Chapter 4

Two-dimensional topological superconductor

The simplest toy model for a two-dimensional topological superconductor is obtained by transcribing the Qi-Wu-Zhang model. The bulk momentum-space Hamiltonian of the Qi-Wu-Zhang model reads

$$\hat{H}_{QWZ}(k) = \begin{pmatrix} \cos k_x + \cos k_y + u & \sin k_x + i \sin k_y \\ \sin k_x - i \sin k_y & -\cos k_x - \cos k_y - u \end{pmatrix}, \tag{4.1}$$

where we used w for the enegy scale of the hopping amplitude. We can reinterpret this as a BdG Hamiltonian, introducing some extra parameters, as

$$\hat{H}_{p+ip}(k) = \begin{pmatrix} -w \cos k_x - w \cos k_y - \mu & -i\Delta \sin k_x + \Delta \sin k_y \\ i\Delta^* \sin k_x + \Delta^* \sin k_y & w \cos k_x + w \cos k_y + \mu \end{pmatrix}. \tag{4.2}$$

The superconducting order parameter in our toy model is not only nonlocal (p-wave), but also direction-dependent. There is a relative phase of i between the Cooper pairs created from $x-$ and $y-$ neighbors. For this reason, this model is called $p_x + ip_y$, or even shorter, $p + ip$. One might worry that this is not too realistic, and indeed, it is not clear whether it is actually realized in nature, although $SrRuO_4$ is a strong candidate.

The corresponding real-space lattice Hamiltonian reads,

$$\begin{aligned} \hat{H}_{p+ip} = \frac{1}{2} \sum_{m,l=1}^{N} \Big(- w \hat{c}^\dagger_{m,l} \hat{c}_{m+1,l} - w \hat{c}^\dagger_{m,l} \hat{c}_{m,l+1} + h.c. \Big) - \mu \sum_{m,l=1}^{N} \hat{c}^\dagger_{m,l} \hat{c}_{m,l} \\ + \frac{1}{2} \sum_{m,l=1}^{N} \Big(\Delta \hat{c}^\dagger_{m+1,l} \hat{c}^\dagger_{m,l} + i\Delta \hat{c}^\dagger_{m,l+1} \hat{c}^\dagger_{m,l} + h.c. \Big). \end{aligned} \tag{4.3}$$

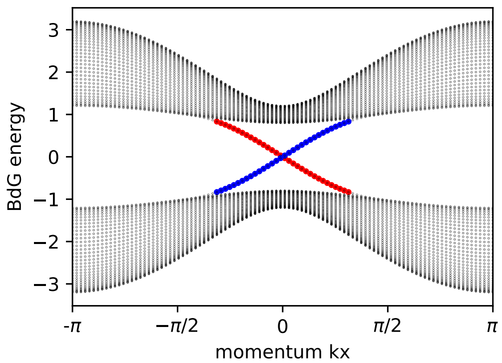

Figure 4.1: Dispersion relation of a strip of $p + ip$ superconductor. Red/blue are states localized on lower/upper edge (with 80% of probability within 2 sites of the boundary). Their wavefunction is equal weight particle and hole, within numerical accuracy.

4.1 Chern number, edge modes

We can apply everything we know about Chern insulators to this two-dimensional topological superconductor (maybe it is time for you to revise the first semester). This can be a gapped system with a bulk topological invariant: the Chern number Q, with

$$
\begin{aligned}
2w < \mu : \quad & Q = 0; & \text{(4.4a)}\\
0 < \mu < 2w : \quad & Q = 1; & \text{(4.4b)}\\
-2w < \mu < 0 : \quad & Q = -1; & \text{(4.4c)}\\
\mu < -2w : \quad & Q = 0. & \text{(4.4d)}
\end{aligned}
$$

Correspondingly, in the gapped topological phases there are edge states, which propagate in one direction only along the edge. Such states are called “chiral”.

The edge states are not Majorana zero modes, but Majorana fermions, branches of the dispersion relation whose negative-energy part is the particle-hole symmetric partner of the positive-energy part. They therefore have to cross $E = 0$ at either $k = 0$ or $k = \pi$. At the crossing point there is a state that is its own particle-home symmetry partner, and thus a Majorana zero mode.

To get more of an intuition for these Majorana fermion modes, we need to do an envelope function approximation for them, as we did for chiral edge modes of Chern insulators in the previous semester. We are looking for eigenstates of the linearized BdG Hamiltonian,

$$\begin{pmatrix} -\mu & \Delta(-\partial_x - i\partial_y) \\ \Delta^*(\partial_x - i\partial_y) & \mu \end{pmatrix} \underbrace{\begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix}}_{\Psi(x,y)} = E \begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix}. \tag{4.5}$$

We take a setup with a boundary tilted at an angle θ with the y-axis (this also gives us an orientation). On the one side of the boundary is the sample, with $\mu > 0$ (trivial). On the other side of the boundary is the vacuum: in this equation, we can realize a vacuum by pushing up the dispersion relation of the electrons, taking μ to large negative values. For simplicity, we take $\Delta = |\Delta| e^{i\phi}$ to be constant. This would involve having a pair potential also in the vacuum, but since there is no density of states at 0 there anyway, this is not a problem.

For each energy E, we are looking for two eigenstates, that are plane-wave-like along the boundary, with wavenumbers to be specified. Actually, we will fix the wavenumber k, and find the corresponding energies E during the calculation; we will then verify if we have found two solutions for every energy. We take rotated coordinates to fit with the boundary:

$$x' = \cos\theta x - \sin\theta y; \qquad \partial_x = \cos\theta \partial_{x'} + \sin\theta \partial_{y'}; \tag{4.6}$$

$$y' = \cos\theta y + \sin\theta x; \qquad \partial_y = \cos\theta \partial_{y'} - \sin\theta \partial_{x'}, \tag{4.7}$$

where the equations on the right were derived using the chain rule, e.g., $\partial_x = \partial_x x' \partial_{x'} + \partial_x y' \partial_{y'}$. Substituting these and $-i\partial_{y'} = k$ into the BdG eigenvalue equation, we obtain

$$\begin{pmatrix} -\mu & \Delta e^{-i\theta}(-\partial_{x'} + k) \\ \Delta^* e^{i\theta}(\partial_{x'} + k) & \mu \end{pmatrix} \begin{pmatrix} u(x') \\ v(x') \end{pmatrix} = E \begin{pmatrix} u(x') \\ v(x') \end{pmatrix}. \tag{4.8}$$

We can now use an Ansatz:

$$u(x') = \pm e^{i(\phi-\theta)} v(x'). \tag{4.9}$$

Substituting this into the eigenvalue equation, we get a system of two equations:

$$\mp\mu e^{i(\phi-\theta)} v + k\Delta e^{-i\theta} v - \Delta e^{-i\theta} \partial_{x'} v = \pm E e^{i(\phi-\theta)} v; \tag{4.10}$$

$$\pm |\Delta| \partial_{x'} v \pm |\Delta| k v + \mu v = E v. \tag{4.11}$$

Now taking $\pm e^{-i(\phi-\theta)}$ times the first equation plus and minus the second equation, we get

$$\pm |\Delta| k = E; \tag{4.12}$$

$$-2\mu v(x') \mp 2 |\Delta| \partial_{x'} v(x') = 0. \tag{4.13}$$

The first equation shows us that these solutions are dispersionless chiral states propagating along the edge, in positive or negative direction. The second equation is solved by integration, and we obtain

$$\Psi(x', y') = \begin{pmatrix} \pm e^{i(\phi-\theta)} \\ 1 \end{pmatrix} \exp\left[\int_0^{x'} \frac{\pm\mu(x'')}{|\Delta|} dx''\right] e^{iky'}. \tag{4.14}$$

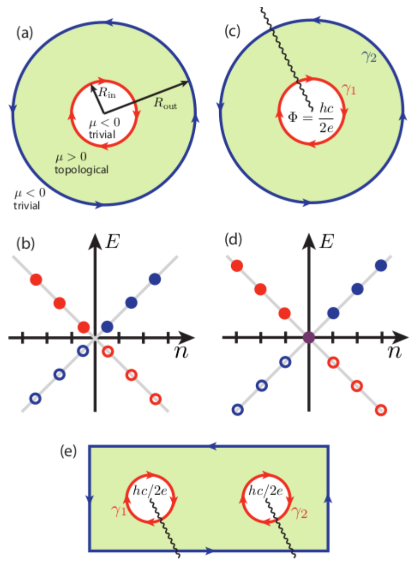

FIG. 4. (a) A topological $p + ip$ superconductor on an annulus supports chiral Majorana edge modes at its inner and outer boundaries. (b) Energy spectrum versus angular momentum n for the inner (red circles) and outer (blue circles) edge states in the setup from (a). Here n takes on half-integer values because the Majorana modes exhibit anti-periodic boundary conditions on the annulus. An $\frac{hc}{2e}$ flux piercing the central trivial region as in (c) introduces a branch cut (wavy line) which, when crossed, leads to a sign change for the Majorana edge modes. The flux therefore changes the boundary conditions to periodic and shifts n to integer values. This leads to the spectrum in (d), which includes Majorana zero-modes γ_1 and γ_2 localized at the inner and outer edges. The two-vortex setup in (e) supports one Majorana zero-mode localized around each puncture, while the outer boundary remains gapped.

Figure 4.2: Figure with caption from the review "New directions in the pursuit of Majorana fermions in solid state systems" by Jason Alicea

Although these are both eigenstates, only one of them is normalizable. When this is a left edge, i.e., $\mu > 0$ for $x' \to \infty$ and $\mu < 0$ for $x' \to -\infty$, it is the solution where the $\pm$ should be taken as $+$, a state propagating in the positive y' direction. On a right edge, i.e., $\mu < 0$ for $x' \to \infty$ and $\mu > 0$ for $x' \to -\infty$, it is the solution where the $\pm$ should be taken as $-$, a state propagating in the negative y' direction.

So for every energy E we have found only one edge state, propagating with velocity $|\Delta|$ along the boundary in a chiral way. The (Nambu) spinor $(u, v)^T$ describing the particle-hole structure of the Majorana edge modes is in the xy plane. Moreover, its angle follows the phase of the superconducting pair potential $\Delta(k)$, corresponding to the direction of propagation of the edge mode.

4.2 Majorana zero modes at the centers of magnetic vortices

If we take a sample of the $p+ip$ superconductor with a disk shape, we find chiral Majorana edge modes around the perimeter. These have allowed wavenumbers along the edge, which are quantized due to the finite size of the sample. They have to cross $E = 0$ at either $k = 0$ or $k = \pi$, and at the crossing point, there should be a Majorana Zero Mode. However, because of the finite size of the sample, wavenumber of the edge modes is quantized: not all wavenumbers are allowed, i.e., compatible with the boundary conditions around the perimeter. Is $k = 0$ an allowed wavenumber for Majorana edge modes on a disk?

Naively, one might expect that the boundary conditions for edge modes are periodic, and thus, $k = 0$, which respects these boundary conditions, is always allowed. However, chiral edge modes also have an internal degree of freedom, their particle-hole structure, which is analogous to a spin-half. And, just like with edge states of Chern insulators, their spin is oriented along the boundary. Therefore, after one round trip, this spin has turned around once, bringing a factor of (-1). Therefore, the boundary conditions required for Majorana fermions are in fact *antiperiodic*. Thus, no edge states at $k = E = 0$.

A way to create a Majorana Zero Mode edge state at $k = 0$ and $E \approx 0$ is to change boundary conditions for edge states by inserting a magnetic field through the middle of the disk. The magnetic field is shielded by the superconductor, falling off exponentially with the distance, with a characteristic London penetration depth λ, as in the Abrikosov vortices. Thus, far away from the vortex core, the magnetic field is no longer present. However, there is an Aharonov-Bohm phase picked up by the electrons, and this results in a twisting of the phase of the superconducting pair potential:

$$\text{vortex at } 0,\ r \gg \lambda\text{:}\ \Delta(x = r\cos\theta, y = r\sin\theta) = e^{i\Phi/\Phi_0\theta}\Delta(x = r, y = 0), \tag{4.15}$$

with Φ denoting the total magnetic flux in the vortex, and $\Phi_0 = e/(\pi\hbar)$ the superconducting flux quantum. Because the pair potential Δ has to be single valued, the magnetic flux inserted in a vortex has to be an integer multiple of the flux quantum.

We can now understand why, for a large disk, inserting a flux quantum through the middle of the disk brings with it a Majorana zero mode on the boundary, at $k = 0$. The Nambu spinor of the edge mode should rotate as we go around the perimeter, because it follows the phase of the pair potential, which follows the direction of propagation along the edge - one rotation for one round trip. However, introducing an odd number of flux quanta in a vortex in the middle of the disk results in an odd number of extra rotations – altogether, an even number of rotations of the spinor, and thus, no extra phase of -1. Hence, not antiperiodic, but periodic boundary conditions.

4.2.1 Gauge transformation

In a numerical model, it is convenient to do a gauge transformation to represent the effects of the vortex with less numerical effort. A gauge transformation changes the phases of terms in a lattice Hamiltonian, such as Eq. (4.3), in such a way that the spectrum is invariant. We start with a real phase field, $\Lambda_{\mathbf{r}} = \Lambda_{m,l} \in \mathbb{R}$, and we transform the creation and annihilation operators,

$$\hat{c}_{\mathbf{r}} \to \hat{c}_{\mathbf{r}} e^{i\Lambda_{\mathbf{r}}}; \qquad \hat{c}_{\mathbf{r}}^\dagger \to \hat{c}_{\mathbf{r}}^\dagger e^{-i\Lambda_{\mathbf{r}}}. \tag{4.16}$$

If we do this transformation of the Hamiltonian, the spectrum does not change: the same Bogoliubov tranformation diagonalizes the Hamiltonian as before, only in terms of the transformed operators. Formulated differently: the above transformation is a unitary tranformation on the BdG Hamiltonian, and therefore does not change the spectrum.

The gauge transformation above can also be realized on the amplitudes of the hopping and superconducting terms in the lattice Hamiltonian. We therefore learn that the following transformation,

$$w_{\mathbf{r}',\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}'}\hat{c}_{\mathbf{r}}; \quad w_{\mathbf{r}',\mathbf{r}} \to w_{\mathbf{r}',\mathbf{r}}e^{-i(\Lambda_{\mathbf{r}}-\Lambda_{\mathbf{r}})}; \tag{4.17}$$

$$\Delta_{\mathbf{r}',\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}'}\hat{c}^\dagger_{\mathbf{r}}; \quad \Delta_{\mathbf{r}',\mathbf{r}} \to \Delta_{\mathbf{r}',\mathbf{r}}e^{-i(\Lambda_{\mathbf{r}}+\Lambda_{\mathbf{r}'})}, \tag{4.18}$$

does not change the spectrum.

An important application is that a position-independent change in the phase of Δ can always be gauged away.

$$\Delta_{\mathbf{r}',\mathbf{r}} \to \Delta_{\mathbf{r}',\mathbf{r}}e^{i\phi} \quad \Leftrightarrow \hat{c}_{\mathbf{r}} \to e^{i\phi/2}\hat{c}_{\mathbf{r}} \tag{4.19}$$

Another interesting application of a gauge transformation is on a vortex carrying one quantum of magnetic flux. Here the phase of the pair potential Δ winds around the vortex core. However, a gauge tranformation can get rid of this winding, using

$$\Lambda(x = r\cos\theta, y = r\sin\theta) = \theta. \tag{4.20}$$

As a result, the phase of the superconductor is uniform. However, all hoppings and pair potentials crossing the line going from the origin to positive infinity along x obtain an extra factor of -1, according to the rules of gauge transformation above. This gives us another way to see that the boundary conditions along the edge change from antiperiodic to periodic as flux quanta are threaded through the center of the disk.

4.2.2 Majorana zero mode at the vortex core

The core of a vortex with odd number of superconducting flux quanta hosts a Majorana zero mode. We can understand this by starting with a Corbino geometry, as in Fig. 4.2. The core is obtained by letting the radius of the inner (red) circle go to zero. In the case with an odd number of flux quanta threading the ring, there is always a Majorana zero mode there with $k = 0$, which has to remain there even if the size of the inner circle is 0.

A Majorana zero mode is an $E = 0$ eigenstate of the BdG Hamiltonian that maps onto itself under particle–hole symmetry. Therefore, we have:

$$\text{Majorana Zero Mode:} \quad u(x) = v(x)^*. \tag{4.21}$$

Thus the Nambu spinor of the Majorana can point in different directions at different positions x, but it is always in the xy plane.

4.3 Physical basics of quantum computing with vortices

Vortices in $p + ip$ superconductors can serve as a platform for topological quantum computation. This works by 1) encoding qubits in groups of vortices, 2) braiding vortices around each other to perform quantum operations, and 3) reading out the qubits. In this section we are going to understand these steps.

4.3.1 Braiding vortices

Let us consider a disk of topological superconductor, with N vortices. Each vortex core has a Majorana zero mode, the corresponding operators are

$$\hat{\gamma}_j = \sum_m u_m^{(j)} \hat{c}_m + u_m^{(j)^*} \hat{c}_m^\dagger. \tag{4.22}$$

Let us consider what happens when we move vortex 1 adiabatically on a round trip around vortex 2. As vortex 1 is moving, its Majorana zero mode experiences a Δ whose phase turns around once. However, at every point x in the wavefunction of γ_1, the Nambu spinor's direction is locked to the phase of $\Delta(x)$. Thus, the Nambu spinor of MZM 1 undergoes a 2π rotation. The same holds for MZM 2 as well. As a result, both Majorana zero modes obtain a factor of 1:

$$\text{Braiding vortex 1 around vortex 2 } : \hat{\gamma}_{1,2} \to -\hat{\gamma}_{1,2}. \tag{4.23}$$

4.4 Exercises

4.4.1 Calculation of Majorana fermion edge states using transfer matrix method

Calculate the Majorana fermion edge states for the lattice model of $p + ip$ superconductor with an edge along the y axis, using a transfer matrix method. Assume that real-valued hopping w and complex-valued superconducting pair potential Δ are constant, but μ can depend on x. Take as Ansatz

$$\Psi(x, y) = \begin{pmatrix} \pm e^{i\phi} \\ 1 \end{pmatrix} e^{iky} \psi(x), \tag{4.24}$$

with $x, y \in \mathbb{Z}$ lattice coordinates, and $\psi(x)$ the wavefunction to be determined. Assume a sharp edge: no hopping to $x < 0$, and take $\psi(0) = 1$. As we did in the long-wavelength approximation, write down the eigenvalue equation, use that to deduce the dispersion relation, and obtain all values of $\psi(x)$ in an iterative way. Solutions that decrease/increase exponentially towards the bulk describe edge states localized to the left/right edge. Under what conditions do you obtain an edge state?

Solution: