achieved with hybrid structures consisting of s-wave SC material and material with spin-orbital coupling.

In this chapter, the fermions are either spinless, or spin-polarized, so that the spin degree of freedom can be ignored. We first consider a continuum version, then a lattice version of the 1D p-wave SC (the Kitaev model). The main references we use on topological superconductor are Bernevig and Hughes, 2013 and Nomura, 2013.

A. Continuum model

The Hamiltonian of the 1D p-wave SC is given as

$$H = \sum_k \left[\varepsilon_k c_k^\dagger c_k + \frac{1}{2}\left(\Delta_k c_k^\dagger c_{-k}^\dagger + \Delta_k^* c_{-k} c_k\right)\right] \quad (1.1)$$

$$= \frac{1}{2}\sum_k (c_k^\dagger c_{-k}) \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta_k^* & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}, \quad (1.2)$$

in which $\varepsilon_k = \hbar^2 k^2/2m - \mu$, and $\Delta_k = \Delta_0 k$. The eigenenergies are,

$$E_\pm(k) = \pm\sqrt{\varepsilon_k^2 + |\Delta_k|^2}. \quad (1.3)$$

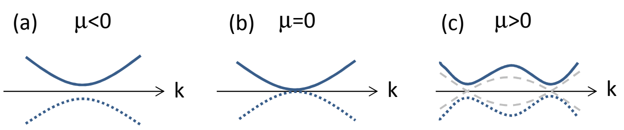

FIG. 1 The energies $\pm E_k$ plotted for 3 chemical potentials.

The eigenstate (u_k, v_k) for energy E_k has the components,

$$u_k = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right)}; \quad v_k = \sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)}\frac{\Delta_k^*}{|\Delta_k|}. \quad (1.4)$$

The particle-hole symmetry has been discussed in Sec. ??.

Near $k = 0$, $\varepsilon_k \simeq -\mu$, and $E_k \simeq |\mu|$. In Fig. 1, we show the dependence of the energy spectrum on the chemical potential. For both $\mu < 0$ and $\mu > 0$, the spectra are gapful. If $\mu = 0$, then $E_+(k), E_-(k)$ touch at $k = 0$.

If $\mu < 0$, then for small k, $u_k \simeq 1, v_k \simeq \Delta_k^*/2|\mu|$. It is known that the Fourier transform of the Cooper pair wave function $g(x)$ is $g(k) = v_k/u_k$ (de Gennes, 1989). So for $\mu < 0$, $g(k) \propto k$. The function $g(k)$ being analytic near $k = 0$ implies that its Fourier transform falls off exponentially at large distance, $g(x) \simeq e^{-x/x_0}$. The phase with $\mu < 0$ is thus called the strong-coupling phase (Read and Green, 2000).

On the other hand, if $\mu > 0$, then for small k, $u_k \simeq |\Delta_k|/2\mu, v_k \simeq 1$ (we have ignored the phase of Δ_k), and $g(k) \propto 1/k$. The sharp peak near small k implies a slow decay of $g(x)$ at large distance. So the phase with $\mu > 0$ is called the weak-coupling phase.

These two phases cannot be adiabatically connected to each other (see p. 198 of Bernevig and Hughes, 2013). Furthermore, the weak-coupling phase has non-trivial topology.

1. Edge state

We now assume $\mu(x > 0) > 0$, and $\mu(x < 0) < 0$, so the 1D space is separated to a weak-coupling phase and a strong-coupling phase (e.g., $\mu(x) = \mu_0 \tanh x$). Ignore terms of order k^2, the BdG equation is,

$$\begin{pmatrix} -\mu(x) & \Delta_0 k \\ \Delta_0 k & \mu(x) \end{pmatrix} \psi = E\psi. \quad (1.5)$$

We are only interested in the edge-state solution. Let $k \to \partial/i\partial x$, and try

$$\psi(x) = \psi_0 e^{-\frac{1}{\Delta_0}\int_0^x dx'\mu(x')}, \quad (1.6)$$

then

$$\begin{pmatrix} -\mu(x) - E & i\mu(x) \\ i\mu(x) & \mu(x) - E \end{pmatrix} \psi_0 = 0. \quad (1.7)$$

At $E=0$, we have a solution,

$$\psi_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{1.8}$$

This is a zero mode localized at the interface.

The Bogoliubov quasiparticle (QP) operator for the zero mode is,

$$\begin{aligned}\gamma_0 &= \int dx\left[u^*(x)\psi(x) + v^*(x)\psi^\dagger(x)\right] \\ &= \frac{e^{i\pi/4}}{\sqrt{2}}\int dx e^{-\frac{1}{\Delta_0}\int_0^x dx'\mu(x')}\left[e^{-i\pi/4}\psi(x) + e^{i\pi/4}\psi^\dagger(x)\right].\end{aligned} \tag{1.9}$$

Removing the overall phase of $\pi/4$, we have

$$\gamma_0^\dagger = \gamma_0. \tag{1.10}$$

That is, the anti-particle of the QP is the same as the QP. Such a fermion is called a **Majorana fermion** (MF). The zero mode is protected by the PH symmetry, as long as it's non-degenerate. For a general introduction to the Majorana fermion, one can read Wilczek, 2009.

B. Kitaev model

We now study the Kitaev model of a 1D p-wave SC (Kitaev, 2001). It is the lattice version of the continuum model introduced in previous section. With the lattice, the topological number can be defined naturally.

Consider a 1D lattice with N sites (lattice constant $a=1$) under periodic BC, $c_{N+1}=c_1$. The Hamiltonian is,

$$\begin{aligned}H &= \sum_{j=1}^{N}\left[-\frac{t}{2}(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}) - \mu c_j^\dagger c_j\right. \\ &\quad \left.+\frac{\Delta_0}{4}\left(c_{j+1}^\dagger c_j^\dagger - c_j^\dagger c_{j+1}^\dagger + h.c\right)\right], t>0, \Delta_0 \in R.\end{aligned} \tag{1.11}$$

With the Fourier transformation,

$$c_j^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{ijk}c_k^\dagger, \tag{1.12}$$

one has

$$\begin{aligned}H &= \sum_k\left[-t\cos k c_k^\dagger c_k - \mu c_k^\dagger c_k\right. \\ &+ \left.\frac{\Delta_0}{4}\left(e^{ik}c_k^\dagger c_{-k}^\dagger - e^{-ik}c_k^\dagger c_{-k}^\dagger + h.c\right)\right].\end{aligned} \tag{1.13}$$

It can be written in matrix form,

$$\begin{aligned}H &= \frac{1}{2}\sum_k (c_k^\dagger c_{-k})\begin{pmatrix} -t\cos k - \mu & i\Delta_0\sin k \\ -i\Delta_0 \sin k & t\cos k + \mu\end{pmatrix}\begin{pmatrix} c_k \\ c_{-k}^\dagger\end{pmatrix} \\ &+ \frac{1}{2}\sum_k t\cos k + \mu.\end{aligned} \tag{1.14}$$

The eigen-energies are,

$$E_\pm(k) = \pm\sqrt{(t\cos k + \mu)^2 + \Delta_0^2\sin^2 k}. \tag{1.15}$$

The energy gap closes when both

$$\begin{cases} \sin k = 0, \\ t\cos k + \mu = 0. \end{cases} \tag{1.16}$$

The gap at $k=0$ closes at $\mu_c = -t$, and the gap at $k=\pi$ closes at $\mu_c = t$. So there are 3 quantum phases within the ranges $\mu < -t$, $|\mu| < t$, and $\mu > t$.

1. Topological number

The 2×2 Hamiltonian matrix can be written in the standard form, $\mathsf{H}(k) = \mathbf{d}\cdot\boldsymbol{\sigma}$, where

$$\mathbf{d} = -(0, \Delta_0\sin k, t\cos k + \mu). \tag{1.17}$$

When k moves from $-\pi$ to π, the tip of $\mathbf{d}(k)$ moves around an ellipse on the $y-z$ plane with a center at $z=-\mu$. If $\mu > t$, then the origin is outside of the elliptical loop, and the winding number of the map $k\to\mathbf{d}(k)$ is zero. If $|\mu|<t$, then the origin is inside the loop, and the winding number is 1. If $\mu < -t$, then the winding number is again 0. To change from 1 to 0, or 0 to 1, the loop needs to cross the origin – at that point the energy gap vanishes.

This indicates that the region $|\mu| < t$ is the topologically non-trivial phase, while the region $|\mu| > t$ is the trivial phase. These two phases with different winding numbers can be distinguished by a Z_2 topological number ν, which is defined as (see Nomura, 2013),

$$(-1)^\nu = \mathrm{sgn}[d_z(0)]\mathrm{sgn}[d_z(\pi)]. \tag{1.18}$$

In our case, $d_z(0) = -t-\mu$, $d_z(\pi) = t-\mu$. It's not difficult to see that the origin can be inside the loop only when these two quantities have opposite signs.

Note: In the phase with $\mu < |t|$, it seems that two systems with $t>0$, $t<0$ would give opposite winding numbers, indicating different topological phases. This is not true. For example, let μ be slightly non-zero, and $\Delta_0 \neq 0$, then the energy gap remains open when t is changed to $-t$, so these two are in the same phase.

2. Kitaev chain with open ends

To study the edge states of an open Kitaev chain, it's convenient to introduce the **Majorana fermion representation**. The usual fermions satisfy the anti-commutation relation,

$$\{c_j, c_{j'}^\dagger\} = \delta_{jj'}. \tag{1.19}$$

Let a_j be Majorana fermion operators, with $a_j^\dagger = a_j$. Define their anti-commutation relations as,

$$\{a_j, a_{j'}^\dagger\} = 2\delta_{jj'}. \tag{1.20}$$

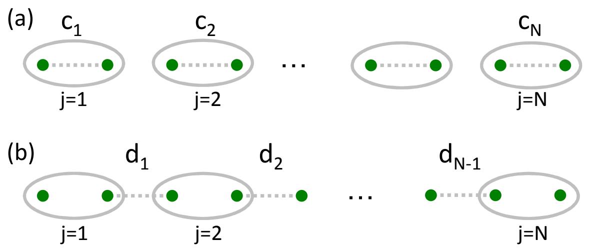

FIG. 2 A Kitaev chain with N sites and open ends. (a) A fermion operator c_j is composed of two MF operators. (b) Using a pair of MFs from different physical fermions to build a fermion operator d_j.

Then, of course, $\{a_j, a_{j'}\} = 2\delta_{jj'}$, and $a_j^2 = 1$ (not zero!).

Decompose a fermion into 2 MFs (see Fig. 2(a)),

$$c_j = \frac{1}{2}(a_{2j-1} + ia_{2j}), \tag{1.21}$$

$$\text{then } c_j^\dagger = \frac{1}{2}(a_{2j-1} - ia_{2j}). \tag{1.22}$$

This is analogous to the decomposition of a complex number to two real numbers. Given Eq. (1.20), one can verify that they do satisfy Eq. (1.19).

Now consider a Kitaev chain with two open ends and N lattice sites ($j = 1, \cdots, N$). The Hamiltonian is,

$$\begin{aligned} H &= -\frac{t}{2}\sum_{j=1}^{N-1} c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} - \mu \sum_{j=1}^{N} c_j^\dagger c_j \\ &+ \frac{\Delta_0}{2}\sum_{j=1}^{N-1} c_{j+1}^\dagger c_j^\dagger + c_j c_{j+1} \qquad (1.23) \\ &= \frac{i}{4}\sum_{j=1}^{N-1}(t+\Delta_0)a_{2j}a_{2j+1} + (-t+\Delta_0)a_{2j-1}a_{2j+2} \\ &- \frac{i}{2}\sum_{j=1}^{N} \mu a_{2j-1}a_{2j}. \qquad (1.24) \end{aligned}$$

Notice that since $(a_{2j}a_{2j+1})^\dagger = -a_{2j}a_{2j+1}$ (anti-hermitian), so the factor i is required.

For simplicity, consider the case with $\Delta_0 = t$, then

$$H = \frac{i}{2}\sum_{j=1}^{N-1} t a_{2j}a_{2j+1} - \frac{i}{2}\sum_{j=1}^{N} \mu a_{2j-1}a_{2j}. \tag{1.25}$$

We know that it is a trivial SC when $|\mu| > t$. When $|\mu| < t$, it is a topological SC with Majorana edge states (see Fig. 3). This fact is trivial when $\mu = 0$: the 2nd term vanishes, and thus the 2 MFs on the ends decouple from the rest of the MFs. That is, there is a lone MF on each end of the chain. Such a conclusion does not change if $\mu \neq 0$. One can consult Kitaev, 2001 for more details.

On the other hand, for the trivial phase ($|\mu| > t$), one can choose $t = 0$ to simplify the Hamiltonian. Then every MF in the chain is coupled with its neighbor, and there is no lone MF at the ends.

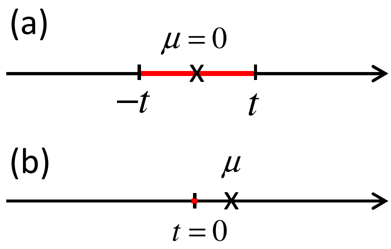

FIG. 3 (a) For $t > 0$, $\mu = 0$ is in the topological phase. (b) For $t = 0$, $\mu > 0$ is in the trivial phase.

Some comments on the realization of Majorana fermions in real 1D systems. p-wave SC is rare, but one can combine s-wave superconductivity with spin-orbit (SO) coupling to produce an effective p-wave SC (Fu and Kane, 2008). In practice, one can put a metal wire on top of a s-wave SC. Either the wire or the SC needs to have the SO coupling. As a result, the electrons in the wire then interact with both the SO coupling and the superconductivity (through the proximity effect). Furthermore, since spin degeneracy could double the number of zero modes and destablize the MFs, magnetic material or magnetic field needs be introduced to break the degeneracy. For example, Nadj-Perge *et al.*, 2014 uses ferromagnetic iron atomic chains on top of a superconducting lead (which has strong SO coupling). Some more discussions can be found in Alicea, 2012.

A brief summary of 1D models with nontrivial topology: In the exercise of Chap **??**, we have studied the SSH model of polyacetylene. In Chap **??**, we introduced the Fu-Kane spin pump. In this Chap we have the Kitaev model of p-wave SC. Other 1D models not covered in this course are, for example, the AKLT model of spin-1 chain, and the Lubensky-Kane model of mechanical chain. They all have non-trivial topology, and they all have robust edge states.

3. Fermion parity of the ground state

As we have explained above, for the topological ground state, there are two Majorana fermions at the ends of the chain. The two MFs have the same degrees of freedom as one ordinary fermion, which can either be occupied or unoccupied. Since the energy of the MFs is zero, these two possible states are both ground states. That is, we expect the topological ground states of the Kitaev chain to be two-fold degenerate. These two states can be characterized by the **fermion parity**, which is explained below.

First, the fermion parity of site-j with fermion number n_j is defined as,

$$(-1)^{n_j} = \begin{cases} +1 \text{ if } n_j = 0, \\ -1 \text{ if } n_j = 1. \end{cases} \tag{1.26}$$

When written in operators, one has ($n_j = c_j^\dagger c_j$)

$$\begin{aligned}(-1)^{n_j} &= e^{i\pi n_j} \quad (n_j^2 = n_j) \\ &= 1 - 2n_j \qquad (1.27)\\ &= -ia_{2j-1}a_{2j}. \qquad (1.28)\end{aligned}$$

We'd like to know if the fermion parity operator commutes with the Hamiltonian. First, one can show that

$$\sum_j [c_j^\dagger c_{j+1}, c_i^\dagger c_i] + h.c. = 0. \qquad (1.29)$$

Second,

$$\begin{aligned}\sum_j [c_j^\dagger c_{j+1}^\dagger, c_i^\dagger c_i] + h.c. &= -c_{i-1}^\dagger c_i^\dagger - c_i^\dagger c_{i+1}^\dagger + h.c. \\ &= 0 \mod 2. \qquad (1.30)\end{aligned}$$

The result is not zero, but since the SC ground state does not have a definite number of Cooper pairs, so when the fermion parity operator is acting within the subspace of the SC ground state, the commutator can be considered as 0. That is, the fermion parity operator 'effectively' commutes with the Hamiltonian.

We thus define the fermion parity operator for the whole system as,

$$\begin{aligned}P_F &= \prod_{j=1}^N (1 - 2c_j^\dagger c_j) \qquad (1.31)\\ &= \prod_{j=1}^N (-ia_{2j-1}a_{2j}), \quad P_F^2 = 1. \qquad (1.32)\end{aligned}$$

Its eigenvalue can only be ± 1: for the trivial phase, it is always $+1$; for the non-trivial phase, it can be $+1$ or -1. This is demonstrated below.

The SC state of the Kitaev model is trivial when $|\mu| > t$. To study its fermion parity, for simplicity, let $\Delta_0 = t$, and just pick up a particular set of parameters with $t = 0, \mu < 0$. Then

$$H = -\frac{i}{2}\sum_{j=1}^N \mu a_{2j-1}a_{2j}. \qquad (1.33)$$

Rewrite $ia_{2j-1}a_{2j} = 2c_j^\dagger c_j - 1$, then

$$H = |\mu| \sum_{j=1}^N \left(c_j^\dagger c_j - \frac{1}{2}\right). \qquad (1.34)$$

Therefore, the ground state is annihilated by c_j, $c_j|0\rangle = 0$. Its fermion parity is $+1$, since

$$\begin{aligned}P_F|0\rangle &= \prod_{j=1}^N (1 - 2c_j^\dagger c_j)|0\rangle \qquad (1.35)\\ &= |0\rangle. \qquad (1.36)\end{aligned}$$

On the other hand, for the non-trivial phase in $|\mu| < t$ ($t > 0$), let $\Delta_0 = t$ and $\mu = 0$, then

$$H = \frac{i}{2}\sum_{j=1}^{N-1} t a_{2j}a_{2j+1}. \qquad (1.37)$$

Since the edge states decouple from the bulk states, instead of Eq. (1.22), for fermions in the bulk ($j = 1, \cdots, N-1$), define (see Fig. 2(b))

$$\begin{aligned}d_j &= \frac{1}{2}(a_{2j} + ia_{2j+1}), \qquad (1.38)\\ \text{then} \quad d_j^\dagger &= \frac{1}{2}(a_{2j} - ia_{2j+1}). \qquad (1.39)\end{aligned}$$

Rewrite $ia_{2j}a_{2j+1} = 2d_j^\dagger d_j - 1$, then

$$H = t\sum_{j=1}^N \left(d_j^\dagger d_j - \frac{1}{2}\right). \qquad (1.40)$$

Therefore, the ground state is annihilated by d_j, $d_j|0\rangle = 0$. To calculate its fermion parity, first rewrite

$$\begin{aligned}P_F &= -ia_1 \prod_{j=1}^{N-1}(-ia_{2j}a_{2j+1})a_{2N} \qquad (1.41)\\ &= -ia_1a_{2N}\prod_{j=1}^{N-1}(1 - d_j^\dagger d_j). \qquad (1.42)\end{aligned}$$

Since $d_j|0\rangle = 0$, we have

$$P_F|0\rangle = (-ia_1a_{2N})|0\rangle. \qquad (1.43)$$

From a pair of edge MFs, one can define a highly non-local fermion,

$$\begin{aligned}f &= \frac{1}{2}(a_1 + ia_{2N}), \qquad (1.44)\\ \text{then} \quad f^\dagger &= \frac{1}{2}(a_1 - ia_{2N}). \qquad (1.45)\end{aligned}$$

The eigenvalues of fermion-number operator can be 0 or 1. The eigenstates are designated as $|0_+\rangle$ and $|0_-\rangle$. That is,

$$\begin{aligned}f^\dagger f|0_+\rangle &= 0, \qquad (1.46)\\ f^\dagger f|0_-\rangle &= |0_-\rangle. \qquad (1.47)\end{aligned}$$

Furthermore,

$$-ia_1a_{2N} = 1 - 2f^\dagger f. \qquad (1.48)$$

Therefore,

$$\begin{aligned}P_F|0_\pm\rangle &= (-ia_1a_{2N}|0_\pm\rangle \qquad (1.49)\\ &= (1 - 2f^\dagger f)|0_\pm\rangle \qquad (1.50)\\ &= \pm|0_\pm\rangle. \qquad (1.51)\end{aligned}$$

That is, the ground states for the non-trivial phase are two-fold degenerate and can be labelled by the fermion parity. It can be considered as a 2-state system that could store 1 qubit of information. Being nonlocal, such a qubit is robust against local perturbations.

Note: Since the fermion operators f operate within a 2D Hilbert space, they can be represented by Pauli matrices,

$$\begin{aligned} f &\simeq \sigma_+ & (1.52)\\ f^\dagger &\simeq \sigma_- & (1.53)\\ 1-2f^\dagger f &\simeq \sigma_z. & (1.54)\end{aligned}$$

Or,

$$\begin{aligned} a_1 &\simeq \sigma_x, & (1.55)\\ a_{2N} &\simeq \sigma_y, & (1.56)\\ -ia_1 a_{2N} &\simeq \sigma_z. & (1.57)\end{aligned}$$

Exercise

1. One can write fermion operators in terms of spin operators,

$$\begin{aligned} a_{2j-1} &= \left(\prod_{k=1}^{j-1}\sigma_k^z\right)\sigma_j^x, & (1.58)\\ a_{2j} &= \left(\prod_{k=1}^{j-1}\sigma_k^z\right)\sigma_j^y. & (1.59)\end{aligned}$$

This is called as the **Jordan-Wigner transformation**. Show that, using this transformation, the Hamiltonian of the Kitaev chain,

$$H = \frac{i}{2}\sum_{j=1}^{N-1} t a_{2j}a_{2j+1} - \frac{i}{2}\sum_{j=1}^{N}\mu a_{2j-1}a_{2j},$$

can be transformed to

$$H = -J_x\sum_{j=1}^{N-1}\sigma_j^x\sigma_{j+1}^x + h\sum_{j=1}^{N}\sigma_j^z, \qquad (1.60)$$

where $J_x = t/2, h = \mu/2$. This is the Hamiltonian of an Ising spin chain in a transverse magnetic field h. Also, show that

$$P_F = \prod_{j=1}^{N}(-ia_{2j-1}a_{2j}) = \prod_{j=1}^{N}\sigma_j^z. \qquad (1.61)$$

Note: There are two possible quantum phases in the Ising chain above: (a) When $|h| < J_x$, the ground state has all the spins either parallel or anti-parallel to the x-axis (two-fold degenerate). (b) When $|h| > J_x$, the ground state has all the spins anti-parallel to the magnetic field (non-degenerate).

2. Show that the inverse of the Jordan-Wigner transformation is given as,

$$\begin{aligned} \sigma_j^+ &= c_j\prod_{k=1}^{j-1}(-1)^{c_k^\dagger c_k}, & (1.62)\\ \sigma_j^- &= c_j^\dagger\prod_{k=1}^{j-1}(-1)^{c_k^\dagger c_k}. & (1.63)\end{aligned}$$

Also,

$$\sigma_j^z = 1 - 2c_j^\dagger c_j. \qquad (1.64)$$

Therefore, one can transform the Hamiltonian of a spin chain to that of a chain with fermions.

References

Alicea, J., 2012, Reports on Progress in Physics **75**(7), 076501.

Bernevig, B. A., and T. L. Hughes, 2013, *Topological Insulators and Topological Superconductors* (Princeton University Press).

Fu, L., and C. L. Kane, 2008, Phys. Rev. Lett. **100**, 096407.

de Gennes, P.-G., 1989, *Superconductivity of metals and alloys* (Addison-Wesley Publishing Co.).

Kitaev, A. Y., 2001, Physics-Uspekhi **44**(10S), 131.

Nadj-Perge, S., I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, 2014, Science **346**(6209), 602.

Nomura, K., 2013, Fundamental theory of topological insulator, unpublished, written in Japanese.

Read, N., and D. Green, 2000, Phys. Rev. B **61**, 10267.

Wilczek, F., 2009, Nat Phys **5**(9), 614.