Topological Superconductors

Lecture notes for the second semester of the course at Eotvos University

April 3, 2016

Chapter 1

Superconductors can be described by single-particle Hamiltonians

In the mean-field approximation, superconductors are described by many-particle Hamiltonians with anomalous terms. These describe the disappearance of two electrons that form a Cooper pair, and the appearance of two electrons from a broken Cooper pair. Because of such processes, the particle number is not conserved, the ground state is a complicated object. Nevertheless, the parity of fermions in the system is conserved, and therefore, the ground state parity is fixed.

1.1 The ground state of a mean-field superconductor can be constructed from its normal modes

The grand canonical Hamiltonian of a superconductor on a 1D lattice of N sites reads,

$$\hat{H} = \sum_{j=1}^{N} \sum_{s=\pm 1} \Big\{ (u_j \pm B_j) \hat{c}_{j,s}^\dagger \hat{c}_{j,s} + t_j \hat{c}_{j+1,s}^\dagger \hat{c}_{j,s} + t_j^* \hat{c}_{j,s}^\dagger \hat{c}_{j+1,s} \Big\} + \sum_j (\Delta_j \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger + \Delta_j^* \hat{c}_{j\downarrow} \hat{c}_{j\uparrow}). \quad (1.1)$$

The position index j is understood modulo N, which means that we have periodic boundary conditions, $N+1 = 1$. Open boundary conditions are obtained by setting $t_N = 0$. The first sum describes the onsite potentials u_j, which includes the chemical potential, the site-dependent Zeeman terms which distinguish between spin up and spin down, and the hopping between neighboring sites with amplitudes t_j. It is the next sum that includes the effect of superconductivity in the mean-field approximation, including the site-dependent pair potential Δ_j. This is here treated as an additional complex parameter, corresponding to the wave function of the Cooper pair condensate. The interpretation of the last term is that Cooper pairs can be broken/created, in which case and two electrons with opposite spins appear/disappear at site j. Both breaking and creating Cooper pairs are procedures with bosonic enhancement factors represented by the complex numbers Δ_j. These amplitudes could be calculated self-consistently, but in these notes, as in a large part of the literature, Δ_j is treated as a parameter, a given complex function of position.

In the mean-field approximation, a superconductor is described by a free Hamiltonian, i.e., quadratic in the electron creation and annihilation operators. Note that although the number of fermions is not conserved, the parity is.

The chain can host at most $2N$ electrons, and so it has 2^{2N} eigenstates. Since this is a free Hamiltonian (quadratic), it can be diagonalized by introducing new fermionic operators,

$$\hat{d}_l = \sum_{j,s} u_{l,j,s}\hat{c}_{j,s} + v_{l,j,s}\hat{c}^\dagger_{j,s}; \tag{1.2}$$

$$\hat{d}^\dagger_l = \sum_{j,s} u^*_{l,j,s}\hat{c}^\dagger_{j,s} + v^*_{l,j,s}\hat{c}_{j,s}. \tag{1.3}$$

We require that the $\hat{d}_l$ obey fermionic commutation relations,

$$\{\hat{d}_l, \hat{d}_m\} = 0; \qquad \{\hat{d}_l, \hat{d}^\dagger_m\} = \delta_{lm}. \tag{1.4}$$

What requirements do the commutation relations impose on the coefficients $u_{l,j,s}$ and $v_{l,j,s}$?

These particles diagonalize the Hamiltonian in the sense that

$$\hat{H} = \sum_{l=1}^{2N} E_l \hat{d}^\dagger_l \hat{d}_l. \tag{1.5}$$

This looks very much like the standard procedure for free Hamiltonians, however, because of the superconducting pair potential, Δ, we cannot take $\hat{d}_l$ to be a linear combination of only electron annihilation operators, $\hat{c}_j$. This means that $\hat{d}_l$ and $\hat{d}^\dagger_l$ are described on the same footing. We can actually use this freedom to ensure that all of the $\hat{d}$ operators describe positive energy excitations:

$$E_l \geq 0. \tag{1.6}$$

This can be achieved by redefining the negative energy fermions as $\hat{d} \leftrightarrow \hat{d}^\dagger$.

Once we have found the operators $\hat{d}_l$, we can easily interpret the spectrum of $\hat{H}$ as consisting of states with a given number of fermions:

$$|0,\ldots,0,0,1\rangle = \hat{d}_1^\dagger |GS\rangle \tag{1.7}$$

$$|0,\ldots,0,1,0\rangle = \hat{d}_2^\dagger |GS\rangle \tag{1.8}$$

$$|0,\ldots,0,1,1\rangle = \hat{d}_2^\dagger \hat{d}_1^\dagger |GS\rangle \tag{1.9}$$

In the above definition, the Ground State $|GS\rangle$ of the Hamiltonian was introduced. This is a complicated state when expressed in the basis of the original fermions $\hat{c}_j$: it is in general a superposition of states with different particle numbers, since the Hamiltonian does not conserve particle number. However, since the Hamiltonian conserves the parity of the particle number, the ground state is a superposition of states with only odd, or only even number of particles ($\hat{c}_l$ fermions).

One way to construct the ground state $|GS\rangle$ is to turn the logic of the previous paragraph around. A state containing no $\hat{c}_l$ fermions, $|0\rangle$, is far from the ground state of the Hamiltonian, and can contain a superposition different number of excitations $\hat{d}$ fermions. Starting from such a simple state, we can take away all the components of it that contain excitations $\hat{d}$: then we are left with $|GS\rangle$, if the initial state had a $|GS\rangle$ component.

$$\hat{d}_{2N}\hat{d}_{2N-1}\ldots\hat{d}_1 |0\rangle = |GS\rangle \text{ or } 0. \tag{1.10}$$

The ground state can be certainly obtained if we remove all single-particle excitations from the mixture of all possible states,

$$|GS\rangle\langle GS| = \hat{d}_{2N}\hat{d}_{2N-1}\ldots\hat{d}_1 \left(\sum_{n_1=0}^{1}\cdots\sum_{n_{2N}=0}^{1} \hat{c}_{2N}^{\dagger n_{2N}}\ldots\hat{c}_1^{\dagger n_1}|0\rangle\langle 0|\hat{c}_1^{n_1}\ldots\hat{c}_{2N}^{n_{2N}}\right)\hat{d}_1^\dagger\hat{d}_2^\dagger\ldots\hat{d}_{2N}^\dagger. \tag{1.11}$$

1.2 The normal modes of a mean-field superconductor are obtained by diagonalizing the Bogoliubov–de Gennes Hamiltonian

The key to understanding the dynamics of the system is finding the coefficients $u_{l,j,s}, v_{l,j,s}$ of the eigenstates $\hat{d}_l$, as in Eq. (1.2). There is a trick to obtain these, called the Bogoliubov–de Gennes formalism, that involves a redundant representation of the states.

We begin by rewriting the Hamiltonian as

$$\hat{H} = \frac{1}{2}\sum_{l=1}^{2N} E_l(\hat{d}_l^\dagger\hat{d}_l - \hat{d}_l\hat{d}_l^\dagger) + \frac{1}{2}\sum_{l=1}^{2N} E_l. \tag{1.12}$$

Using a practical shorthand, this can be written as:

$$\hat{\mathbf{c}}^\dagger = (\hat{c}^\dagger_{1,\uparrow}, \hat{c}^\dagger_{1,\downarrow}, \ldots, \hat{c}^\dagger_{N,\uparrow}, \hat{c}^\dagger_{N,\downarrow}); \tag{1.13}$$

$$\hat{H} = \sum_{\alpha,\beta} \left(\hat{c}^\dagger_\alpha h_{\alpha,\beta} \hat{c}_\beta + \frac{1}{2} \hat{c}^\dagger_\alpha \Delta_{\alpha,\beta} \hat{c}^\dagger_\beta + + \frac{1}{2} \hat{c}_\beta \Delta^*_{\alpha,\beta} \hat{c}_\alpha \right); \tag{1.14}$$

$$\hat{H} = \frac{1}{2} \begin{pmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{pmatrix} \mathcal{H} \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} + \frac{1}{2} \mathrm{Tr} h; \tag{1.15}$$

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}, \tag{1.16}$$

where $\mathcal{H}$ is the matrix of the Bogoliubov-de Gennes Hamiltonian. The factors of $1/2$ were placed conveniently so as not to conflict with Eq. (1.1). Hermiticity of $\hat{H}$ implies h is Hermitian, and therefore, $h^* = h^T$. Since the electrons are fermions, Δ can be chosen to be a complex antisymmetric matrix, i.e.,

$$h_{\alpha,\beta} = h^*_{\beta,\alpha}; \tag{1.17}$$

$$\Delta_{\alpha,\beta} = -\Delta_{\beta,\alpha}. \tag{1.18}$$

Using these choices, the PHS symmetry, represented by $\Sigma_X K$, right away:

$$\Sigma_X = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}; \tag{1.19}$$

$$\Sigma_X \mathcal{H}^\star \Sigma_X = -\mathcal{H}. \tag{1.20}$$

Using the particle-hole symmetry of $\mathcal{H}$, we can diagonalize it using only the positive energy eigenstates,

$$\mathcal{H} \begin{pmatrix} u^*_j \\ v^*_j \end{pmatrix} = E_j \begin{pmatrix} u^*_j \\ v^*_j \end{pmatrix}, \quad \text{for } j = 1, \ldots, N; \tag{1.21}$$

$$\mathcal{H} \begin{pmatrix} v_j \\ u_j \end{pmatrix} = -E_j \begin{pmatrix} v_j \\ u_j \end{pmatrix}, \quad \text{for } j = 1, \ldots, N, \tag{1.22}$$

where the jth eigenvector of $\mathcal{H}$ was written as $(u_j, v_j)^\dagger$, with u_j and v_j both N-component vectors. Remember that $\mathcal{H}$ was a Hermitian matrix, and thus its eigenvectors form an orthonormal basis. We can then express $\mathcal{H}$ as

$$\mathcal{H} = \sum_j E_j \begin{pmatrix} u^*_j \\ v^*_j \end{pmatrix} \begin{pmatrix} u_j & v_j \end{pmatrix} - \sum_j E_j \begin{pmatrix} v_j \\ u_j \end{pmatrix} \begin{pmatrix} v^*_j & u^*_j \end{pmatrix} \tag{1.23}$$

Comparison with Eq. (1.12) reveals that the u's and the v's are truly the coefficients of the $\hat{c}$'s in the eigenmodes of the system, the $\hat{d}$ fermions, as per Eq. (1.2). Orthonormality of the eigenvectors translates to the required anticommutation relations.

1.3 Simplest case: single site

As an illustrative case, we consider the simplest mean-field superconductor, consisting of a single site. The Hamiltonian reads

$$\hat{H} \quad = \quad -\mu(\hat{c}_\uparrow^\dagger \hat{c}_\uparrow \ + \ \hat{c}_\downarrow^\dagger \hat{c}_\downarrow) \ + \ B(\hat{c}_\uparrow^\dagger \hat{c}_\uparrow \ - \ \hat{c}_\downarrow^\dagger \hat{c}_\downarrow) \ + \ \Delta \hat{c}_\uparrow^\dagger \hat{c}_\downarrow^\dagger \ + \ \Delta^* \hat{c}_\downarrow \hat{c}_\uparrow. \quad (1.24)$$

For such a small system, we can actually calculate everything in the Hilbert space of all states:

$$\hat{H} = \begin{pmatrix} |0\rangle & |\uparrow\downarrow\rangle & |\downarrow\rangle & |\uparrow\rangle \end{pmatrix} \begin{pmatrix} 0 & \Delta^* & & \\ \Delta & -2\mu & & \\ & & -\mu - B & \\ & & & -\mu + B \end{pmatrix} \begin{pmatrix} \langle 0| \\ \langle\uparrow\downarrow| \\ \langle\downarrow| \\ \langle\uparrow| \end{pmatrix} \quad (1.25)$$

$$(1.26)$$

This 4 by 4 matrix is composed of 2 blocks of 2 by 2 matrices, both of which have the form $X\sigma_x + Y\sigma_y + Z\sigma_z$. Since such matrices will occur often later on, we derive their spectrum here:

$$\begin{pmatrix} Z & X - iY \\ X + iY & -Z \end{pmatrix} \begin{pmatrix} X - iY \\ \pm E - Z \end{pmatrix} = \pm E \begin{pmatrix} X - iY \\ \pm E - Z \end{pmatrix}; \quad E = \sqrt{X^2 + Y^2 + Z^2}. \quad (1.27)$$

In our case,

$$E = \sqrt{|\Delta|^2 + \mu^2}. \quad (1.28)$$

The energy levels are shown in Fig. 1.1. We can interpret the energy levels by introducing μ, B and Δ sequentially. First, μ shifts the energy of all levels, depending on the number of

For weak magnetic fields, $B^2 < \mu^2 + \Delta^2$, the ground state is $|GS\rangle = -\Delta^* |0\rangle + (E + \mu) |\uparrow\downarrow\rangle$. For weak Δ, this can be approximated as $|GS\rangle \approx |0\rangle + \Delta/\mu |\uparrow\downarrow\rangle$.

The spectrum of $\hat{H}$ is symmetric around $E = -\mu$. This symmetry has nothing to do with superconductivity, it is a generic feature of free Hamiltonians, which can be explained simply. All energy levels can be obtained from the bottom up, starting with $|GS\rangle$, and adding particles $\hat{d}$, as indicated by the slashed lines. Alternatively, one can go top-down: with the state where all d fermions are present, and subtract the d's. The symmetry point can be shifted by onsite potentials, but is always there.

We now calculate this simplest case using the BdG formalism.

$$\hat{H} = \frac{1}{2} \begin{pmatrix} \hat{c}_\uparrow^\dagger & \hat{c}_\downarrow^\dagger & \hat{c}_\uparrow & \hat{c}_\downarrow \end{pmatrix} \underbrace{\begin{pmatrix} -\mu + B & 0 & 0 & \Delta \\ 0 & -\mu - B & -\Delta & 0 \\ 0 & -\Delta^* & \mu - B & 0 \\ \Delta^* & 0 & 0 & \mu + B \end{pmatrix}}_{\mathcal{H}} \begin{pmatrix} \hat{c}_\uparrow \\ \hat{c}_\downarrow \\ \hat{c}_\uparrow^\dagger \\ \hat{c}_\downarrow^\dagger \end{pmatrix}$$

$$(1.29)$$

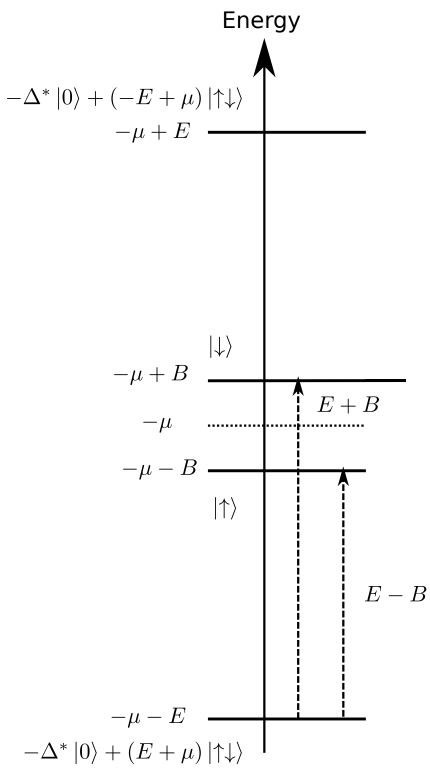

Figure 1.1: Energy levels of a single-site superconductor.

The BdG matrix $\mathcal{H}$ falls apart to two 2×2 matrices:

$$u^* \hat{c}_\uparrow + v^* \hat{c}_\downarrow^\dagger : B \pm E; \qquad \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \Delta \\ \mu \pm E \end{pmatrix} \tag{1.30}$$

$$u^* \hat{c}_\downarrow + v^* \hat{c}_\uparrow^\dagger : -B \pm E; \qquad \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -\Delta \\ \mu \pm E \end{pmatrix}. \tag{1.31}$$

These are 4 different d operators. However, they are not independent:

$$\left[\Delta^* \hat{c}_\uparrow + (\mu \pm E)\hat{c}_\downarrow^\dagger\right]^\dagger = (\mu \pm E)\, \hat{c}_\downarrow + \Delta\, \hat{c}_\uparrow^\dagger. \tag{1.32}$$

To compare the fermions on the rhs with the fermions from the "second batch", note that

$$\frac{\mu \pm E}{\Delta} = \frac{-\Delta^*}{\mu \mp E}, \tag{1.33}$$

which follows from $E^2 = \mu^2 + \Delta^2$.

In the weak magnetic field case, $B^2 < \mu^2 + |\Delta|^2$, the positive energy Bogoliubov operators are:

$$\hat{d}_1 = -\Delta^* \hat{c}_\downarrow + (\mu + E)\hat{c}_\uparrow^\dagger; \tag{1.34}$$

$$\hat{d}_2 = \Delta^* \hat{c}_\uparrow + (\mu + E)\hat{c}_\downarrow^\dagger. \tag{1.35}$$

To check consistency, you can verify that the recipe for the ground state based on the BdG formalism gives the same $|GS\rangle$ as calculated above,

$$|GS\rangle = \hat{d}_1 \hat{d}_2 |0\rangle = \hat{d}_1 \hat{d}_2 |\uparrow\downarrow\rangle. \tag{1.36}$$

1.4 Hopping

In a longer chain, it is more convenient to order the operators according to site first, then according to creation or annihilation, then spin. This makes the PHS less transparent, but it is easier to link with a general tight binding Hamiltonian.

$$\frac{1}{2} \begin{pmatrix} \hat{c}_{1,\uparrow}^\dagger & \hat{c}_{1,\downarrow}^\dagger & \hat{c}_{2,\uparrow}^\dagger & \hat{c}_{2,\downarrow}^\dagger & \hat{c}_{1,\uparrow} & \hat{c}_{1,\downarrow} & \hat{c}_{2,\uparrow} & \hat{c}_{2,\downarrow} \end{pmatrix} \mathcal{H} \begin{pmatrix} \hat{c}_{1,\uparrow} \\ \hat{c}_{1,\downarrow} \\ \hat{c}_{2,\uparrow} \\ \hat{c}_{2,\downarrow} \\ \hat{c}_{1,\uparrow}^\dagger \\ \hat{c}_{1,\downarrow}^\dagger \\ \hat{c}_{2,\uparrow}^\dagger \\ \hat{c}_{2,\downarrow}^\dagger \end{pmatrix} \tag{1.37}$$

1.5 p-wave SC

(Introduction to *p*-wave).

Assume no s-wave Δ, only p-wave. The simplest model is a spin polarized chain:

$$\hat{H} = \sum_j V_j \hat{c}_j^\dagger \hat{c}_j + \sum_j \left(\Delta_j^* \hat{c}_{j+1} \hat{c}_j - t_j \hat{c}_j^\dagger \hat{c}_{j+1} + h.c. \right) \tag{1.38}$$

We use the convention of the Alicea review, without the unnecessary factor of 1/2.

The BdG Hamiltonian reads

$$\mathcal{H} = \begin{pmatrix} V_1 & 0 & -t_1 & \Delta_1 & & & -t_N^* & -\Delta_N \\ 0 & -V_1 & -\Delta_1^* & t_1^* & & & \Delta_N^* & t_N \\ -t_1^* & -\Delta_1 & V_2 & 0 & -t_2 & \Delta_2 & & \\ \Delta_1^* & t_1 & 0 & -V_2 & -\Delta_2^* & t_2^* & & \\ & & -t_2^* & -\Delta_2 & V_3 & 0 & -t_3 & \Delta_3 \\ & & \Delta_2^* & t_2 & 0 & -V_3 & -\Delta_3^* & t_3^* \\ -t_N & \Delta_N & & & -t_3^* & -\Delta_3 & V_N & 0 \\ -\Delta_N^* & t_N^* & & & \Delta_3^* & t_3 & 0 & -V_N \end{pmatrix}, \tag{1.39}$$

where we supressed the 2×2 zero matrices for better readability.

This can be written as

$$\sum_j \hat{d}_j^\dagger U_j \hat{d}_j + \sum_j \hat{d}_j^\dagger T_j \hat{d}_{j+1} \tag{1.40}$$

using the notation $\hat{d}_j^\dagger = (c_j\dagger, c_j)$. This has the same form as a usual nearest neighbor hopping Hamiltonian, with

$$U_j = V_j \sigma_z; \qquad T_j = -\sigma_z \mathrm{Re}\, t_j - i \mathrm{Im}\, t_j + i\sigma_y \mathrm{Re}\,\Delta_j + i\sigma_x \mathrm{Im}\,\Delta_j. \tag{1.41}$$

In the translation invariant bulk, we can look for eigenstates of $\mathcal{H}$ in the form of $\hat{d}_j = \hat{d}_1 e^{ikj}$. This choice of sign of k is so we have the same formulas as for ordinary Hamiltonians. Bear in mind though, that because of the extra complex conjugation, we have $d(k) = \sum_j (\hat{d}_{j,1}^* c_j + \hat{d}_{j,2}^* c_j^\dagger) e^{-ikj}$. The BdG Hamiltonian reads,

$$\mathcal{H}(k) = U + (T + T^\dagger)\cos k + i(T - T^\dagger)\sin k; \tag{1.42}$$

$$\mathcal{H}(k) = (V - 2\,\mathrm{Re}\, t \cos k)\sigma_z + 2 \sin k (\mathrm{Im}\, t - \sigma_y \mathrm{Re}\,\Delta - \sigma_x \mathrm{Im}\,\Delta). \tag{1.43}$$

To see the antiunitary symmetries of this Hamiltonian, consider its complex conjugate (remember that we conjugate in real space, meaning k flips sign too):

$$K\mathcal{H}(k)K = (V - 2\,\mathrm{Re}\, t \cos k)\sigma_z + 2 \sin k (\mathrm{Im}\, t + \sigma_y \mathrm{Re}\,\Delta - \sigma_x \mathrm{Im}\,\Delta). \tag{1.44}$$

There is a sign flip in the term proportional to σ_0, this cannot be undone by conjugation via a unitary operator. This means that we can only have TRS if

$t \in \mathbb{R}$. Even then, we would need to undo the sign flip the σ_x term only, which cannot be done in a unitary way. So we have TRS, represented by K, only if both t and Δ are real.

For PHS, all terms in $\mathcal{H}$ need to undergo a sign flip. We need an extra sign flip for the σ_z and the σ_y terms, which can be achieved by a σ_x operator:

$$\sigma_x K \mathcal{H}(k) K \sigma_x = \sigma_x \mathcal{H}(-k) \sigma_x = -\mathcal{H}(k). \tag{1.45}$$

Thus, we have PHS, represented by $\sigma_x K$ which squares to $+1$, and possibly also TRS, represented by K, which squares to $+1$. So we are either in class D, or in BDI. We look at class D first.

Express the topological invariant via the polarization.

For a 2-band Hamiltonian, this has a practical graphical representation.

$$\mathcal{H}(k) = \vec{h}(k)\vec{\sigma} = h_x(k)\sigma_x + h_y(k)\sigma_y + h_z(k)\sigma_z; \tag{1.46}$$

$$K\mathcal{H}(k)K = \mathcal{H}^*(-k) = \vec{h}(-k)\vec{\sigma}^* = h_x(-k)\sigma_x - h_y(-k)\sigma_y + h_z(-k)\sigma_z; \tag{1.47}$$

$$\sigma_x K \mathcal{H}(k) K \sigma_x = h_x(-k)\sigma_x + h_y(-k)\sigma_y - h_z(-k)\sigma_z; \tag{1.48}$$

This gives as requirement for PHS,

$$h_{x,y}(k) = -h_{x,y}(-k); \qquad h_z(k) = h_z(-k). \tag{1.49}$$

At the TRI momenta $k = 0$ and $k = \pi$, this simplifies to $h_{x,y}(k = 0, \pi) = 0$. Since the gap has to remain open, we have 4 distinct options as to the sign of $h_z(0)$ and $h_z(\pi)$. Consider the path of the unit vector of $\vec{h}(k)$,

$$\vec{n}(k) = \vec{h}(k) / \left| \vec{h}(k) \right|, \tag{1.50}$$

on the Bloch sphere. Looking at the path from the North Pole, it either comes back there from $k = 0 \to \pi$, in which case, the path looks like an 8, or goes to the South Pole, in which case it looks like a 0. Because of PHS, the path from $k = 0 \to -\pi$ is the mirror image of the path from $k = 0 \to \pi$. In the "8" case, this mirroring undoes any Berry phase obtained, so the polarization is 0. In the "0" case, it ensures that the surface of the sphere is cut into 2 equal halves, thus giving a Berry phase of π, polarization of 1/2.

We can express the topological invariant in a straightforward way in the basis where PHS is represented by K, i.e., after transformation by σ_x (by Σ_x in the general case).

Chapter 2

The Kitaev Wire is mapped to the SSH model using Majorana Fermions

2.1 The Kitaev Wire and the SSH model are in the same universality class

The Kitaev wire has the same fundamental symmetries as the SSH model, as listed in Table 2.1. Therefore the BdG Hamiltonian of the Kitaev wire can host robust edge states.

2.1.1 The mapping is made explicit by a basis transformation

To map the Kitaev wire onto the SSH model, we can use a unitary rotation to map σ_x to σ_z. This is achieved by

$$\mathcal{H}' = e^{i\pi/4\,\sigma_y}\mathcal{H}e^{-i\pi/4\,\sigma_y} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\mathcal{H}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{2.1}$$

	Kitaev	SSH	Kitaev MF
PHS (+1)	$\sigma_x\mathcal{H}^*\sigma_x = -\mathcal{H}$	$\sigma_z H_{\text{SSH}}^*\sigma_z = -H_{\text{SSH}}$	$\mathcal{A}^* = \mathcal{A}$
TRS (+1)	$\mathcal{H}^* = \mathcal{H}$	$H_{\text{SSH}}^* = H_{\text{SSH}}$	$\sigma_z\mathcal{A}^*\sigma_z = -\mathcal{A}$
CS	$\sigma_x\mathcal{H}\sigma_x = -\mathcal{H}$	$\sigma_z H_{\text{SSH}}\sigma_z = -H_{\text{SSH}}$	$\sigma_z\mathcal{A}\sigma_z = -\mathcal{A}$

Table 2.1: The symmetries of the Kitaev wire and the Su–Schrieffer–Heeger (SSH) model. In the last column, the representation of the symmetries on the real matrix $\mathcal{A}$ representing the Kitaev wire with Majorana Fermions.

Substituting Eq. (1.16), this corresponds to

$$\mathcal{H}' = \begin{pmatrix} i(\operatorname{Im} h + \operatorname{Im}\Delta) & -\operatorname{Re} h + \operatorname{Re}\Delta \\ -\operatorname{Re} h - \operatorname{Re}\Delta & i(\operatorname{Im} h - \operatorname{Im}\Delta) \end{pmatrix}. \tag{2.2}$$

This is a Hermitian matrix because h is Hermitian and Δ is antisymmetric.

On the level of the fermion operators, this corresponds to

$$\hat{H} - \frac{1}{2}\mathrm{Tr}h = \frac{1}{8}\begin{pmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \mathcal{H} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} \tag{2.3}$$

$$= \frac{1}{8}\begin{pmatrix} \hat{\mathbf{b}} & i\hat{\mathbf{a}} \end{pmatrix} \mathcal{H}' \begin{pmatrix} \hat{\mathbf{b}} \\ -i\hat{\mathbf{a}} \end{pmatrix}, \tag{2.4}$$

where we introduced Majorana fermions according to

$$\hat{b}_j = \hat{c}_j + \hat{c}_j^\dagger; \tag{2.5a}$$

$$\hat{a}_j = \frac{\hat{c}_j - \hat{c}_j^\dagger}{i}. \tag{2.5b}$$

These so-called Majorana fermions are often used to treat superconducting systems. They are self-adjoint fermionic operators, so that for any j, l:

$$\{\hat{a}_j, \hat{b}_l\} = 0; \tag{2.6}$$

$$\{\hat{a}_j, \hat{a}_l\} = \{\hat{b}_j, \hat{b}_l\} = \delta_{jl}. \tag{2.7}$$

The symmetries of $\mathcal{H}'$ are represented by the same operators as those of the SSH model.

2.1.2 A next basis transformation to Majorana Fermions makes the role of PHS more transparent

Since it is PHS that plays a central role, it is worthwhile to make yet another basis transformation that simplifies its representation. We define

$$\mathcal{H}'' = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \mathcal{H}' \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}. \tag{2.8}$$

We then have

$$\mathcal{H}''^* = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \mathcal{H}'^* \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \sigma_z \mathcal{H}'^* \sigma_z \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} = -\mathcal{H}''. \tag{2.9}$$

In other words, $\mathcal{H}''$ is a Hermitian matrix with all elements purely imaginary. Thus it can be written as i times a real antisymmetric matrix,

$$\mathcal{H}'' = i\mathcal{A}; \quad A_{mn} \in \mathbb{R} \quad \text{for } m, n = 1, \ldots, 2n; \tag{2.10}$$

$$\mathcal{A} = -i \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \mathcal{H} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} = \begin{pmatrix} \operatorname{Im} h + \operatorname{Im}\Delta & \operatorname{Re} h - \operatorname{Re}\Delta \\ -\operatorname{Re} h - \operatorname{Re}\Delta & \operatorname{Im} h - \operatorname{Im}\Delta \end{pmatrix}. \tag{2.11}$$

On the level of the Fock-space Hamiltonian, this corresponds to rewriting it in terms of the Majorana fermions,

$$\hat{H} - \frac{1}{2}\mathrm{Tr}h = \frac{i}{8}\begin{pmatrix}\hat{\mathbf{b}} & \hat{\mathbf{a}}\end{pmatrix}\mathcal{A}\begin{pmatrix}\hat{\mathbf{b}} \\ \hat{\mathbf{a}}\end{pmatrix}. \tag{2.12}$$

Time-reversal and chiral symmetries

If the matrix elements of $\mathcal{H}$ are all real, we also have time-reversal symmetry. This translates to reality of matrix elements of $\mathcal{H}'$, and thus,

$$\sigma_z \mathcal{H}''^* \sigma_z = \mathcal{H}''; \tag{2.13}$$

$$\sigma_z \mathcal{A}^* \sigma_z = -\mathcal{A}. \tag{2.14}$$

In the time-reversal symmetric case, get chiral symmetry for free, which is represented on $\mathcal{H}''$ in the same way as in the SSH model,

$$\sigma_z \mathcal{H}'' \sigma_z = -\mathcal{H}''; \tag{2.15}$$

$$\sigma_z \mathcal{A} \sigma_z = -\mathcal{A}. \tag{2.16}$$

2.1.3 The Kitaev wire is more robust

The topological protection of the edge states in the SSH model depended on two fragile features: the robustness of the chiral symmetry and the indivisibility of the unit cell. An isolated edge state can be moved away from 0 energy by breaking chiral symmetry. This is easily realized, e.g., using an onsite potential. On the other hand, just changing the chain termination by adding an extra site is enough to move a bound state from 0 energy as well.

In the Kitaev wire, both the particle-hole symmetry and the indivisibility of the unit cell are hardwired into the formalism, and therefore are robust. Thus Majorana fermions as end states are more robust.

2.2 Majorana fermion operators have simple properties

Given a set $\underline{\hat{\gamma}}$ of Majorana fermions,

$$\underline{\hat{\gamma}} = \{\hat{\gamma}_1, \hat{\gamma}_2 \ldots, \hat{\gamma}_{2n}\} = a_1, b_1, a_2, b_2, \ldots, a_n, b_n, \tag{2.17}$$

we consider some of their properties.

2.2.1 Majorana fermions transform well under real orthogonal transformations

If we mix Majorana fermion operators using a real orthogonal transformation,

$$\underline{\hat{\eta}} = \underline{\underline{\mathcal{O}}}\,\underline{\hat{\gamma}}, \tag{2.18}$$

$$\tag{2.19}$$

the new operators $\hat{\eta}_j$ are also Majorana fermions.

This property is useful later when we use the Pfaffian.

2.2.2 For complex pair potential, there is a more practical way to introduce Majorana fermions

The norm of the Majorana fermions is chosen so that for any site, $\hat{a}_j^2 = \hat{b}_j^2 = 1$. It is simple to see that the only way to introduce these operators is:

$$\hat{b}_j = e^{-i\phi_j/2}\hat{c}_j + e^{i\phi_j/2}\hat{c}_j^\dagger; \tag{2.20a}$$

$$\hat{a}_j = -i\left(e^{-i\phi_j/2}\hat{c}_j - e^{i\phi_j/2}\hat{c}_j^\dagger\right). \tag{2.20b}$$

These relations can be inverted to give

$$\hat{c}_j = \frac{e^{i\phi_j/2}}{2}(\hat{b}_j + i\hat{a}_j); \tag{2.21a}$$

$$\hat{c}_j^\dagger = \frac{e^{-i\phi_j/2}}{2}(\hat{b}_j - i\hat{a}_j). \tag{2.21b}$$

The Hermitian ("real") Majorana fermion operators are the "real parts" and "imaginary parts" of the original ("complex") fermion operators $\hat{c}$. There is a free parameter ϕ_j, which we can set to the phase of the p-wave order parameter: $\Delta_j = \Delta_j e^{i\phi_j}$, with Δ_j denoting its absolute value.

Rewriting the Hamiltonian in terms of the Majorana operators introduced in Eq. (2.20) above, corresponds to a transformation on the Bogoliubov-de Gennes Hamiltonian. Starting from Eq. (1.15), we have:

The matrix A associated to the BdG Hamiltonian is real and skew-symmetric.

2.3 Pfaffian and the ground-state parity

The fermion parity of the ground state is a topological invariant of a 0-dimensional superconductor. In the noninteracting case it can be directly computed from the Bogoliubov-de Gennes Hamiltonian using the Pfaffian.

2.3.1 Pfaffian

In this section we review the Pfaffian, an important tool for skew symmetric matrices.

We consider an $M \times M$ skew symmetric matrix A, with matrix elements a_{lm}, i.e.,

$$A^T = -A; \quad a_{lm} = -a_{ml}. \tag{2.22}$$

The determinant of such a matrix is a homogeneous Mth order polynomial of its matrix elements.

If the matrix is odd dimensional, $M = 2N + 1$, its determinant vanishes;

$$M = 2N + 1: \quad \det A = \det A^T = \det(-A) = (-1)^{2N+1} \det A = -\det A. \tag{2.23}$$

If, on the other hand, the matrix is even dimensional, the determinant can be written as the complete square of a homogeneous $M/2$th order polynomial of the matrix elements. This polynomial is known as the Pfaffian.

$$M = 2N: \quad \det A = (\mathrm{Pf} A)^2. \tag{2.24}$$

Its definition and further properties follow below.

The Pfaffian is a homogeneous polynomial of the matrix elements

The polynomial is defined in the following way. Consider the partitions of the indices $\{1, 2, \ldots, 2N\}$ into pairs, without regard to order,

$$\alpha = \{(j_1, m_1), (j_2, m_2), \cdots, (j_n, m_n)\}, \tag{2.25}$$

with $j_n < m_n$ for every $n = 1, \ldots, N$, and $j_1 < j_2 < \ldots < j_N$. We can regard each partition as a permutation,

$$\pi_\alpha = \begin{bmatrix} 1 & 2 & 3 & 4 & \cdots & 2n-1 & 2n \\ i_1 & j_1 & i_2 & j_2 & \cdots & i_n & j_n \end{bmatrix}. \tag{2.26}$$

The Pfaffian is

$$\mathrm{Pf}(A) = \sum_{\alpha \in \Pi} \mathrm{sgn}(\pi_\alpha) a_{i_1,j_1} a_{i_2,j_2} \cdots a_{i_n,j_n}. \tag{2.27}$$

Important properties

We list some important properties of the Pfaffian, which are easy to prove or are detailed in the notes by Haber.

For a block-diagonal matrix, we have

$$A_1 \oplus A_2 = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}; \tag{2.28}$$

$$\mathrm{Pf}(A_1 \oplus A_2) = \mathrm{Pf}(A_1)\mathrm{Pf}(A_2). \tag{2.29}$$

For an arbitrary $2N \times 2N$ matrix B,

$$\mathrm{Pf}(BAB^T) = \det(B)\mathrm{Pf}(A). \tag{2.30}$$

The Pfaffian is related to the normal form

The Householder transformations are normally used to bring a real symmetric matrix to a tridiagonal form. They are conjugations by suitably chosen orthogonal matrices P_j, each has determinant -1. See the note attached.

Take a real and skew-symmetric matrix A.

$$P_{2N} \dots P_2 P_1 A P_1 P_2 \dots P_{2N} = A_{\mathrm{tri}}, \tag{2.31}$$

where

$$A_{\mathrm{tri}} = \begin{pmatrix} 0 & \lambda_1 & 0 & 0 & \dots & 0 \\ -\lambda_1 & 0 & \lambda_2 & 0 & \dots & 0 \\ 0 & -\lambda_2 & 0 & \ddots & \dots & \vdots \\ & & \ddots & 0 & \ddots & \\ 0 & & & \ddots & 0 & \lambda_{N-1} \\ \vdots & & \vdots & & -\lambda_{N-1} & 0 \end{pmatrix} \tag{2.32}$$

It can easily be shown that the Pfaffian of such a matrix is the product of half of the λ,

$$\mathrm{Pf}(A_{\mathrm{tri}}) = \lambda_1 \lambda_3 \dots \lambda_{N-1}. \tag{2.33}$$

Using the property in Eq. (2.30) above,

$$\mathrm{Pf}(A) = \det(P_1)\det(P_2)\dots\det(P_{2N})\mathrm{Pf}(A_{\mathrm{tri}}) = \lambda_1 \lambda_3 \dots \lambda_{N-1}. \tag{2.34}$$

2.4 Pfaffian of the Bogoliubov-de Gennes Hamiltonian is the ground state parity

2.5 Exercises

Express the Hamiltonian in the Majorana basis. Show that in the simple cases a) $\Delta = t = 0$ and b) $\mu = 0$, $\Delta = \pm\mu$ the Hamiltonian can be diagonalized easily. What are the independent fermionic operators d?