Topological Origin of Zero-Energy Edge States in Particle-Hole Symmetric Systems

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A criterion to determine the existence of zero-energy edge states is discussed for a class of particle-hole symmetric Hamiltonians. A “loop” in a parameter space is assigned for each one-dimensional bulk Hamiltonian, and its topological properties, combined with the chiral symmetry, play an essential role. It provides a unified framework to discuss zero-energy edge modes for several systems such as fully gapped superconductors, two-dimensional d-wave superconductors, and graphite ribbons. A variance of the Peierls instability caused by the presence of edges is also discussed.

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deformation of a Hamiltonian from a reference Hamiltonian with exact zero-energy edge states, in conjunction with a symmetry.

In the following, let us focus on a loop on a 2D plane that contains the origin \( O \) in \( \mathbf{R} \) space. We crown such loops with a superscript \( \mathbf{s} \) as a reminder, thereby referred to as \( \ell^s \).

As a prescription for creating edges, we adopt \( e_c \) for a while. Let \( (\ell, E, p) \) denote an edge state of \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e_c) \) with energy \( E \), localizing at \( p = L(R) \) where \( L(R) \) represents the left(right) edge. We assume a state which appears within the bulk energy gap is localized at either end of the sample for an infinite system. A state localized at both ends also may appear, which is a superposition made from two independent edge states localized at the left and the right. We will show

(A) If \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e_c) \) has an edge state at nonzero energy \( |\ell^s, E \neq 0, p\rangle \), it also has \( |\ell^s, -E, p\rangle \), which localizes at the same edge with the opposite energy.

First, note that we can restrict ourselves to loops on the \( XY \) plane, since an arbitrary 2D plane can be rotated to the \( XY \) plane by a unitary transformation: a global SO(3) rotation in \( \mathbf{R} \) space, which amounts to a SU(2) transformation on \( e_c \), for each site. To prove the statement, it is essential that the particle-hole symmetry is promoted to the chiral symmetry for \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e_c) \). Since all the hopping \( t_{x,y} \) is zero for loops on the \( XY \) plane, the Hamiltonian can be expressed as 
\[ \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e_c) = (c_1^e, c_1^o) H^0_{\mathbf{s}}(\ell), \quad H^0_{\mathbf{s}}(\ell) = \begin{pmatrix} 0 & \ell \otimes \sigma_z \end{pmatrix}. \]

Then, \( \Gamma := 1 \otimes \sigma_z \) anticommutes with \( H \), \( \Gamma H \Gamma = -H \), which we call the chiral symmetry. Consequently, if \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e_c) \) has an edge mode \( |\psi\rangle = |\ell^s, E \neq 0, p\rangle \), it also has an edge mode with energy \( -E \), \( \Gamma |\psi\rangle = |\ell^s, -E, q\rangle \). Moreover, since \( \Gamma \) is a purely local operator which only changes the phase of \( c_1 \), i.e., it does not “mix” the coordinate in the real space, \( |\psi\rangle \) and \( \Gamma |\psi\rangle \) should be localized at the same edge, \( q = p \). Notice that the above discussion is not applicable for \( E = 0 \), since both \( |\psi\rangle \) and \( \Gamma |\psi\rangle \) have the same energy, and hence can be the equivalent state.

Next, we further assume that \( \ell^s \) is continuously deformed into a unite circle \( \ell_c \) centered at \( O \), such that the loop is always on the 2D plane and does not cross \( O \) during the deformation (Fig. 1). For a loop \( \ell^s \) with this property, we write as \( \ell^s \sim \ell_c \) henceforth. We can prove that

(B) \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell^s \sim \ell_c, e_c) \) has at least a pair of edge states at zero energy.

To see this, we focus on \( \mathbf{R}(k) = (\cos k, -\sin k, 0) \) and the corresponding Hamiltonian \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell_c, e_c) = \sum_{\ell=1}^{N_c} c_{\ell}^0 |\ell, 0\rangle \langle 0, \ell| + \text{H.c.} \). Since \( c_{\ell}^0, c_{\ell}^e, c_{\ell}^o, c_{\ell}^n \) do not appear in \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e_c) \), there are two exact zero-energy levels, which localize at \( x = 1 \) and \( x = N_c \), i.e., \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell_c, e_c) \) has two edge states \( |\ell_c, 0, L\rangle \) and \( |\ell_c, 0, R\rangle \) [19]. By assumption, we can deform \( \ell_c \) into \( \ell^s \) continuously. During the deformation, \( |\ell_c, 0, L\rangle \) and \( |\ell_c, 0, R\rangle \) do not go away from zero energy, since we can apply (A), and the bulk energy gap does not collapse. Although other edge states \( |E, p\rangle \) and \( |E, p\rangle \) may appear in pairs from the bulk energy bands, since the number of edge modes localized at \( L/R \) is always odd, there must exist at least a pair of zero-energy states.

Although we have concerned ourselves with a certain type of edge \( e_c \), let us next consider to adiabatically modify \( e_c \). As far as the modified prescription does not break the chiral symmetry, the perturbed Hamiltonian also supports exact zero-energy edge states, since perturbations at the edges do not collapse the energy gap. Thus, we have shown

(C) For a prescription \( e^* \) that respects the chiral symmetry, \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell^s \sim \ell_c, e^*) \) possesses at least a pair of zero-energy states.

In summary, there are three conditions for \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell, e) \) to support zero-energy edge states: (A) \( \ell \) is on a 2D plane that contains \( O \), (B) \( \ell \) is continuously deformed to \( \ell_c \) without crossing \( O \), (C) \( e \) respects the chiral symmetry, \( (e^*) \).

We have established our main results, and a few comments are in order. First, notice that the edge states discussed here are not at exact zero-energy for a finite system, though \( |\ell_c, 0, L\rangle \) and \( |\ell_c, 0, R\rangle \) are exact zero-energy states. This is allowed since an assumption for the statement (A) does not hold for a finite system size. In this case, a state localized at both ends cannot be decomposed into two independent edge states, which we can regard as a hybridized state made from the two edge modes at the left and the right. In \( N_c \to \infty \), this state becomes degenerate with another hybridized state.

Second, consider a unit circle \( \ell^s_c \) that encloses \( O \) \( n \) times \( (n \text{ odd}) \). \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell^s_c, e_c) \) can be diagonalized in the same way as \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell_c, e_c) \), resulting in \( 2n \) exact zero-energy states. Then, by the same discussion, a class of Hamiltonians \( \mathcal{H}_{\text{edge}}^{\mathbf{s}}(\ell^s \sim \ell_c, e^*) \) have at least one pair of edge states at \( E = 0 \).

We go on to applications of the present results. We adopt \( e_c \) as a prescription for creating edges unless otherwise stated. First, we discuss fully gapped systems and edge states. Especially, we comment on a topological aspect of 2D SC with a full gap, whose examples include \( d + id \) SC states.
and the chiral $p$-wave SC [6–11]. For these SC, we can define an integer called the Chern number, the nonzero value of which implies the existence of edge states connecting the upper and the lower bands as known in the QHE [5]. The present results are consistent with this discussion. For 2D systems with edges, we first Fourier transform along a direction parallel to the edge to get a family of 1D Hamiltonians parametrized by the wave number along the edge. Then, we can apply the present discussions for each 1D Hamiltonian. Since the nonzero Chern number implies there exists a loop which is on a plane and encloses $\mathcal{O}$ [11], both the topological argument and the present results lead to existence of zero-energy edge modes. For fully gapped systems, edge modes are expected to be stable even in the presence of electron-electron interaction as far as the bulk energy gap is not collapsed.

Although the topological argument is only applicable for fully gapped systems, our results here are not restricted to gapped cases and can be applicable also for gapless cases in arbitrary dimensions. Here, as an application, we consider surface states for $d_{x^2-y^2}$-wave SC. In Ref. [12], a semiclassical approach was employed to show that the sign change of the pair potential at a $(110)$ surface gives rise to existence of edge states, which can be used as a phase sensitive probe to detect pairing symmetries. It was also pointed out that the Andreev equation for the present system is closely related to Witten’s supersymmetric quantum mechanics [13,20]. Here, we discuss this issue with a lattice regularization.

Consider 2D $d_{x^2-y^2}$-wave SC \( \mathcal{H}^{\text{bulk}} = \sum_r [c_r \text{c}_r + c_r^\dagger \text{c}_{r+} + \text{c}_r^\dagger \text{c}_{r+y} + \text{H.c.} + \text{c}_r^\dagger \text{h}_0 \text{c}_r] \), where \( \text{c}_r \) is an electron annihilation operator on a sublattice \( \mathcal{O} \), \( \text{c}_r^\dagger \) is the creation operator, \( \text{h}_0 = [\alpha_0 \cdot \mu] \). (We set \( t = \Delta = 1, \mu = 0 \) as an example.) We terminate this system and consider $(110)$ surfaces first. Fourier transforming along the \( y' \) direction in Fig. 2(a), we obtain a family of 1D Hamiltonians parametrized by \( k_{y'} \). The corresponding loops are \( \mathbf{R}_{k_{y'}}(k_x) = [2 \cos(k_x - k_{y'}) - 2 \cos k_x, 0, 2 \cos(k_x - k_{y'}) + 2 \cos k_x] \). For a given \( k_{y'} \), \( 1 + \cos k_x(X/2)^2 + (1 - \cos k_x)(Z/2)^2 = 2 \sin^2 k_{y'} \) is satisfied, which is an ellipse on the XZ plane enclosing \( \mathcal{O} \). Thus, from the above discussion, the present system supports zero-energy surface states for all \( k_{y'} \) except at the gap-closing points \( k_{y'} = \pm \pi, 0 \), where the loop collapses into a line segment.

On the other hand, for $(100)$ surfaces, we obtain \( \mathbf{R}_k(k_x) = [2(\cos k_x - \cos k_x), 0, 2(\cos k_x + \cos k_x)] \), which is a line segment on the XZ plane for all \( k_{y'} \). Zero-energy edge states are not expected to exist for this case. We have verified numerically this prediction in Fig. 2(b).

Let us comment on an interplay between zero-energy edge states and interactions for the present case. If we treat the problem self-consistently, coexistence of $is$- or $id_{x^2-y^2}$-wave order parameters with $d_{x^2-y^2}$ waves near the surface is possible for the $(110)$ surface, locally breaking the time-reversal symmetry [21]. This can be interpreted based on the present discussions as follows. Since edge states with different \( k_{y'} \) are all degenerate at \( E = 0 \), they are expected to cause a Peierls-like instability. In the presence of interactions, parameters in a single-particle Hamiltonian \( t, \Delta, \Delta' \) near the edges might be effectively modified in order to lift the degeneracy and thereby lower the ground state energy. However, since these zero-energy edge states 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 \( is \) or \( id_{x^2-y^2} \) components near the boundary indeed breaks the chiral symmetry to lift the degeneracy of edge modes, while a purely real order parameter cannot do it.

We turn to edge states in graphite ribbons. There are several types of edges for a graphite ribbon, such as zigzag, bearded, and armchair edge [14]. Defining \( c_{x/} = c_\ast \) and \( c_{z/}^\dagger = c_\ast \), where \( c_{z/} \) is an electron annihilation operator on a sublattice \( \bullet/ \), we can apply our formalism to graphite ribbons. Notice that we have several options for choosing \( c_{z/} \) to form a spinor \( \epsilon \), since they live on different sites. When we truncate the system, these choices lead to different shapes of edges (Fig. 3). Taking an appropriate pair for each type of edge as indicated in Fig. 3, we can discuss in parallel to the above SC example. The existence of zero-energy edge states is predicted for the zigzag and the bearded cases, while we do not expect zero-energy edge states for an armchair edge, which is confirmed by a numerical calculation (see Fig. 3). These zero-energy edge modes are continuously connected to the gapless bulk spectrum, forming a flat band and a sharp peak in density of states at the Fermi energy. This might trigger an
instability in the presence of electron-electron or electron-phonon interactions, which leads to, for example, a magnetic polarization near the boundaries [14].

To conclude, we have established a criterion to determine the existence of zero-energy edge modes in terms of bulk properties and the chiral symmetry. Our strategy is to make use of the chiral symmetry and a continuous deformation of a reference Hamiltonian with exact zero-energy edge states. The present discussions are applicable for both gapped and gapless systems in arbitrary dimensions.

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[18] Note that for a finite system with PBC, the loop is actually a discrete set of points.
[19] \( \mathcal{H}_{edge}[\ell_i, e_i] \) can be diagonalized as \( \mathcal{H}_{edge}[\ell_i, e_i] = \sum_{i=1}^{N_y} \left[ d_{i+1/2}^{+} d_{i+1/2}^{-} - d_{i-1/2}^{+} d_{i-1/2}^{-} \right] \) by a unitary transformation \( d_{i+1/2}^+ := (c_i^+ \pm c_{i+1}^-)/\sqrt{2} \).