Note: Zero modes at disclination defects in C_4-symmetric superconductors

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Abstract

For the zero modes at disclination defects discussed by Teo–Hughes [1], I numerically confirmed the existence of zero modes for a model of a $p_x + ip_y$-wave superconductor.

Consider a system with fourfold rotation symmetry,

$$\hat{C}_4 f_i^\dagger(x,y)\hat{C}_4^{-1} = f_j^\dagger(-y,x)u_{ji}. \tag{1}$$

Using this symmetry transformation, one can introduce a disclination defect into the model. A disclination defect can be introduced using only the C_4 symmetry; when translation symmetry is also present, Teo–Hughes [1] gave a momentum-space formula for the $\mathbb{Z}_2$ invariant that characterizes the zero mode. In this note I only record the numerical results for the zero mode and do not verify the Teo–Hughes formula.

1 Model

I explain the introduction of a disclination defect using a $p_x + ip_y$ superconductor as an example. Put a complex fermion $f_{\boldsymbol{x}}^\dagger$ on each integer lattice site, with $\boldsymbol{x} \in \mathbb{Z}^2$. The model on an infinitely extended plane is

$$\hat{H} = \sum_{\boldsymbol{x}} \left(t f_{\boldsymbol{x}+\hat{x}}^\dagger f_{\boldsymbol{x}} + t f_{\boldsymbol{x}+\hat{y}}^\dagger f_{\boldsymbol{x}} + \text{h.c.} \right) + \frac{1}{2}\sum_{\boldsymbol{x}} \left\{ \Delta(\boldsymbol{x}) \left(i f_{\boldsymbol{x}+\hat{x}}^\dagger f_{\boldsymbol{x}}^\dagger - f_{\boldsymbol{x}+\hat{y}}^\dagger f_{\boldsymbol{x}}^\dagger \right) + \text{h.c.} \right\}. \tag{2}$$

Here $\Delta(\boldsymbol{x})$ is a site-dependent complex number. When $\Delta(\boldsymbol{x})$ is constant, the model has the C_4 symmetry defined by the following transformation:

$$\hat{C}_4 f_{\boldsymbol{x}}^\dagger \hat{C}_4^{-1} = \pm e^{\frac{\pi i}{4}} f_{c_4\boldsymbol{x}}^\dagger, \qquad \hat{C}_4^4 = (-1)^F. \tag{3}$$

Here $c_4\boldsymbol{x} = (-y,x)$. The sign ambiguity comes from fermion-parity symmetry. Because $\hat{C}_4^4 = (-1)^F$, note that the $(-1)^F$ symmetry may be regarded as part of the $\mathbb{Z}_8$ generated by the $\hat{C}_4$ symmetry. In what follows I consider the case where $\Delta(\boldsymbol{x})$ is constant and write $\Delta(\boldsymbol{x}) \equiv \Delta$.

Introduce a disclination defect. First remove the degrees of freedom in the first quadrant. More concretely, remove the degrees of freedom with $x \geq 0$ and $y > 0$. Next, construct the hopping term in the y direction for the degrees of freedom on the half line $x > 0$, $y = 0$ by using the C_4 rotation symmetry. More explicitly, define

$$\sum_{x>0,y=0} \left\{ t(\hat{C}_4 f_{\boldsymbol{x}+\hat{y}}^\dagger \hat{C}_4^{-1}) f_{\boldsymbol{x}} + \frac{1}{2}\Delta(-1)(\hat{C}_4 f_{\boldsymbol{x}+\hat{y}}^\dagger \hat{C}_4^{-1}) f_{\boldsymbol{x}}^\dagger \right\} + \text{h.c.} \tag{4}$$

$$= \sum_{x>0,y=0} \left\{ t\left(\pm e^{\frac{\pi i}{4}}\right) f_{c_4\boldsymbol{x}-\hat{x}}^\dagger f_{\boldsymbol{x}} + \frac{1}{2}\Delta(-1)\left(\pm e^{\frac{\pi i}{4}}\right) f_{c_4\boldsymbol{x}-\hat{x}}^\dagger f_{\boldsymbol{x}}^\dagger \right\} + \text{h.c.} \tag{5}$$

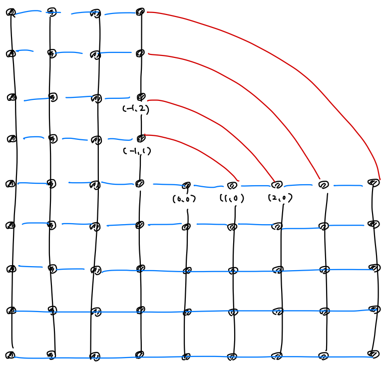

Figure 1: A disclination defect constructed from a site-centered C_4 rotation.

See Fig. 1.

For a numerical implementation it suffices to proceed as follows. Let L be a natural number and take the sites to be $x, y = -L, \dots, L$. The momentum-space model is

$$\mathcal{H}(\boldsymbol{k}) = (t\cos k_x + t\cos k_y - \mu)\tau_z + \begin{pmatrix} 0 & \Delta(\sin k_x + i\sin k_y) \\ \Delta^*(\sin k_x - i\sin k_y) & 0 \end{pmatrix}_\tau . \tag{6}$$

The site-centered C_4 symmetry is

$$u(\boldsymbol{k})H(\boldsymbol{k})u(\boldsymbol{k})^{-1} = H(c_4\boldsymbol{k}), \qquad u(\boldsymbol{k}) = U, \qquad U = \pm e^{\frac{\pi i}{4}\tau_z}. \tag{7}$$

To obtain the real-space model, take the hopping matrix $h(n_x, n_y)$ in the directions $n_x, n_y \in \mathbb{Z}$ to be

$$h(n_x, n_y) = \frac{1}{(2\pi)^2}\int dk_x dk_y\, e^{in_xk_x + in_yk_y}\mathcal{H}(\boldsymbol{k}). \tag{8}$$

The action of the C_4 rotation on sites is

$$C_4 : (x, y) \mapsto (-y, x). \tag{9}$$

Consider open boundary conditions in both the x and y directions. The model without a disclination defect is

$$\begin{aligned} \mathcal{H}(\boldsymbol{x}, \boldsymbol{x}') = \delta_{\boldsymbol{x}+\hat{x},\boldsymbol{x}'}t(1,0) + \delta_{\boldsymbol{x},\boldsymbol{x}'+\hat{x}}t(-1,0) + \delta_{\boldsymbol{x}+\hat{y},\boldsymbol{x}'}t(0,1) \\ + \delta_{\boldsymbol{x},\boldsymbol{x}'+\hat{y}}t(0,-1) + \delta_{\boldsymbol{x},\boldsymbol{x}'}t(0,0). \end{aligned} \tag{10}$$

To obtain the model with a disclination defect from the above model $\mathcal{H}$, first delete hopping terms involving degrees of freedom that do not exist. More explicitly, reset

$$\mathcal{H}(\boldsymbol{x} + \hat{x}, \boldsymbol{x}) = \mathcal{H}(\boldsymbol{x}, \boldsymbol{x} + \hat{x}) = 0, \qquad x = -1, \dots, L-1, \quad y = 1, \dots, L, \tag{11}$$

$$\mathcal{H}(\boldsymbol{x} + \hat{y}, \boldsymbol{x}) = \mathcal{H}(\boldsymbol{x}, \boldsymbol{x} + \hat{y}) = 0, \qquad x = 0, \dots, L, \quad y = 0, \dots, L-1, \tag{12}$$

$$\mathcal{H}(\boldsymbol{x}, \boldsymbol{x}) = E_{\text{big}}, \qquad x = 0, \dots, L, \quad y = 1, \dots, L. \tag{13}$$

Here $E_{\text{big}} \gg 1$ is chosen appropriately so that these states do not appear among the low-energy eigenvalues. The part glued by the C_4 rotation symmetry is set to

$$\mathcal{H}((-1, x), (x, 0)) = Ut(0, 1), \qquad \mathcal{H}((x, 0), (-1, x)) = t(0, -1)U^{-1}, \qquad x = 1, \dots, L. \tag{14}$$

Figure 2 shows an example of density plots of eigenstates.

Under this setup, changing the signs of the parameters t, μ, and $U = \pm e^{\frac{\pi i}{4}\tau_z}$ and numerically checking whether zero modes are present gives the following result.

- A zero mode localized at the disclination defect appears only in the parameter region where the absolute value of the Chern number is 1, namely $|\mu| < 2|t|$ and $\mu \neq 0$, and only for $U = -e^{\frac{\pi i}{4}\tau_z}$.

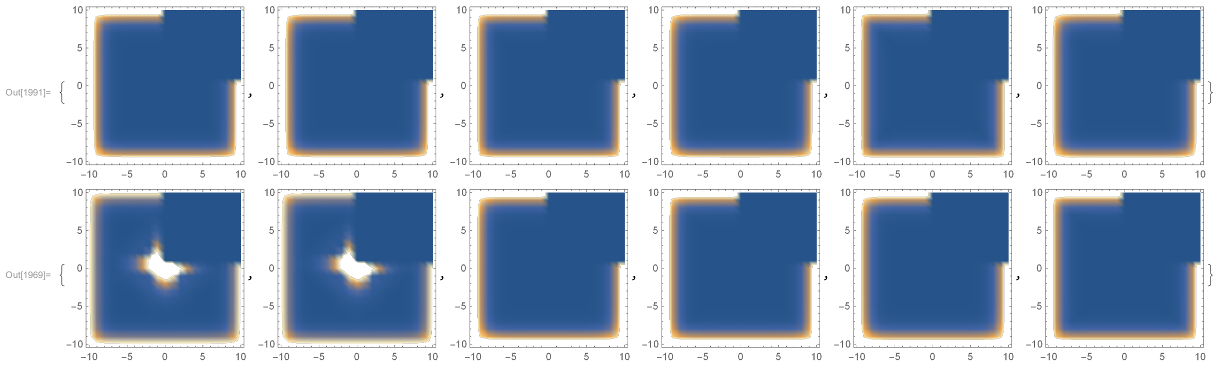

Figure 2: Density plots of energy eigenstates for $L = 10$, $t = 1$, $\mu = 1.2$, and $\Delta = 1$. The six states with the smallest absolute values of the eigenvalues are shown. The upper panel is for $U = e^{\frac{\pi i}{4}\tau_z}$, while the lower panel is for $U = -e^{\frac{\pi i}{4}\tau_z}$. Edge states originating from the nonzero Chern number can be observed. Because of finite-size effects, the disclination zero mode forms superposition states with the edge zero modes.

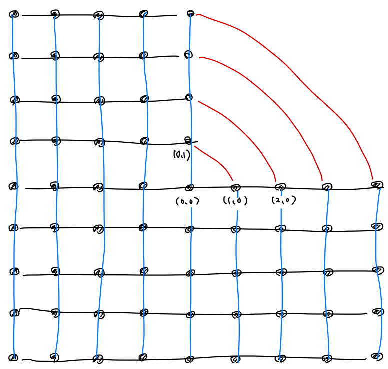

Figure 3: A disclination defect centered at $(1/2, 1/2)$.

1.1 Taking the center of the C_4 rotation to be $(1/2, 1/2)$

Since the model has translation symmetry, it also has a C_4 rotation symmetry centered at $(1/2, 1/2)$:

$$c_4 : (x, y) \mapsto (-y + 1, x). \tag{15}$$

The corresponding disclination defect is shown in Fig. 3.

Whether a disclination zero mode is present changes compared with the case of a C_4 rotation centered at $(0, 0)$. The symmetry in momentum space is

$$u(\boldsymbol{k})\mathcal{H}(\boldsymbol{k})u(\boldsymbol{k})^{-1} = \mathcal{H}(c_4\boldsymbol{k}), \qquad u(\boldsymbol{k}) = Ue^{ik_y}, \qquad U = \pm e^{\frac{\pi i}{4}\tau_z}. \tag{16}$$

Notice the factor e^{ik_y}. This factor affects the invariants at high-symmetry points in momentum space.

Construct the model with the disclination defect as follows. First delete hopping terms involving degrees of freedom that do not exist. More explicitly, reset

$$\mathcal{H}(\boldsymbol{x} + \hat{x}, \boldsymbol{x}) = \mathcal{H}(\boldsymbol{x}, \boldsymbol{x} + \hat{x}) = 0, \qquad x = 0, \ldots, L-1, \quad y = 1, \ldots, L, \tag{17}$$

$$\mathcal{H}(\boldsymbol{x} + \hat{y}, \boldsymbol{x}) = \mathcal{H}(\boldsymbol{x}, \boldsymbol{x} + \hat{y}) = 0, \qquad x = 1, \ldots, L, \quad y = 0, \ldots, L-1, \tag{18}$$

$$\mathcal{H}(\boldsymbol{x}, \boldsymbol{x}) = E_{\text{big}}, \qquad x = 1, \ldots, L, \quad y = 1, \ldots, L. \tag{19}$$

The part glued by the C_4 rotation symmetry is set to

$$\mathcal{H}((0,x),(x,0)) = Ut(0,1), \qquad \mathcal{H}((x,0),(0,x)) = t(0,-1)U^{-1}, \qquad x = 1,\dots,L. \tag{20}$$

Figure 2 shows an example of density plots of eigenstates.

Under this setup, changing the signs of the parameters t, μ, and $U = \pm e^{\frac{\pi i}{4}\tau_z}$ and numerically checking whether zero modes are present gives the following result.

- In the parameter region where the absolute value of the Chern number is 1, namely $|\mu| < 2|t|$ and $\mu \neq 0$, a zero mode localized at the disclination defect appears in the following two cases: (i) t and μ have the same sign and $U = -e^{\frac{\pi i}{4}\tau_z}$; (ii) t and μ have opposite signs and $U = e^{\frac{\pi i}{4}\tau_z}$.

2 Comments

Introducing a disclination defect is equivalent to considering the model on a cone. In particular, when the line defect introduced by a twisted boundary condition can be "undone" by a $U(1)$ phase rotation of the complex fermion, the model is equivalent to a model on a cone in which the parameters vary adiabatically in real space. Zero modes of a $p_x + ip_y$ superconductor on a cone in this situation are discussed in [2]. Since the zero modes are stable as long as the bulk gap is preserved, for a cone with an arbitrary opening angle there should be an index theorem similar to the winding of the phase of the gap function, or a semiclassical topological invariant.

References

[1] Jeffrey C. Y. Teo and Taylor L. Hughes, "Existence of Majorana-Fermion Bound States on Disclinations and the Classification of Topological Crystalline Superconductors in Two Dimensions," Phys. Rev. Lett. **111**, 047006 (2013).

[2] A. Quelle, C. Morais Smith, T. Kvorning, and T. H. Hansson, "Edge Majoranas on locally flat surfaces: The cone and the Möbius band," Phys. Rev. B **94**, 125137 (2016).