Emergent Majorana Fermions in Topological Superconductors

In this project, we learn how to realize Majorana fermions in two-dimensional condensed matter systems. We take the simplest route by employing topological superconductors and find that Majorana fermions may emerge at interfaces between topological different regions.

A. The model: chiral p-wave superconductor

We consider a lattice model Hamiltonian for a chiral p-wave superconductor on a square lattice with a lattice spacing a,

$$\begin{aligned} H_0 &= H_t + H_\mu + H_\Delta \\ H_t &= \sum_j -t(f_j^\dagger f_{j+\hat{x}} + f_j^\dagger f_{j-\hat{x}} + f_j^\dagger f_{j+\hat{y}} + f_j^\dagger f_{j-\hat{y}}) \\ H_\mu &= -\tilde{\mu}\sum_j f_j^\dagger f_j \\ H_\Delta &= -\sum_j \Delta(f_j f_{j+\hat{x}} + i f_j f_{j+\hat{y}}) + \Delta^*(f_{j+\hat{x}}^\dagger f_j^\dagger - i f_{j+\hat{y}}^\dagger f_j^\dagger) \end{aligned} \tag{1}$$

where $f_j(f_j^\dagger)$ is a fermion annihilation (creation) operator at a site j. We introduce j to specify a lattice point vector,

$$j \equiv (x_j, y_j), \tag{2}$$

where x_j, y_j are integers setting the lattice spacing to be unity ($a \equiv 1$). The Bravais vectors of the square lattice $\hat{x}, \hat{y}$ (unit vectors) are introduced,

$$\hat{x} \equiv (1,0), \quad \hat{y} \equiv (0,1). \tag{3}$$

Note that the imaginary number (i) in the pairing terms plays a significant role in our discussion, which is a consequence of broken time-reversal-symmetry.

Q1) Discuss physical meaning of H_t, H_μ, H_Δ.

B. Bogoliubov-de-Gennes Hamiltonian

Let us put our system on a torus whose size is $(L \times L)$, so the translational symmetries are well-defined. The model Hamiltonian can be rewritten as

$$H_0 = \frac{1}{2}\sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \mathcal{H}_{\mathbf{k}} \Psi_{\mathbf{k}}, \tag{4}$$

by performing the Fourier transformation with a two-component Nambu spinor (Ψ_k) and 2×2 matrix in the particle-hole space ($\mathcal{H}_{\mathbf{k}}$),

$$\Psi_{+\mathbf{k}} = \begin{pmatrix} f_{+\mathbf{k}} \\ f_{-\mathbf{k}}^\dagger \end{pmatrix}, \quad \mathcal{H}_{\mathbf{k}} = \begin{pmatrix} \epsilon(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta(\mathbf{k})^* & -\epsilon(\mathbf{k}) \end{pmatrix} \equiv \epsilon(\mathbf{k})\tau^z + \mathrm{Re}\Delta(\mathbf{k})\tau^x - \mathrm{Im}\Delta(\mathbf{k})\tau^y \equiv \sum_{a=x,y,z} \mathcal{H}_{\mathbf{k}}^a \tau^a, \tag{5}$$

upto a trivial constant shift. The Nambu spinor is useful to understand the properties of excitations made of particles and holes whose real space expression is obtained by using the inverse Fourier transformation,

$$\Psi(\mathbf{x}) = \frac{1}{\sqrt{L^2}}\sum_{\mathbf{k}} \Psi_{+\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} = \begin{pmatrix} f(\mathbf{x}) \\ f^\dagger(\mathbf{x}) \end{pmatrix}. \tag{6}$$

Note that the spinor field operator, $\Psi(\mathbf{x})$, expression can be used without the translational symmetry.

Q2) Show

$$\epsilon(\mathbf{k}) = -2t(\cos(k_x) + \cos(k_y)) - \tilde{\mu}, \quad \Delta(\mathbf{k}) = 2i\Delta(\sin k_x + i \sin k_y). \tag{7}$$

It is instructive to consider the long wave-length limit ($\mathbf{k} \to 0$), where the effective continuum model becomes

$$H_0 \to H_0^{\text{eff}} = \frac{1}{2}\sum_{\mathbf{k}}^{\Lambda} \Psi_{\mathbf{k}}^{\dagger} \begin{pmatrix} \frac{\mathbf{k}^2}{2m} - \mu & 2i\Delta(k_x + ik_y) \\ -2i\Delta^*(k_x - ik_y) & -\frac{\mathbf{k}^2}{2m} + \mu \end{pmatrix} \Psi_{\mathbf{k}}, \tag{8}$$

where the shifted chemical potential ($\mu = \tilde{\mu} + 4t$) and the short wave-length cutoff (Λ) are introduced. It is easy to check $m = (2t)^{-1}$.

C. Topological Invariant

The Bogoliubov-de-Gennes Hamiltonian form (Eq. (4)) is useful to find a topological invariant. The eigenenergy with a momentum $\mathbf{k}$ is readily obtained by diagonalizing the Bloch Hamiltonian, $\mathcal{H}(\mathbf{k})$, giving

$$E_{\pm}(\mathbf{k}) = \pm\sqrt{\epsilon(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2}. \tag{9}$$

Let us define a unit vector,

$$\mathbf{n}(\mathbf{k}) = \big(\frac{\mathcal{H}_{\mathbf{k}}^x}{E_+(\mathbf{k})}, \frac{\mathcal{H}_{\mathbf{k}}^y}{E_+(\mathbf{k})}, \frac{\mathcal{H}_{\mathbf{k}}^z}{E_+(\mathbf{k})}\big). \tag{10}$$

In the thermodynamic limit, $L \to \infty$, the topological invariant is defined as

$$C[\mathbf{n}(\mathbf{k})] = \frac{1}{4\pi}\int_{T^2} \mathbf{n}(\mathbf{k}) \cdot \big(\frac{\partial \mathbf{n}(\mathbf{k})}{\partial k_x} \times \frac{\partial \mathbf{n}(\mathbf{k})}{\partial k_y}\big) = \frac{1}{4\pi}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\int_{-\pi}^{\pi}\frac{dk_y}{2\pi}\mathbf{n}(\mathbf{k}) \cdot \big(\frac{\partial \mathbf{n}(\mathbf{k})}{\partial k_x} \times \frac{\partial \mathbf{n}(\mathbf{k})}{\partial k_y}\big). \tag{11}$$

Q3) Calculate and plot $C[\mathbf{n}(\mathbf{k})]$ for $-4 < \mu/t < 4$.

Check that the quantum critical point of the topological phase transition is $\mu = 0$.

D. Edge mode

Since $\mu < 0$ and $\mu > 0$ have different topological invariants, it is natural to consider a interface geometry by replacing the constant chemical potential with a chemical potential function, $\mu \to \mu(x, y)$ such that $\mu(x, y) = \mu(x) = -\mu_0$ for $x < 0$ and $\mu(x, y) = \mu(x) = +\mu_0$ for $x > 0$. Then, the chemical potential function is invariant under the translation along the y direction, so the momentum k_y is well-defined.

In this geometry, the single-particle Hamiltonian can be rewritten as

$$H_0^{\text{eff}} \doteq \frac{1}{2}\begin{pmatrix} -\mu(x) & 2i|\Delta|\Big(-i\frac{d}{dx} + ik_y\Big) \\ -2i|\Delta|\Big(-i\frac{d}{dx} - ik_y\Big) & +\mu(x) \end{pmatrix} \tag{12}$$

in the continuum effective model. The quadratic dependence $\mathbf{k}^2$ is ignored since we are interested in the long wave-length limit.

We want to solve the eigenvalue problem with H_0^{eff} and use the ansatz solution,

$$|\Psi_{k_y}; (x, y)\rangle = e^{ik_y y} e^{-\frac{1}{2|\Delta|}\int_0^x \mu(x')dx'} |\phi_0\rangle. \tag{13}$$

For $k_y = 0$, the eigenvalue problem becomes

$$H_0^{\rm eff}|\Psi_0;(x,y)\rangle = 0 \quad \rightarrow \quad \begin{pmatrix} -\mu(x) & \mu(x) \\ -\mu(x) & \mu(x) \end{pmatrix} |\phi_0\rangle = 0 \quad \rightarrow \quad |\phi_0\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{14}$$

Q3) Show that the constant spinor $|\phi_0\rangle$ gives the energy eigenvalue, $E(k_y) = -2|\Delta|k_y$, for $H_0^{\rm eff}$, in the interface geometry.

The factor $e^{-\frac{1}{2|\Delta|}\int_0^x \mu(x')dx'}$ of $|\Psi_{k_y};(x,y)\rangle$ indicates that the solution is localized near the interface, and the form of $E(k_y) = -2|\Delta|k_y$ indicates that the eigenstate is *chiral and gapless*.

To see the meaning of the chiral gapless excitations, let us recall the spinor field operator ($\Psi(\mathbf{x})$) and its mode expansion,

$$\Psi(\mathbf{x}) = \begin{pmatrix} f(\mathbf{x}) \\ f^\dagger(\mathbf{x}) \end{pmatrix} = \sum_{k_y} e^{ik_y y} e^{-\frac{1}{2|\Delta|}\int_0^x \mu(x')dx'} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \gamma_{k_y} + \cdots, \tag{15}$$

where $\cdots$ are for the eigenmodes which are not localized at the interface.

The mode expansion shows that the creation and annihilation operators satisfy the condition, $\gamma_{k_y} = \gamma^\dagger_{-k_y}$, which gives the edge Majorana field operator,

$$\gamma(y) = \gamma^\dagger(y). \tag{16}$$