Topological Majorana and Dirac Zero Modes in Superconducting Vortex Cores

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We provide an argument based on flux insertion to show that certain superconductors with a nontrivial topological invariant have protected zero modes in their vortex cores. This argument has the flavor of a two-dimensional index theorem and applies to disordered systems as well. It also provides a new way of understanding the zero modes in the vortex cores of a spinless $p_x + ip_y$ superconductor. Applying this approach to superconductors with and without time-reversal and spin-rotational symmetry, we predict the necessary and sufficient conditions for protected zero modes to exist in their vortices.

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Fermionic zero-energy modes (eigenstates of the Hamiltonian whose energy is zero) are expected to occur as localized excitations of vortices of certain superconductors such as a spinless $p_x + ip_y$ superconductor. These modes, also called Majorana modes, have attracted a fair bit of recent theoretical attention due to the fact that they can obey non-Abelian statistics and have potential applications in decoherence free quantum computation [1–4]. While vortices in ordinary s-wave superconductors also have subgap modes which have energy of order Δ^2/E_f, in a $p_x + ip_y$ superconductor the lowest lying modes are predicted to be at zero energy [5].

Various topological arguments have been advanced to explain the existence of the Majorana modes [6–11]. Nevertheless, a general and simple 2D topological argument using standard mathematical techniques that can emulate the success of the Jackiw-Rebbi theory for solitons and zero modes in 1D [12] has been elusive.

Here, we present a new argument for the existence of the zero modes which is quite general and relies neither on an analytic solution of the Bogoliubov–de Gennes (BdG) equations nor on dimensional reduction or the quasiclassical approximation. We hope that this will be particularly useful in the context of recent efforts to find Majorana modes in systems other than a $p_x + ip_y$ superconductor [13]. We discuss and contrast our method with some previous topological methods in the study of vortices towards the end of this Letter. A second aspect of this work is a systematic study of the different symmetry classes in the Altland-Zirnbauer classification and a prediction of the zero modes in these systems based on the topological class.

Using a flux insertion argument, we first show that a certain class of insulators with π flux inserted through a plaquette have exact zero-energy eigenstates which are topologically protected in the sense that their existence is connected to the Hall conductance of the insulator. We then use these to deduce the conditions for protected zero modes to exist in the superconductors. This argument thus has the flavor of a 2D index theorem.

Consider a gapped 2D tight binding insulator on an infinite lattice with an even number of orbitals, $2s$ per site. The Hamiltonian can be written in the form $\mathcal{H} = \sum_{i,j} \Psi_i^\dagger H_{ij} \Psi_j$, where H_{ij} is a $2s \times 2s$ dimensional matrix and $\Psi_j = (\psi_{j,\alpha})^T$, where j is an index for the position and α for the orbital. The Fermi energy is set to zero.

In the first instance, we study systems with neither spin-rotational symmetry (SRS) nor time-reversal symmetry (TRS). We further restrict our study to Hamiltonians $\mathcal{H}$ which posses a symmetry analogous to that of BdG Hamiltonians. In other words, we assume the existence of an antiunitary operator S such that $S\mathcal{H}S^{-1} = -\mathcal{H}$. Furthermore, we assume that S acting on single particle position eigenkets in the Hilbert space produces a linear combination of kets at the same position, i.e., $S\Psi_j S^{-1} = U_j \Psi_j$, and U_j is a $2s \times 2s$ dimensional unitary matrix. The symmetry under S also implies that $U_i H_{ij} U_j^{-1} = -H_{ij}^*$.

Consider the effect of flux insertion through an infinitesimal tube in an infinite sample of such a system. Each hopping term in the matrix H_{ij} gets multiplied by the phase factor $\exp[i(e/\hbar)\int_j^i \boldsymbol{dr}\cdot\boldsymbol{A}]$, where the integral is along the hopping path to be and $\boldsymbol{A}$ is the vector potential due to the flux tube. It is easy to verify that, due to the BdG symmetry, $S\mathcal{H}(\boldsymbol{A})S^{-1} = -\mathcal{H}(-\boldsymbol{A})$, where $\mathcal{H}(\boldsymbol{A})$ is the Hamiltonian of the system with the vector potential $\boldsymbol{A}$. It follows that if $\mathcal{H}(\phi)$ is the Hamiltonian in the presence of a flux ϕ, then $S\mathcal{H}(\phi)S^{-1} = -\mathcal{H}(-\phi)$. Thus if $\mathcal{H}(\phi)$ has an eigenstate with eigenvalue E, then $\mathcal{H}(-\phi)$ has an eigenstate with eigenvalue $-E$.

Now suppose the system has a quantized Hall conductance of $pe^2/2\pi\hbar$. Then as a flux of $2\pi\hbar/e$ is adiabatically inserted through the flux tube, a total charge of pe flows in from infinity towards the flux tube [14]. In an infinite sample, the total spectral flow, i.e., the total number of states which cross the gap at the Fermi surface from below minus the number of states which cross it from above, is equal to p [14,15].

Let $n(\phi)$ be the number of eigenstates of the Hamiltonian whose energy is zero at the flux ϕ.

A schematic example of the energy spectrum of extended states close to the Fermi energy as a function of flux is plotted in Fig. 1. The function $n(\phi)$ is nonzero only for $\phi \in \{\phi_a, \phi_b, \frac{2\pi\hbar}{2e}, \phi_c, \phi_d\}$, where $\phi_c = 2\pi - \phi_a$ and $\phi_d = 2\pi - \phi_b$. The above discussion implies that $n(2\pi - \phi) = n(\phi)$.

Apart from the states which traverse the gap and thus cross the Fermi energy an odd number of times, there might also be states which cross the Fermi energy an even number of times as shown in the figure. Thus, the total number of zero-energy states at all fluxes is $p + 2m$, where p is the total Chern number of the ground state. It follows that when p is odd, $n(0) + n(2\pi\hbar/2e) = 2k + 1$, where k is some integer.

At zero flux, the Fermi energy lies in a gap. Thus, $n(0) = 0$, which in turn implies that $n(2\pi\hbar/2e)$ is an odd integer when p is odd. Since the integer p is a topological invariant, which cannot change under small transformations of the Hamiltonian, the zero mode is topologically protected.

We now use this result to study superconductors. In the remainder of the Letter, we are frequently going to consider Hamiltonians with $2s$ degrees of freedom per site, and we write such matrices in the form

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{12}^{\dagger} & M_{22} \end{pmatrix}. \tag{1}$$

Consider a tight binding BCS Hamiltonian for fermions hopping on a lattice which can be written in the form $\mathcal{H}_S = \sum_{i,j} \Psi_i^{N\dagger} H_{ij}^B \Psi_j^N$, where $\Psi_i^N = (\varphi_{i,\gamma}, \varphi_{i,\gamma}^{\dagger})^T$ is a Nambu spinor. Here, i and j stand for positions, and γ is an index for the orbitals and spin which runs from 1 to s. The matrix H^B is the BdG Hamiltonian which is of the form of Eq. (1) with $M_{11} = h$, $M_{12} = \Delta$, and $M_{22} = -h^T$, where h is the single particle Hamiltonian and Δ is the gap matrix. We can map the Hamiltonian $\mathcal{H}_S$ to the Hamiltonian of an insulator $\mathcal{H}_I$ (which we call the associated insulator) given by $\mathcal{H}_I = \sum_{ij} \Psi_i^{\dagger} H_{ij}^B \Psi_j$, where $\Psi_j = (\psi_{j,\alpha}, \psi_{j,\beta})^T$.

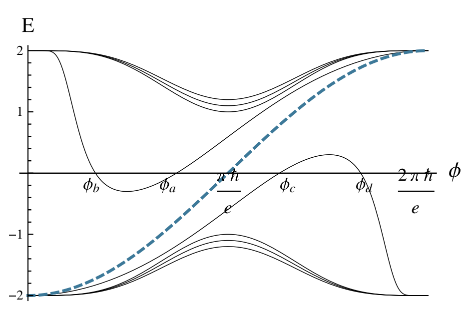

FIG. 1 (color online). A schematic plot of the energy E versus ϕ, where ϕ is the flux inserted through a plaquette of the insulator with Bogoliubov symmetry. Only states which lie close to the Fermi energy at $\phi = 0$ are shown. The dashed line is the single energy curve which traverses the gap as the flux is changed from 0 to $2\pi\hbar/e$.

We first study BdG Hamiltonians with neither TRS nor SRS. Imagine inserting an infinitesimal tube containing a flux of $2\pi\hbar/2e$ through the center of a plaquette in such a way that the low-energy configuration where the current $j \propto (\nabla\phi - eA)$ vanishes is attained. In this configuration, the phase winds around by 2π around the flux tube. Let r_i and θ_i be, respectively, the distance from the origin and the polar angle of site i in a coordinate system with the origin located at the position of the flux tube. Then the single particle terms in the Hamiltonian transform as $h_{ij} \to h'_{ij} = h_{ij} e^{i(e/\hbar)\int d\mathbf{r}\cdot \mathbf{A}} = h_{ij} e^{i(\theta_i - \theta_j)/2}$, where $\mathbf{A}$ is chosen to be $\frac{\hbar}{2e}\nabla(\theta)$, while the gap matrix transforms as $\Delta_{ij} \to \Delta'_{ij} = \Delta e^{i(\theta_i + \theta_j)/2}$.

The BdG eigenvalue equation in the presence of the vortex is thus $H'\psi = E\psi$, where $\psi = (u, v)^T$ and H' has the form of Eq. (1) with $M_{11} = h'$, $M_{12} = \Delta'$, and $M_{22} = -(h')^T$. Let $\tilde{u}_i = u_i$, $\tilde{v}_i = e^{i\theta_i} v_i$. Then $\tilde{\psi} = (\tilde{u}, \tilde{v})^T$ satisfies the eigenvalue equation $H''\tilde{\psi} = E\tilde{\psi}$, where H'' can be written in the form of Eq. (1) with $M_{11} = h'$, $M_{12} = \Delta''$, $M_{22} = -(h'')$, $h''_{ij} = h_{ji} e^{i(\theta_i - \theta_j)/2}$, and $\Delta''_{ij} = \Delta_{ij} e^{i(\theta_i - \theta_j)/2}$.

We now replace the superconductor with the associated insulator $\mathcal{H}_I$ with the same flux configuration, i.e., half a quantum of flux inserted at the origin, which lies at the center of a plaquette. It is easy to verify that $\mathcal{H}_I(\pi)$ can be written as $\sum_{ij} \Psi_i^{\dagger} H''_{ij} \Psi_j$ with H'' as given above. Furthermore, $\mathcal{H}_I$ satisfies $S\mathcal{H}_I S^{-1} = -\mathcal{H}_I$, since it is derived from a BdG Hamiltonian and the analysis for the zero modes for insulators made previously can therefore be used.

The necessary and sufficient condition for the existence of an exact zero-energy mode which is localized around the flux tube is therefore that the Hall conductance of $\mathcal{H}_I$ is $pe^2/2\pi\hbar$, where p is odd [16]. If this condition is met, it follows that there is a zero-energy mode localized around the plaquette containing the tube. Since the Hall conductance is a robust topological invariant, the existence of the zero mode for the superconductor is also topologically protected. The Hall conductance for noninteracting Hamiltonians is one of the most well studied topological invariants in condensed matter physics [14,15] and can readily be computed in terms of the projection operator for the ground state [17].

It is important to note that the spectral equivalence holds only for flux tubes which contain multiples of $2\pi\hbar/2e$ flux, and this does not imply that arbitrary flux configurations of the two systems have the same spectrum. In this context, it is interesting to note that spectral flow of vortex core states occurs during the motion of a vortex in a supercurrent and is associated with forces on the vortex (see Ref. [18] and references therein).

A more realistic description of a vortex would include a finite region larger than a single plaquette where the magnetic field is nonzero rather than the situation considered above where the flux is confined to a single plaquette. The more realistic Hamiltonian describing such a vortex may be written as a sum $\mathcal{H} = \mathcal{H}_0 + V$, where $\mathcal{H}_0$ is the

Hamiltonian which corresponds to the idealized vortex discussed above and V is a local perturbation in the sense that $V_{ij} = 0$ sufficiently far from the vortex. If there is an odd number of Majorana zero-energy states, then the Hilbert space of the idealized vortex has one unpaired fermionic mode. No local perturbation such as V can alter the Hilbert space structure. It follows that the zero mode persists in the more realistic configuration. It also follows from the above arguments that there is an odd (even) number of zero modes for vortices whose phase winds around the vortex by an odd (even) multiple of 2π for superconductors whose auxiliary insulators have a Hall conductance which is an odd multiple of $e^2/2\pi\hbar$.

We now intend to study superconductors in the other symmetry classes in the Altland-Zirnbauer classification scheme [19] starting with superconductors which are TRS invariant and belong to class DIII. As before, we first study the corresponding insulators with time-reversal symmetry which are classified by a Z_2 invariant. Their Hamiltonians have the property that they can be continuously deformed to one which can be written as the sum of two Hamiltonians, each of which has an odd (even) Hall conductance if the Hamiltonian has a nontrivial (trivial) topological invariant. When flux is introduced through a narrow flux tube for these insulators, by using arguments very similar to those used above for the insulators which break time-reversal symmetry, one can show that the number of pairs of zero modes at π flux is odd for the case when the invariant is nontrivial and even when the invariant is trivial.

Superconductors in class DIII are classified by a Z_2 invariant [20] and can be mapped onto insulators with time-reversal symmetry whose Hamiltonians satisfy $S\mathcal{H}S^{-1} = -\mathcal{H}$ and which have the same spectrum, exactly as in the case of superconductors without TRS or SRS. Using this mapping and the results for the corresponding insulators stated in the previous paragraph, one can show that these superconductors have an odd number of Kramers pairs of zero-energy modes if and only if they belong to the nontrivial topological class. In the presence of a more realistic vortex configuration, time-reversal symmetry is broken near the vortex core. However, if there is an odd number of vortices and if the magnetic fields far from the cores vanish, then there will still be one robust pair of zero-energy edge modes. These may be regarded as a single Dirac mode.

Hamiltonians of superconductors with SRS but not TRS fall in the class C of the Altland-Zirnbauer symmetry classes [19]. These Hamiltonians may be regarded as the sum of $\mathcal{H}_\uparrow = (\psi_\uparrow^\dagger, \psi_\downarrow)H_\uparrow(\psi_\uparrow, \psi_\downarrow^\dagger)^T$ and $\mathcal{H}_\downarrow = (\psi_\downarrow^\dagger, \psi_\uparrow)H_\downarrow(\psi_\downarrow, \psi_\uparrow^\dagger)^T$ [19], where $H_\uparrow$ and $H_\downarrow$ have the form of Eq. (1) with $M_{11} = h$, $M_{12} = \Delta$, $M_{22} = -h^T$ and $M_{11} = h$, $M_{12} = -\Delta$, $M_{22} = -h^T$, respectively. The spectra of $H_\uparrow$ and $H_\downarrow$ are identical. If $(u, v)^T$ written in the particle-hole basis is a zero mode of $H_\uparrow$, then $(u, -v)^T$ is a zero mode of $H_\downarrow$. The superconductor may be mapped onto an insulator $\mathcal{H}_I$, which is the sum of two single particle Hamiltonians $\mathcal{H}_{I,\uparrow}$ and $\mathcal{H}_{I,\downarrow}$ and which may be regarded as separate systems. The condition that in the presence of a vortex the matrix $H_\uparrow$ has an odd number of zero modes is, as deduced in the study of Hamiltonians of class D, that the Hall conductance of the corresponding insulator $\sigma_{xy}(\mathcal{H}_{I,\uparrow})2\pi\hbar/e^2$ is an odd integer. The net Hall conductance $\sigma_{xy}(H_I)$ is twice that of $H_{I,\uparrow}$ and is always an even integer. Thus, when the Hall conductance of $\mathcal{H}_I$ has the form $2pe^2/2\pi\hbar$, where p is an odd integer, the system has an odd number of pairs of zero modes in its vortices, while when p is even the system has an even (or zero) number of pairs of zero modes.

Superconductors with both TRS and SRS, which belong to the class CI, may be regarded as belonging to the trivial Z_2 class of superconductors with TRS. These superconductors thus have no topologically protected zero modes in their vortex cores. Ordinary s-wave superconductors with spin-rotation symmetry fall in this class and are thus predicted to have no topologically protected zero modes.

Our results are summarized in Table I. Most continuum models can be simulated to an arbitrary degree of accuracy by a series of lattice models. Since the results derived above are not limited to a particular tight binding model, one expects that the analysis presented above extends also to continuum models.

To test these ideas, we have performed computer simulations for a tight binding superconductor on a square lattice with the following Hamiltonian:

$$H = \frac{1}{2}\sum_{i,j}\{\alpha c_{i,j}^\dagger c_{i,j} - (c_{i,j+1}^\dagger c_{i,j} + c_{i+1,j}^\dagger c_{i,j}) + i(c_{i+1,j}^\dagger c_{i,j}^\dagger - c_{i,j}^\dagger c_{i+1,j}^\dagger) - (c_{i,j+1}^\dagger c_{i,j}^\dagger - c_{i,j}^\dagger c_{i,j+1}^\dagger)\} + \text{H.c.}$$

The Hamiltonian is gapless at $\alpha = 2$. For α close to 2, the low-energy effective Hamiltonian for this model resembles that of a $p_x + ip_y$ superfluid [Eq. (1) of Ref. [2]] whose superconducting equivalent is possibly realized in strontium ruthenate. For $0 < \alpha < 2$, the corresponding auxiliary insulator has a nontrivial Hall conductance and in accordance with our arguments above, we find numerically the existence of a localized zero mode associated with an isolated vortex in the energy spectrum. On the

TABLE I. Conditions for superconductors in the various symmetry classes to support protected zero modes in vortex cores or edges, expressed as conditions on $\mathcal{H}_I$, the insulator associated with the superconductor. The last column indicates whether there is a single protected Majorana mode (M) or a protected pair of modes (D). No protected modes exist for the class CI.

Class	TRS	SRS	Condition on $\mathcal{H}_I$	Mode
D	No	No	$\sigma_{xy}e^2/h = 2k - 1$	M
C	No	Yes	$\sigma_{xy}e^2/h = 2(2k - 1)$	D
DIII	Yes	No	Nontrivial Z_2	D
CI	Yes	Yes	...	...

other hand, for $2 < \alpha$, the Hall conductance of the auxiliary insulator vanishes and there is no localized zero mode at an isolated vortex. When more than one vortex is considered, there is a splitting in the energy levels, and the magnitude of the splitting when the two vortices are a distance d apart is proportional to the overlap between two zero-energy eigenstates of an isolated vortex placed at the same distance. The splitting therefore falls exponentially as the distance between the vortices.

Finally, we note that the arguments made above are also applicable in the case when there is a mobility gap in the absence of flux rather than a gap to all states since the states within the mobility gap have zero Chern number and their energies return to their initial values when the flux inserted varies from 0 to $2\pi\hbar/e$.

It is useful to compare this method to other topological methods used in the analysis of zero modes in vortices. The BdG equations for the vortex core states can be reduced to a set of coupled first-order equations which can be solved to yield a spectrum which is linear in the generalized angular momentum [9,21]. In 3D systems, the spectral asymmetry index $N(k_z)$ [i.e., the difference between the number of positive and negative eigenvalues of the BdG equations as defined in Eq. (1) of Ref. [22]] can be calculated doing a gradient expansion of the Greens function. If $N(k_z)$ changes sign as a function of k_z, this indicates the presence of an anomalous branch of zero modes and topological invariants can be defined to detect this change of sign. One may treat the BdG Hamiltonian at a quasiclassical level as a function of the impact parameter b of the classical trajectory and position and momentum (x, p_x) along a classical trajectory. The existence of anomalous branches can be inferred from the zeros of the classical energy $E(b, x, p_x)$ and can also be expressed as a topological invariant [23]. The flat band in the spectrum in certain types of vortices [5] can be argued to be topological stable by applying various discrete symmetries such as time-reversal and particle-hole exchange to the spectrum [24].

An alternative approach is presented in Sec. 23.2 of Ref. [9]. The energy $E(Q)$ of the low-lying modes can be written as $E = -mp_f b\omega_0$ [10]. The right-hand side of this equation can be treated as an effective Hamiltonian, with the operator $Q = bp_f$, which is the angular momentum, being written as $-i\frac{\partial}{\partial\theta}$, where θ is the angle of the classical trajectory of the particle. This together with the boundary conditions which depend on the form of the pairing and the order parameter provides a condition for when Q is integer and when it is half integer.

The key difference between this class of arguments and the one used here is that, in our analysis, we do not use the quasiclassical approximation and hence our method applies to cases where this approximation cannot easily be used. Examples include topological superconductors where the Fermi momentum might be small such as recent proposals of proximity-induced superconductors and superconductors with impurities which lack translational symmetry even in the absence of a vortex. In both cases, the Chern number can be calculated to determine the existence of zero modes.

In summary, we have provided a simple and general argument which shows that certain topological classes of superconductors have topologically protected, robust zero modes, which can either be unpaired Majorana modes or come in pairs. We applied this analysis to the various symmetry classes of superconducting Hamiltonians.

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