Zero-energy edge states and their origin in particle-hole symmetric systems: symmetry and topology

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Abstract

We propose a criterion to determine the existence of zero-energy edge states for a class of particle-hole symmetric systems. A loop is assigned for each system, and its topology and a symmetry play an essential role. Applications to d-wave superconductors are demonstrated.

Key words: zero-energy edge states; d-wave superconductivity; graphite ribbons; coexistence of different order parameters

Introduction When a quantum system is terminated to a finite size, it may support a state localized at the boundaries. The appearance of such states is a hallmark of a phase degree of freedom specific to quantum mechanical systems, and has been investigated in the context of, say, quantum Hall or Haldane spin systems. In addition to these gapped cases, edge states in gapless systems have attracted a great deal of interest recently. For example, zero-energy edge states (ZES) at a (110) surface in d-wave superconductors (SC) have been observed via a tunneling spectroscopy. [1,2,3] Graphite ribbons are also known to support ZES, which lead to several physical consequences such as spin polarization near the boundaries. [4] In this article, we present a criterion to tell whether a certain system supports ZES. Our criterion is built on a symmetry and topology. Applications to ZES in d-wave SC is demonstrated. We also discuss an instability caused by ZES for d-wave SC: the emergence of the time-reversal symmetry breaking superconducting order parameters near (110) surfaces. [5]

Criterion for ZES A class of systems that we are concerned with is described by the following single-

particle hamiltonian:

$$\mathcal{H} = \sum_{x,x'} \boldsymbol{c}_x^\dagger h_{x,x'} \boldsymbol{c}_{x'}, \ h_{x,x'} = \begin{bmatrix} t_{x,x'} & \Delta_{x,x'} \\ \Delta'_{x,x'} & -t_{x,x'} \end{bmatrix} = h_{x',x}^\dagger,$$

where $t_{x,x'}, \Delta_{x,x'}, \Delta'_{x,x'} \in \mathbb{C}$, and $\boldsymbol{c}_x^\dagger = (c_{x\uparrow}^\dagger, c_{x\downarrow})$ denotes electron creation/annihilation operators at site x. The system is defined on a 1D lattice, with its total number of the lattice sites being N_x, and $x = 1, \cdots, N_x$.

Our criterion for ZES is stated in terms of the bulk properties of the system and the shapes of edges. The bulk property of the system is easily captured by adopting the periodic boundary condition. With the periodic boundary condition, the above hamiltonian can be transformed to

$$\mathcal{H}^{\text{bulk}} = \sum_k \boldsymbol{c}_k^\dagger \boldsymbol{R}(k) \cdot \sigma \, \boldsymbol{c}_k,$$

where $k \in (-\pi, \pi] = S^1$ is the crystal momentum, and $\sigma_{X,Y,Z}$ the Pauli matrices. All bulk properties are encoded in the Fourier-transformed matrix element $\boldsymbol{R}(k) \in \mathbb{R}^3$, from which we can identify a loop $\ell : k \in S^1 \to \boldsymbol{R}(k) \in \mathbb{R}^3$ for each 1D Hamiltonian $\mathcal{H}^{\text{bulk}}$. A system with a certain type of edges is then generated by truncating a bulk Hamiltonian $\mathcal{H}^{\text{bulk}}$. We

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refer a prescription for creating edges as e. Generally, e represents an impurity potential at an edge, coexistence of different order parameters near boundaries in superconducting systems, etc. We write a system characterized by ℓ and e as $\mathcal{H}^{\text{edge}}[\ell, e]$. Then, we ask if $\mathcal{H}^{\text{edge}}[\ell, e]$ supports ZES localized at either end of the sample for given ℓ and e.

Our criterion to tell the existence of ZES is summarized as follows[6]:

(A) The loop ℓ is on a plane cutting the origin $\mathcal{O}$ of the three-dimensional $\boldsymbol{R}$-space. For loops that satisfy this condition, we can find an operator Γ which anticommutes with $\mathcal{H}^{\text{bulk}}[\ell]$. We call this property as chiral symmetry. Γ is equivalent to $\mathbf{1}_{N_x} \otimes \sigma_Z$ upto an arbitrary SU(2) transformation, where $\mathbf{1}_{N_x}$ acts on a site index, while σ_Z on a spin index.

(B) ℓ can be continuously deformed to ℓ_c without crossing $\mathcal{O}$, where ℓ_c is a unit circle on the plane. $(\ell \sim \ell_c)$

(C) e respects the chiral symmetry. That is, $\mathcal{H}^{\text{edge}}[\ell, e]$ anticommutes with Γ.

If the conditions (A)-(C) are satisfied, there exists at least a pair of ZES, one of which localized at the right edge and the other at the left edge.

For 2D or higher-dimensional systems with edges, we first Fourier transform along directions parallel to the edge, to get a family of 1D Hamiltonians parametrized by the wave number along the edge. Then, the present results are applicable for each 1D Hamiltonian.

As an application of the present results, let us discuss 2D $d_{x^2-y^2}$-wave SC with surfaces. In Fig.(1a) and (1b), a family of loops in $\boldsymbol{R}$-space and the energy spectrum is shown for $d_{x^2-y^2}$-wave SC with (a) (110) and (b)(100) surfaces. For the (110) case, loops are an ellipsis on the XZ-plane enclosing $\mathcal{O}$ except at $k_{y'} = \pm\pi, 0$ ($k_{y'}$ is the wave number along the edges). Thus, the above criterion tells us there are ZES for the (110) case. On the other hand, we do not expect ZES for the (100) case since loops collapse into a line segment. We have verified numerically this prediction in Fig. (1b).

Peierls-like instability and the chiral symmetry breaking Since edge states with different $k_{y'}$ are all degenerate at $E = 0$, they are expected to cause a Peierls-like instability. In presence of interactions, parameters in a single particle Hamiltonian t, Δ, Δ' near the edges might be effectively modified in order to lift the degeneracy, and thereby lower the ground state energy. However, since these ZES are stable to perturbations which respect the chiral symmetry (Statement (C)), such modifications should be accompanied with the breaking of the chiral symmetry near the boundaries. The emergence of, say, is or id_{xy} components near the boundary can breaks the chiral symmetry to lift the degeneracy of edge modes. On the other hand,
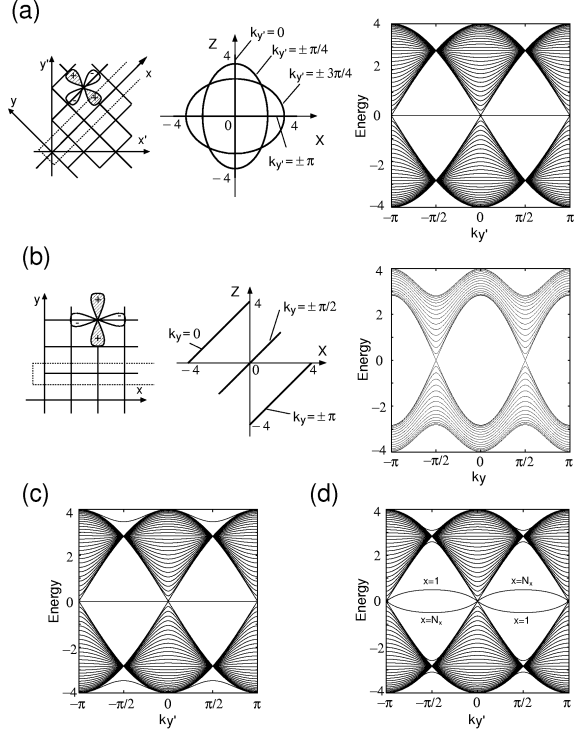

Fig. 1. Loops in the $\boldsymbol{R}$-space and the corresponding energy spectrum for $d_{x^2-y^2}$ SC with (a) (110) and (b) (100) surfaces. Energy spectra with introduction of (c) s and (d) is order parameter near a (110) surface. An edge mode localized at the site 1, N_x is indicated by $x = 1, N_x$.

a purely real order parameter cannot do it. Indeed, it has been revealed via a quasi-classical study that coexistence of is- or id_{xy}-wave order parameter with $d_{x^2-y^2}$-wave near the surface is possible for the (110) surface. [5]

This is explicitly demonstrated in Fig. (1c) and (1d). With the introduction of is order parameter near a (110) surface in $d_{x^2-y^2}$ SC, the flat band formed by edge states develops a finite dispersion. On the other hand, introduction of s order parameter does not break the chiral symmetry, and hence cannot lift the degeneracy.

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