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.

Depending on several parameters such as hopping integrals or chemical potentials, and also on underlying crystalline lattices, a large variety of electronic structures are realized in condensed matter physics. Electron correlations also give rise to plenty of quantum phases, forming nontrivial quasiparticle band structures. An interesting consequence of a rich band structure is the existence of edge states that may appear when boundaries are present. In the quantum Hall effect (QHE), this issue was discussed in terms of the origin of the quantization of a Hall conductance [1–5]. Recently, the ideas developed in the QHE have also been extended for other gapped many-body systems and become essential to describing the topological nature of several quantum phases [6–11].

Apart from these examples for gapped systems, edge states in gapless systems have attracted much attention recently. Examples of these are d-wave superconductor (SC) with edges [12,13] or graphite ribbons [14], where the existence of edge states strongly depends on the shape of the edges. For d-wave SC with edges, the zero bias conductance peak due to zero-energy edge states was observed via tunneling spectroscopy [15,16].

The issue addressed in this Letter is how to infer the existence of zero-energy eigenstates localized on the boundaries in terms of properties of the bulk and the symmetry. We first consider one-dimensional (1D) systems with a particle-hole symmetry and then apply the results to systems in higher dimensions. Especially, we will demonstrate applications to fully gapped SC in conjunction with the Chern number, 2D d-wave SC, and graphite ribbons. In addition to these examples, the present Letter is also applicable to zero modes in the 1D molecule polyacetylene [17] and quantum spin systems.

We start with the following single-particle Hamiltonian on a 1D lattice:

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

where $t_{x,x'}$, $\Delta_{x,x'}$, $\Delta'_{x,x'} \in \mathbb{C}$, and $\mathbf{c}_x^\dagger = (c_{x\uparrow}^\dagger, c_{x\downarrow})$ denotes electron creation/annihilation operators at site x. The total

number of the lattice sites is N_x and $x = 1, \ldots, N_x$. This Hamiltonian includes the Bogoliubov–de Gennes Hamiltonian both for singlet and (some of) triplet SC.

In the following, we consider two types of Hamiltonians: the bulk Hamiltonian and the edge Hamiltonian. As for the bulk Hamiltonian, assuming that the system is translationally invariant, $h_{x,x'} = h(x - x')$, and adopting a periodic boundary condition (PBC), we can perform the Fourier transformation to obtain $\mathcal{H}^{\text{bulk}} = \sum_k \mathbf{c}_k^\dagger h_k \mathbf{c}_k = \sum_k \mathbf{c}_k^\dagger [\begin{smallmatrix} \xi_k & \Delta_k \\ \Delta_k^* & -\xi_k \end{smallmatrix}] \mathbf{c}_k$, where $\mathbf{c}_x = 1/\sqrt{N_x} \sum_k e^{ikx} \mathbf{c}_k$, $k \in (-\pi, \pi] = S^1$ is the crystal momentum, and $\xi_k \in \mathbb{R}$, $\Delta_k \in \mathbb{C}$. Since $(\sigma_Y h_k \sigma_Y)^* = -h_k$ ($\sigma_{X,Y,Z}$ represent the Pauli matrices), eigenvalues E and $-E$ always appear in a pair for each k, which we call the particle-hole symmetry. Let us introduce a convenient parametrization for $\mathcal{H}^{\text{bulk}}$ in k space

$$h_k = \mathbf{R}(k) \cdot \sigma,$$

where $\mathbf{R}(k) = (X, Y, Z) := (\text{Re}\Delta_k, -\text{Im}\Delta_k, \xi_k) \in \mathbb{R}^3$. In this parametrization, the energy eigenvalues are given by $E(k) = \pm|\mathbf{R}(k)|$. The origin $\mathcal{O} \in \mathbb{R}^3$ corresponds to the gap-closing point. For a given $k \in S^1$, there exists a one to one correspondence between a point in 3D space $\mathbf{R}(k)$ and h_k, and hence we can identify a loop $\ell: k \in S^1 \to \mathbf{R}(k) \in \mathbb{R}^3$ for each 1D Hamiltonian $\mathcal{H}^{\text{bulk}}$; for a given parametrized loop, we can always reconstruct $\mathcal{H}^{\text{bulk}}$ by inverse Fourier transformation [18]. We write $\mathcal{H}^{\text{bulk}}[\ell]$ for the Hamiltonian which corresponds to ℓ hereafter.

An edge Hamiltonian $\mathcal{H}^{\text{edge}}$ is generated by truncating a bulk Hamiltonian $\mathcal{H}^{\text{bulk}}[\ell]$ in a certain way. We refer to an edge Hamiltonian as $\mathcal{H}^{\text{edge}}[\ell, e]$, where e represents a prescription for creating edges. For example, a natural way of truncation is to prohibit all the matrix elements across N_x, i.e., set $h_{x,x'} = 0$ if $N_x \in [x, x']$, which we call e_c. Generally, e can represent an impurity potential at an edge, coexistence of different order parameters near boundaries in superconducting systems, etc. Then we ask if $\mathcal{H}^{\text{edge}}[\ell, e]$ supports zero-energy states localized at either end of the sample for given ℓ and e. Our strategy to answer this question is to consider a continuous

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 $\mathcal{O}$ in $\mathbf{R}$ space. We crown such loops with a superscript $*$ as a reminder, thereby referred to as ℓ^*. As a prescription for creating edges, we adopt e_c for a while. Let $|\ell, E, p\rangle$ denote an edge state of $\mathcal{H}^{\mathrm{edge}}[\ell, e_c]$ 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 $\mathcal{H}^{\mathrm{edge}}[\ell^*, e_c]$ has an edge state at nonzero energy $|\ell^*, E \neq 0, p\rangle$, it also has $|\ell^*, -E, p\rangle$, 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 $\mathbf{c}_x$ for *each site*. To prove the statement, it is essential that the particle-hole symmetry is promoted to the chiral symmetry for $\mathcal{H}^{\mathrm{edge}}[\ell^*, e_c]$. Since all the hopping $t_{x',x}$ is zero for loops on the XY plane, the Hamiltonian can be expressed as $\mathcal{H}^{\mathrm{edge}}[\ell^*, e_c] = (\mathbf{c}_\uparrow^\dagger, \mathbf{c}_\downarrow)H(\begin{smallmatrix}\mathbf{c}_\uparrow\\\mathbf{c}_\downarrow^\dagger\end{smallmatrix})$, $H = \begin{bmatrix} \mathbf{0} & \mathcal{D} \\ \mathcal{D}^\dagger & \mathbf{0} \end{bmatrix}$. Then, $\Gamma := \mathbf{1} \otimes \sigma_Z$ anticommutes with H, $\Gamma H \Gamma = -H$, which we call the chiral symmetry. Consequently, if $\mathcal{H}^{\mathrm{edge}}[\ell^*, e_c]$ has an edge mode $|\psi\rangle = |\ell^*, E \neq 0, p\rangle$, it also has an edge mode with energy $-E$, $\Gamma|\psi\rangle = |\ell^*, -E, q\rangle$. Moreover, since Γ is a purely local operator which only changes the phase of $c_\uparrow$, 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 ℓ^* is continuously deformed into a unite circle ℓ_c centered at $\mathcal{O}$, such that the loop is always on the 2D plane and does not cross $\mathcal{O}$ during the deformation (Fig. 1). For a loop ℓ^* with this property, we write as $\ell^* \sim \ell_c$ henceforth. We can prove that

(B) $\mathcal{H}^{\mathrm{edge}}[\ell^* \sim \ell_c, e_c]$ 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 $\mathcal{H}^{\mathrm{edge}}[\ell_c, e_c] = \sum_{x=1}^{N_x - 1} \mathbf{c}_x^\dagger \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \mathbf{c}_{x+1} + \mathrm{H.c.}$ Since $c_{1\downarrow}, c_{1\downarrow}^\dagger, c_{N_x\downarrow}, c_{N_x\uparrow}^\dagger$ do not appear in $\mathcal{H}^{\mathrm{edge}}[\ell_c, e_c]$, there are two exact zero-energy levels, which localize at $x = 1$ and $x = N_x$, i.e., $\mathcal{H}^{\mathrm{edge}}[\ell_c, e_c]$ has two edge states $|\ell_c, 0, L\rangle$ and $|\ell_c, 0, R\rangle$ [19]. By assumption, we can deform ℓ_c into ℓ^* 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, $\mathcal{H}^{\mathrm{edge}}[\ell^* \sim \ell_c, e^*]$ possesses at least a pair of zero-energy states.

In summary, there are three conditions for $\mathcal{H}^{\mathrm{edge}}[\ell, e]$ to support zero-energy edge states: (A) ℓ is on a 2D plane that contains $\mathcal{O}$, (ℓ^*), (B) ℓ is continuously deformed to ℓ_c without crossing $\mathcal{O}$, $(\ell \sim \ell_c)$, and (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 $N_x \to \infty$, this state becomes degenerate with another hybridized state.

Second, consider a unit circle ℓ_c^n that encloses $\mathcal{O}$ n times (n:odd). $\mathcal{H}^{\mathrm{edge}}[\ell_c^n, e_c]$ can be diagonalized in the same way as $\mathcal{H}^{\mathrm{edge}}[\ell_c, e_c]$, resulting in $2n$ exact zero-energy states. Then, by the same discussion, a class of Hamiltonians $\mathcal{H}^{\mathrm{edge}}[\ell^* \sim \ell_c^n, e^*]$ 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
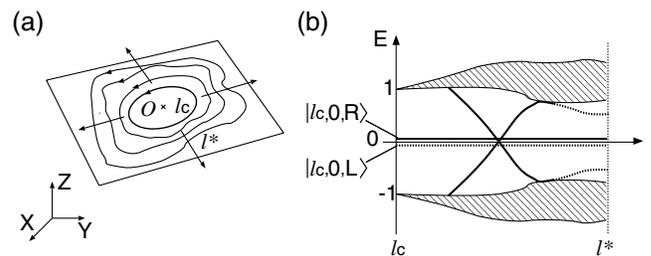
FIG. 1. (a) Continuously deforming ℓ_c into a loop $\ell^* \sim \ell_c$. During the deformation, the loop is kept on the 2D plane without crossing $\mathcal{O}$. (b) A possible energy spectrum during the deformation. A thick/broken line represents an edge mode localized at R/L.

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 $\mathcal{H}^{\text{bulk}} = \sum_r^{\text{PBC}}[\mathbf{c}_r^\dagger h_x \mathbf{c}_{r+x} + \mathbf{c}_r^\dagger h_y \mathbf{c}_{r+y} + \text{H.c.} + \mathbf{c}_r^\dagger h_0 \mathbf{c}_r]$, where $h_x = \begin{bmatrix} t & \Delta \\ \Delta & -t \end{bmatrix}$, $h_y = \begin{bmatrix} t & -\Delta \\ -\Delta & -t \end{bmatrix}$, and $h_0 = \begin{bmatrix} \mu & 0 \\ 0 & -\mu \end{bmatrix}$. (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 $k_{y'}$, $(1 + \cos k_{y'})(X/2)^2 + (1 - \cos k_{y'})(Z/2)^2 = 2\sin^2 k_{y'}$ is satisfied, which is an ellipsis 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 $\mathbf{R}_{k_y}(k_x) = [2(\cos k_x - \cos k_y), 0, 2(\cos k_x + \cos k_y)]$, 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_{xy}-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
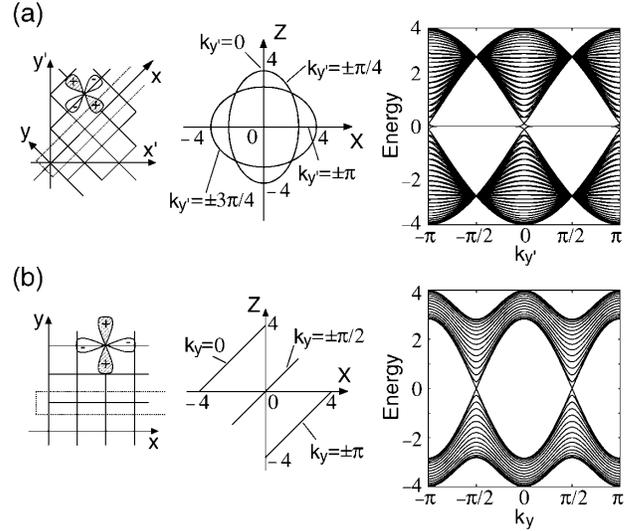
FIG. 2. Loops in $\mathbf{R}$ space and the energy spectrum of $d_{x^2-y^2}$-wave SC with (a) (110) and (b) (100) surfaces. Dotted squares show a choice of unit cell in Fourier transforming along the edges. The calculation is for $N_x = 50$ for (110) surfaces and $N_x = 30$ for (100) surfaces.

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, 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 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_{xy} 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 $c_\uparrow = c_\bullet$ and $c_\downarrow^\dagger = c_\circ$, where $c_{\bullet/\circ}$ is an electron annihilation operator on a sublattice $\bullet/\circ$, we can apply our formalism to graphite ribbons. Notice that we have several options for choosing $c_{\bullet/\circ}$ to form a spinor $\mathbf{c}$, 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
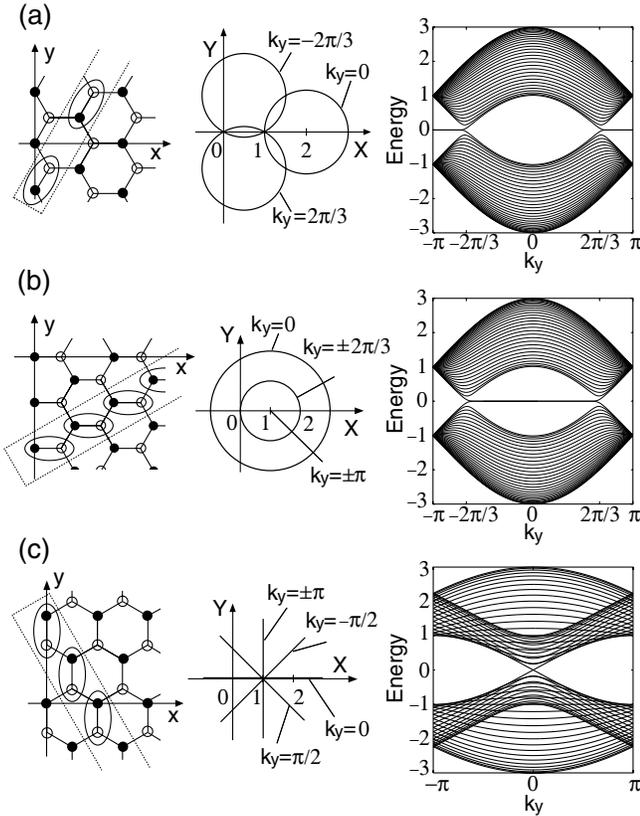
FIG. 3. Loops in **R** space and the energy spectrum of a graphite ribbon with (a) zigzag, (b) bearded, and (c) armchair edges. The ovals indicate how to form a spinor **c** for each edge, and dotted squares show a choice of unit cell in Fourier transforming along the edges. The loops corresponding to a one-parameter family of Hamiltonians are (a) $\mathbf{R}_{k_y}(k_{x'}) = [\cos(k_y - k_{x'}) + 1 + \cos k_y, -\sin(k_y - k_{x'}) + \sin k_y, 0]$, (b) $[\cos k_{x'} + \cos(k_y - k_{x'}) + 1, \sin k_{x'} - \sin(k_y - k_{x'}), 0]$, (c) $[\cos(k_{x'} + k_y) + \cos k_{x'} + 1, -\sin(k_{x'} + k_y) + \sin k_{x'}, 0]$. Here we have taken all the hopping integrals equal to unity, and k_y is a wave number along the edges. The calculation is for $N_{x'} = 30$ for zigzag and bearded edges and $N_{x'} = 29$ for armchair edges.

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] $\mathcal{H}^{\text{edge}}[\ell_c, e_c]$ can be diagonalized as $\mathcal{H}^{\text{edge}}[\ell_c, e_c] = \sum_{x=1}^{N_x-1}[d^\dagger_{+,x+1/2}d_{+,x+1/2} - d^\dagger_{-,x+1/2}d_{-,x+1/2}]$ by a unitary transformation $d^\dagger_{\pm,x+1/2} := (c^\dagger_{x\uparrow} \pm c_{x+1\downarrow})/\sqrt{2}$.
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