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Quantizing Majorana fermions in a superconductor

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A Dirac-type matrix equation governs surface excitations in a topological insulator in contact with an s-wave superconductor. The order parameter can be homogenous or vortex valued. In the homogenous case a winding number can be defined whose nonvanishing value signals topological effects. A vortex leads to a static, isolated, zero-energy solution. Its mode function is real and has been called “Majorana.” Here we demonstrate that the reality/Majorana feature is not confined to the zero-energy mode but characterizes the full quantum field. In a four-component description a change in basis for the relevant matrices renders the Hamiltonian imaginary and the full, space-time-dependent field is real, as is the case for the relativistic Majorana equation in the Majorana matrix representation. More broadly, we show that the Majorana quantization procedure is generic to superconductors, with or without the Dirac structure, and follows from the constraints of fermionic statistics on the symmetries of Bogoliubov-de Gennes Hamiltonians. The Hamiltonian can always be brought to an imaginary form, leading to equations of motion that are real with quantized real-field solutions. Also we examine the Fock space realization of the zero-mode algebra for the Dirac-type systems. We show that a two-dimensional representation is natural, in which fermion parity is preserved.

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I. INTRODUCTION

Majorana bound states arise as zero-energy states in two-dimensional (2D) systems involving superconductors in the presence of vortices. 1-4 These zero modes have attracted much attention recently, in part, because of the possibility that they can realize “half-qubits” within topological quantum computing schemes. 3 The basic idea is that two far away Majorana bound states, real fermions, can be put together into a complex fermion acting on a two-dimensional Hilbert space spanned by the states |0⟩ and |1⟩. Hence, two Majorana fermions comprise one qubit, which is protected against the environment if the vortices binding the Majorana fermions are kept far away from each other.

The first example of a zero mode in a two-dimensional superconductor was presented in Ref. 1. More recently it has been stated that the proximity effect at the interface between an s-wave superconductor and the surface of a topological insulator can be described by a planar Dirac equation, 4 providing a physical realization of the mathematical structure of Ref. 1. Other examples of Majorana bound states arise in systems with a nonrelativistic kinetic term and a p = p x ± ip y interaction with a vortex order parameter (i.e., p-wave superconductors). 2,3 These types of bound states have been the subject of much recent interest. 5-8 The focus of the discussions of Majorana fermions in superconductors have focused thus far on the zero modes.

However, Majorana’s original work 9 was actually quite more general and did not address a single mode but instead a whole field. What he showed was that it was possible to construct a representation of the Dirac equation that admits purely real solutions. The particles that follow from his construction are their own antiparticles and thus necessarily neutral. What was striking about Majorana’s proposal was that these particles were fermions—bosonic neutral particles represented by real fields are common, pions, and vector bosons, such as photons, being simple examples (see Ref. 10 for a perspective on Majorana fermions).

In this paper we look at three issues regarding the quantization of Majorana fermions, beyond simply the zero modes, in superconductors. First, we look specifically at the case of Dirac-type systems describing s-wave-induced superconductivity on the surface of topological insulators. There, we find that the entire ψ field of the superconductor model (and not merely particular modes) obeys equations that are analogous to the Majorana equations of particle physics. The equations of motion for the fields can be brought to a real form, and the fermionic solutions are real and therefore their own antiparticles. Indeed, other than the fact that surface states are 2D, the topological insulator-superconductor system can be brought to the exactly same form that was discussed in Majorana’s original formulation of real relativistic fermions.

Second, we note various topological features of the Dirac-type model. We compute the Pontryagin index associated with the k-space dispersion, and find it to be ±1/2, which is an indication of the existence of zero modes in the presence of vortices. We then present the Fock space-level structures that accommodate an isolated, zero-energy state, which arises in the presence of a vortex. In particular, we show that fermion parity can be preserved, even with a single zero-energy state. As we discussed above the Majorana zero modes are usually thought of “half” qubits, as two of them make up a complex fermion with a two-dimensional Hilbert space. Here we ruffle this simple view by quantizing the theory in the infinite plane in the presence of a single vortex. A sole Majorana zero mode exists but a two-dimensional Hilbert space remains. In a finite system, another zero mode would appear at the edge, which is however absent in the infinite plane.
Third, we show that the Majorana quantization procedure that we discuss for the Dirac-type equations describing $s$-wave-induced superconductivity on the surface of topological insulators does extend, more broadly, to any superconductor. A description of Bogoliubov-de Gennes (BdG) Hamiltonians using Majorana modes has been noted by Senthil and Fisher\textsuperscript{11} for systems where spin-rotational symmetry is broken (classes D and DIII of Ref. 12). Here we show rather generically that lack of spin-rotation symmetry is not a necessity and thus classes C and CI of Ref. 12 also realize Majorana fermions. All one actually needs is to have fermions and hence these results hold for any superconducting system made of half-integer spin particles, regardless of the size of the spin. What we show is that the constraints imposed by fermionic statistics on the symmetries of Bogoliubov-de Gennes Hamiltonians always allow one to bring the Hamiltonian in the Nambu representation to an imaginary form. In turn, Schrödinger’s equation with this imaginary Hamiltonian leads to a real equation of motion for the fields, as in Majorana’s construction. The real-field solutions in the constrained doubled Nambu space can then be quantized as Majorana fields.

II. QUANTUM STRUCTURE OF THE SUPERCONDUCTING MODEL

Let us start by analyzing the planar Dirac-type systems realized on the surface of a topological insulator, placed in proximity to an $s$-wave superconductor. The Hamiltonian density for the model under discussion acts on two spatial dimensions:\textsuperscript{1,14}

$$H = \psi^\dagger p_+ \psi_1 + \psi^\dagger p_- \psi_1 - \mu(\psi^\dagger \psi_1 + \psi^\dagger \psi_1) + \Delta \psi^\dagger \psi_1 + \Delta^* \psi_1 \psi_1.$$  

(1)

Here $\psi_1$ are electron field amplitudes, $p_\pm = -i \partial_\pm \mp \partial_x$, $\mu$ is the chemical potential (which was omitted in the Ref. 1) and $\Delta(r)$ is the order parameter that is constant in the homogeneous case or takes a vortex profile in the topologically interesting case: $\Delta(r) = v(r)e^{i\theta}$, in circular coordinates. Equivalently, in a two-component notation

$$H = \psi^\dagger(\sigma \cdot p - \mu) \psi_1 + \frac{1}{2} \Delta \psi^\dagger i\sigma^2 \psi_1 - \frac{1}{2} \Delta^* \psi i\sigma^2 \psi_1.$$  

(2)

Now $\psi = (\psi^\dagger \psi^\dagger)$ and $\sigma$ comprises the two Pauli matrices ($\sigma^3, \sigma^2$). The $(2+1)$-dimensional equations of motion for Eqs. (1) and (2)

$$i\partial_t \psi_1 = p_- \psi_1 - \mu \psi_1 + \Delta \psi^\dagger_1,$$

$$i\partial_t \psi_2 = p_+ \psi_1 - \mu \psi_1 - \Delta^* \psi_1$$  

(3)

can be presented in two-component matrix notation.

$$i\partial_t \psi = (\sigma \cdot p - \mu) \psi + \Delta i\sigma^2 \psi^*.$$  

(4)

When the chemical potential is absent, and $\Delta$ is constant, the above system is a $(2+1)$-dimensional version of the $(3+1)$-dimensional, two component Majorana equation, which in $(3+1)$-dimensional space-time describes chargeless spin 1/2 fermions with “Majorana mass” $|\Delta|$.\textsuperscript{13}

A static solution to Eq. (3), equivalently Eq. (4), with a vortex profile for $\Delta$, can be readily found. It corresponds to a zero-energy mode. With $f$ and $g$ real in the Ansatz

$$\psi_1 = f(r)exp\{-i\pi/4 - V(r)\},$$

$$\psi_2 = g(r)exp[i(\theta + \pi/4) - V(r)],$$

$$V'(r) = v(r).$$  

(5)

Equation (3) reduces to

$$(rg)' = \mu rf,$$

$$f' = - \mu g.$$  

(6)

(Dash signifies $r$—differentiation). Regular solutions are Bessel functions

$$f(r) = NJ_0(\mu r),$$

$$g(r) = NJ_1(\mu r)$$  

(7)

with $N$ as a real normalization constant.\textsuperscript{14}

While the static, zero-energy mode is readily obtained from Eq. (3), for the finite-energy modes, we must take account of the fact that $\psi_1$, $\psi_2$ mix with their complex conjugates. Therefore, one cannot separate the time dependence with an energy phase. Correspondingly one cannot construct a Hamiltonian energy eigenvalue problem, which is the usual first step in the quantization procedure. Progress is achieved by doublings the system with a four-component spinor.

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi^\dagger_1 \\ -\psi^\dagger_2 \end{pmatrix} = \begin{pmatrix} \psi \\ i\sigma^2 \psi^* \end{pmatrix}.$$  

(8)

An extended Hamiltonian density $\mathcal{H}$ leads to equations for $\Psi$, which are just two copies of Eq. (3) or (4).

$$\mathcal{H} = \frac{1}{2} \Psi^\dagger \sigma \cdot p - \mu \frac{\Delta}{\Delta^* - \sigma \cdot p + \mu} \Psi = \frac{1}{2} \Psi^\dagger T \Psi.$$  

(9)

Here $T$ denotes transposition. Because the last two components of $\Psi$ are constrained by their relation to the first two, $\Psi$ satisfies the (pseudo-) reality constraint

$$C\Psi^\dagger = \Psi,$$  

(10)

with $C = C^{-1} = C^T = C^\dagger = \begin{pmatrix} 0 & i\sigma \tau_1 \\ i\sigma \tau_1 & 0 \end{pmatrix}$.

To proceed, one ignores the constraint in Eq. (10) on $\Psi$ and works with an unconstrained four-spinor $\Phi = (\psi 0)$. Time can now be separated with the usual phase Ansatz and the energy eigenvalue spectrum can be found.

$$i\hbar \dot{\Phi} = i\partial_t \Phi, \quad \Phi = e^{-iE \hbar t} \Phi_E, \quad \hbar \dot{\Phi}_E = E \Phi_E.$$  

(11)

These are the Bogoliubov-de Gennes equations for the superconductor problem. In the particle physics application, the
unconstrained four-component equation is just the Dirac equation describing charged spin 1/2 fermions. When the (pseudo-) reality constraint is imposed, one is dealing with the four-component version of the Majorana equation.\textsuperscript{13}

Observe that $h$ in Eq. (9) possesses the conjugation symmetry
\begin{equation}
C^{-1} h C = - h^*,
\end{equation}
which has the consequence that to each positive-energy eigenmode there corresponds a negative-energy mode.

\begin{equation}
C \Phi^*_f E = \Phi_{-E}.
\end{equation}

A quantum field may now be constructed by superposing the energy eigenmodes $\Phi_E$ with appropriate creation and annihilation quantum operators. It is here that we again encounter the Majorana construction: the unconstrained fermion four-spinor $\Phi$ is like a “Dirac” fermion spinor, governed by a Hamiltonian, which satisfies a conjugation symmetry in Eq. (12) that leads to Eq. (13). Then the spinor $\Psi$, which satisfies the (pseudo-) reality constraint in Eq. (10), is like a Majorana spinor, viz., a Dirac spinor obeying a (pseudo-) reality condition.

With the eigenmodes one can construct a quantum field $\hat{\Phi}$. It can be an unconstrained Dirac field operator.

\begin{equation}
\hat{\Phi} = \sum_{E>0} a_E e^{-iE \hat{t}} \Phi_E + \sum_{E<0} b_E^* e^{iE \hat{t}} \Phi_E^*
= \sum_{E>0} a_E e^{-iE \hat{t}} \Phi_E + \sum_{E<0} b_E^* e^{iE \hat{t}} C \Phi_E^*.
\end{equation}

Here the $a_E$ operator annihilates positive-energy excitations (conduction band) and the $b_E^*$ operator creates negative-energy excitations (valence band). Since $\hat{\Phi}$ is unconstrained, $a$ and $b$ are independent operators. Their conventional anticommutators ensure that the unconstrained fields satisfy Dirac anticommutation relations.

\begin{equation}
\{ \hat{\Phi}_j (r), \hat{\Phi}_j (r') \} = 0,
\end{equation}
\begin{equation}
\{ \hat{\Phi}_j (r), \hat{\Phi}_j^* (r') \} = \delta_{jj} \delta (r - r').
\end{equation}

For the superconductor/topological insulator system under consideration $\hat{\Phi} \mapsto \Psi$ and the quantum field $\hat{\Psi}$ satisfies the constraint
\begin{equation}
C_{ij} \hat{\Psi}_j = \hat{\Psi}_i.
\end{equation}

This is achieved by setting $b = a$ in Eq. (14).

\begin{equation}
\hat{\Psi} = \sum_{E>0} (a_E e^{-iE \hat{t}} \Phi_E + a_E^* e^{iE \hat{t}} C \Phi_E^*).
\end{equation}

Owing to the constraint in Eq. (16) the anticommutators take a Majorana form.

\begin{equation}
\{ \hat{\Psi}_j (r), \hat{\Psi}_j (r') \} = C_{ij} \delta (r - r'),
\end{equation}
\begin{equation}
\{ \hat{\Psi}_j (r), \hat{\Psi}_j^* (r') \} = \delta_{jj} \delta (r - r').
\end{equation}

These also follow from Eq. (17) with $a_E$, $a_E^*$ obeying conventional anticommutators. We have ignored possible zero-energy states; they will be discussed at length below.

In the final result in Eq. (17), $\hat{\Psi}$ retains the Majorana feature of describing excitations that carry no charge. This is true for the entire quantum field $\Psi$, not only for its zero-energy modes (if any), which are emphasized in the condensed-matter literature. Explicitly we see this by examining the conserved current that is constructed with the unconstrained Dirac field $\Phi$.

\begin{equation}
(\rho, J) = \left( \Phi_i^* \Phi_i^* \Phi_i, \left[ \sigma^0 0 \right] \Phi_i^* \right).
\end{equation}

When the above is evaluated on the constrained field $\Psi$, all terms vanish. This is to be expected for a Majorana field which carries no charge.

One may also consider a chiral current constructed with the Dirac field $\Phi$.

\begin{equation}
(\rho_5, J_5) = \left( \Phi_i^* \left[ \begin{array}{cc} I & 0 \\ 0 & -I \end{array} \right] \sigma_{ij} \Phi_i^* \right). \tag{20}
\end{equation}

But with nonvanishing $\Delta$ this is not conserved.

\begin{equation}
\frac{\partial}{\partial t} \rho_5 + \nabla \cdot J_5 = - 2i \gamma_5 \left( \begin{array}{cc} 0 & \Delta \\ -\Delta^* & 0 \end{array} \right) \Phi_i^*.
\end{equation}

These results persist when the constraint in Eq. (16) is imposed on $\Phi \mapsto \Psi$.

\begin{equation}
(\rho_5, J_5) \Rightarrow 2(\psi^T \psi, \psi^T \sigma \psi),
\end{equation}
\begin{equation}
\frac{\partial}{\partial t} \rho_5 + \nabla \cdot J_5 \Rightarrow 2\Delta \psi^T \sigma^2 \psi + 2\Delta^* \psi^T \sigma^2 \psi.
\end{equation}

Thus no conserved current is present in the superconductor model in Eq. (1).

The Majorana/reality properties are obscured by the representation of the Dirac matrices employed in presenting the $4 \times 4$ Hamiltonian $h$ in Eq. (9). As written, the matrices in $h$ are given in the Weyl representation.

\begin{equation}
\alpha = \left( \begin{array}{cc} \sigma^0 & 0 \\ 0 & -\sigma^0 \end{array} \right), \quad \beta = \left( \begin{array}{cc} I & 0 \\ 0 & -I \end{array} \right), \quad \gamma_5 = \left( \begin{array}{cc} I & 0 \\ 0 & -I \end{array} \right).
\end{equation}

$h = \alpha \cdot p - \mu \gamma_5 + \beta \Delta_R - i \beta \gamma_5 \Delta_I$.\textsuperscript{25}

$\Delta_{R,I}$ are the real and imaginary parts of the order parameter. One may pass to the Majorana representation by conjugating with the unitary matrix

\begin{equation}
V = \left( \begin{array}{cc} Q_- & Q_+ \\ Q_+ & -Q_- \end{array} \right) e^{i\pi/4}, \quad Q_{\pm} = \frac{1}{2} (1 \pm \alpha^2).
\end{equation}

Then $h$ becomes

\begin{equation}
V^{-1} h V = \left( \begin{array}{cccc}
-p_y & p_x \sigma^1 + i \Delta_I \\
p_x \sigma^1 - i \Delta_I & p_y \\
-\mu \sigma^2 - \Delta_R \sigma^2 \\
-\Delta_R \sigma^2 + \mu \sigma^2
\end{array} \right).
\end{equation}

This is manifestly imaginary and the conjugation matrix $C$ in Eq. (10) becomes the identity so that the (pseudo-) reality constraint on $\Psi$ becomes a reality condition.\textsuperscript{17}
III. HOMOGENEOUS ORDER PARAMETER

For constant $\Delta=me^{i\omega}$, we pass to momentum space with an $e^{i\mathbf{k}\cdot r}$ Ansatz in Eq. (11). The energy eigenvalue is
\[
E = \pm \sqrt{(k \pm \mu)^2 + m^2}
\]
(28)
with no correlation among the signs. For fixed $k$ there are two ($\pm \mu$) positive-energy solutions and two negative-energy solutions. They become doubly degenerate at $\mu=0$. The degeneracy occurs because at $\mu=0$, $h$ commutes with $S=(0, e^{-i\omega^2 \sigma_3})$ when the phase $\omega$ of $\Delta$ is constant. The energy in Eq. (28) is nonvanishing for all values of the parameters; there is no zero-energy state.

The operators $a_{E}$, $a_{E}^\dagger$ and the eigenmodes $\Phi_{E}$, which are explicitly presented in Appendix A, are labeled by the momentum $\mathbf{k}$ and a further $(+,-)$ variety describing the twofold dependence on $\mu$ of $E_{z}=\sqrt{(k \pm \mu)^2 + m^2}$ (29).

The quantum operator $\hat{\Psi}$ is constructed as in Eq. (17), which with notational changes $[a_{E} \rightarrow a_{n}(\mathbf{k}) ; \Phi_{E} \rightarrow \Phi_{n}(\mathbf{k}); n= (+,-)]$ reads explicitly
\[
\hat{\Psi}(t, \mathbf{r}) = \sum_{n} \int \frac{d^2k}{(2\pi)^2} \left[ a_{n}(\mathbf{k}) e^{-i(E_{\mathbf{k}} - k \cdot \mathbf{r})/\hbar} \Phi_{n}(\mathbf{k}) \right.
\]
\[
+ a_{n}^{\dagger}(\mathbf{k}) e^{i(E_{\mathbf{k}} - k \cdot \mathbf{r})/\hbar} \Phi_{n}(\mathbf{k}) \left. \right] (29)
\]
with positive-energy eigenfunction $\Phi_{n}(\mathbf{k})$ carrying energy $E_{n}$. The conjugation condition in Eq. (13) now states that $\Phi_{n}^{\dagger}(\mathbf{k})$ is a negative energy solution at $(-\mathbf{k})$.

Actually we can suppress the lower two components of $\Phi_{n}(\mathbf{k})$ in Eq. (29), because they repeat the information contained in the upper two components, owing to the subsidiary condition in Eq. (16). In this way from the four-component spinors recorded in Appendix A, we arrive at a mode expansion for the electron field operators $\hat{\psi}_{\uparrow, \downarrow}$.

\[
\hat{\psi}_{\uparrow, \downarrow} = \left( \begin{array}{c} \varphi_{\uparrow} \\ \varphi_{\downarrow} \end{array} \right) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ i \end{array} \right), \quad |\varphi\rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ -i \end{array} \right), \quad \varphi \text{ arises as } \hat{k} = \hat{0} \cos \varphi + \hat{3} \sin \varphi. \quad \text{One verifies that Eq. (30) satisfies Eq. (3).}
\]

The Majorana character of this expression manifests itself in that the particle annihilation operators $a_{\pm}$, associated with the positive energy eigenvalues $E_{\pm}$, are partnered with their Hermitian adjoint creation operators $a_{\pm}^{\dagger}$, which are associated with the negative-energy $-E_{\pm}$ modes. By contrast, for a Dirac field the negative-energy modes are associated with the antiparticle creation operators $b_{\pm}^{\dagger}$, which anticommute with $a_{\pm}$, $a_{\pm}^{\dagger}$. In other words, in the Majorana field operator in Eq. (30) the antiparticle (hole) states are identified with the particle states.

IV. TOPOLOGICAL NUMBERS

When $\mu$ is absent and $S$ commutes with $h$, we may equivalently work with $h'=Sh$, which possesses the same eigenvectors as $h$, common with the eigenvectors of $S$. However, $h'$ has the appealing form
\[
h' = \Sigma_{S} n^{a} \quad (a=1,2,3).
\]
(31)

Here $n^{i}=\hat{k}^{i}(\mathbf{k})$ and $n^{3}$ is $\Delta e^{-i\omega}=m$, i.e., the constant phase of $\Delta$ is removed so $m$ is a real constant but of indefinite sign. The matrices $\Sigma_{a}$

Here $|\pm\rangle$ are the two-component eigenvectors of $\sigma^{i} \hat{k}^{i} |\pm\rangle = \frac{1}{\sqrt{2}} (|\varphi\rangle \pm i |\bar{\varphi}\rangle)$, where $\varphi$ arises as $\hat{k} = \hat{0} \cos \varphi + \hat{3} \sin \varphi$. One verifies that Eq. (30) satisfies Eq. (3).

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The nonvanishing answer $\pm 1/2$, depending only on the sign of $m$, is evidence that the model belongs to a topologically nontrivial class. It is also a hint that topologically protected zero modes exist in the presence of a vortex. (Although vortex-based zero modes are also present for $\mu \neq 0$, we do
not know how to define a winding number in that case.)

We can understand the fractional value for \( N \). The unit vector

\[
\hat{n}^\alpha = (k \cos \varphi, k \sin \varphi, m) / \sqrt{k^2 + m^2}
\]

maps \( R^{(2)} \) (\( \neq S^{(2)} \)) to \( S^{(2)} \). When \( k \) begins at \( k = 0 \), \( \hat{n}^\alpha \) is at the north or south pole \( (0, 0, \pm 1) \). As \( k \) ranges to \( \infty \), \( \hat{n}^\alpha \) covers a hemisphere (upper or lower) and ends at the equator of \( S^{(2)} \). Thus only one half of \( S^{(2)} \) is covered.

V. SINGLE-VORTEX ORDER PARAMETER

When \( \Delta \) takes the vortex form, \( \Delta(\mathbf{r}) = v(r)e^{i\theta} \), Eq. (11) possesses an isolated zero-energy mode

\[
\Psi_0^\alpha = \left( \frac{\psi_0^\alpha}{i\sigma^2\psi_0^\ast} \right)
\]

with \( \psi_0^\alpha \) determined by Eqs. (5) and (7). Note that

\[
CP\Psi_0^\alpha = \Psi_0^\ast.
\]

There are also continuum modes.

The operator field \( \hat{\Psi} \) is now given by an expansion such as Eq. (17), except there is an additional contribution due to the zero mode controlled by the operator \( A \).

\[
\hat{\Psi} = \sum_{E > 0} (a_E e^{-iE\Phi_F} + a_E^\dagger e^{iE\Phi_F^\ast}) + A \sqrt{2}\Psi_0^\alpha.
\]

(The \( \sqrt{2} \) factor will be explained later.) Due to Eqs. (16) and (39), \( A \) is Hermitian \( A = A^\dagger \), anticommutes with \( (a_E, a_E^\dagger) \) and obeys

\[
\{A, A\} = 2A^2 = 1.
\]

The question arises: how is \( A \) realized on states? Two possibilities present themselves: two disconnected one-dimensional representations or one two-dimensional representation. In the first instance, we take the ground state to be an eigenstate of \( A \). The possible eigenvalues are \( \pm \frac{1}{2} \), so there are two ground states, \( |0+\rangle \) with eigenvalue \( +\frac{1}{2} \), and \( |0−\rangle \) with eigenvalue \( −\frac{1}{2} \). No local operator connects the two and the two towers of states built upon them

\[
\left\{ a_E^\dagger a_{E'}^\dagger \ldots |0\pm\rangle \right\}
\]

define two disconnected spaces of states. Moreover, one observes that \( A \) has a nonvanishing expectation value \( \langle 0\pm | A | 0\pm \rangle = \pm \frac{1}{2} \). Since \( A \) is a fermionic operator, fermion parity is lost.\(^{21}\)

In the second possibility, with a two-dimensional realization, we suppose that the vacuum is doubly degenerate: call one “bosonic” \( |b\rangle \), the other “fermionic” \( |f\rangle \), and \( A \) connects the two

\[
A|f\rangle = \frac{1}{\sqrt{2}}|b\rangle,
\]

\[
A|b\rangle = \frac{1}{\sqrt{2}}|f\rangle.
\]

(Phase choice does not loose generality.) Again there are two towers of states

\[
\left\{ a_E^\dagger a_{E'}^\dagger \ldots |f\rangle, \quad \left[ a_E^\dagger a_{E'}^\dagger \ldots |b\rangle \right]\right\}
\]

but now \( A \) connects them. With this realization, fermion parity is preserved when \( |b\rangle \) and \( |f\rangle \) are taken with opposite fermion parity. Of course since \( A \) is Hermitian, it can be diagonalized by the eigenstates.

\[
|0+\rangle = \frac{1}{\sqrt{2}}(|b\rangle + |f\rangle),
\]

\[
|0−\rangle = \frac{1}{\sqrt{2}}(|b\rangle − |f\rangle).
\]

This regains the two states of the two one-dimensional realizations. But the combination \( |b\rangle ± |f\rangle \) violates fermion parity as it superposes states with opposite fermion parity.

There does not seem to be a mathematical way to choose between the two possibilities. But physical arguments favor the fermion parity preserving realization. First of all, there is no reason to abandon fermion parity; if possible it should be preserved since it is a feature of the action. Also arguments against combining states of opposite fermion parity may be given: Since bosons and fermions transform differently under \( 2\pi \)-spatial rotations; the \( |0\pm\rangle \) states in Eq. (44) are not rotationally covariant but transform into each other. [This argument is completely convincing in a \((3 + 1)\)-dimensional theory. In \((2 + 1)\) dimensions the anyon possibility clouds the picture, and in \((1 + 1)\) dimensions the argument cannot be made, because spatial rotations do not occur.] Furthermore, time inversion transformations work differently on bosons and fermions: \( T^2 \) is \( I \) for bosons and \( −I \) for fermions. The superposed states in Eq. (44) are not invariant under \( T^2 \), rather they transform into each other. [This argument can be made for \((2 + 1)\) dimensional models, but in \((1 + 1)\) dimensions spin is absent so the fermion parity violating option cannot be ruled out. Furthermore, the fermion-boson equivalence of \((1 + 1)\)-dimensional models obscures the status of fermion-boson mixing. Indeed it is argued within supersymmetry that fermion parity is lost in the presence of solitons in \((1 + 1)\) dimensions “due to boundary effects.”]\(^{22}\)

[Any argument based on time inversion transformations requires viewing the complex valued vortex configuration as arising from the degrees of freedom of an enlarged model, in which the vortex emerges from the dynamics of the extended model (Abrikosov, Ginzburg, and Landau). Otherwise, a vortex background is not \( T \) invariant.]

In the next section we examine the vortex/antivortex background and argue that the two-state, two-dimensional, fermion parity preserving realization can be established. The physical picture that emerges is that there are two towers of states, one built on an “empty” zero-energy state \( |b\rangle \), the other on the “filled” zero-energy state \( |f\rangle \), and the \( A \) operator, which connects the two “vacua,” fills or empties the zero-energy state.

VI. VORTEX/ANTIVORTEX ORDER PARAMETER

Insight on physical states in the presence of a vortex in a superconductor adjoined to a topological insulator can be
gotten by considering a vortex/antivortex background. The zero-energy mode for considering an antivortex at the origin, \( \Delta(r) = v(r)e^{-i\theta} \), is given by

\[
\psi_i = N J_0(\mu r) \exp \{i \pi/4 - V(r) \},
\]

\[
\psi_i = N J_1(\mu r) \exp \{-i(\theta + \pi/4) - V(r) \}.
\]

To simplify the discussion, we omit the chemical potential and evaluate \( V(r) = f dr' v(r') \) with the asymptotic form of \( v(r) \rightarrow m \). Thus the zero-energy mode for the vortex becomes, approximately

\[
\psi_0^\pm = Ne^{-i\pi/4}e^{-mr} \begin{pmatrix} 1 \\ 0 \end{pmatrix}
\]

while the antivortex at \( r = R \), in the same approximation leads to

\[
\psi_0^\pm = Ne^{i\pi/4}e^{-m|r-R|} \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]

The corresponding four spinors that solve Eq. (11) at zero energy are

\[
\Psi_0^\pm = \begin{pmatrix} Ne^{-i\pi/4}e^{-mr} \\ 0 \\ 0 \\ -Ne^{i\pi/4}e^{-mr} \end{pmatrix}.
\]

\[
\Psi_0^0 = \begin{pmatrix} 0 \\ Ne^{i\pi/4}e^{-m|r-R|} \\ Ne^{-i\pi/4}e^{-m|r-R|} \\ 0 \end{pmatrix}.
\]

Consider now a configuration with a vortex at the origin and an antivortex at \( R \). No zero mode is present in the spectrum of \( h \); rather there are two bound states, one with positive, exponentially small energy \( \epsilon = e^{-mR} \) and the other with equal magnitude, but opposite sign.

The former, called \( \Phi^\mp \), consists of portions localized at the origin (vortex) and at \( r = R \) (antivortex). The latter is given by \( \Phi^\pm = \mathcal{C}\Phi^\mp \) and has similar structure. Both contribute unambiguously to the expansion of the quantum field operator \( \hat{\Psi} \), the former with an annihilation operator, the latter with a creation operator.

\[
\hat{\Psi} = \hat{\Psi}_{\text{cont}} + a_\epsilon e^{-i\epsilon t}\Phi^\epsilon + a^\dagger_\epsilon e^{i\epsilon t}\mathcal{C}\Phi^\epsilon. \quad (48)
\]

The first term on the right is the continuum contribution, as in Eq. (40). The Fock space spectrum is clear. There is a vacuum state \( |\Omega\rangle \) annihilated by \( a_\epsilon \)

\[
a_\epsilon |\Omega\rangle = 0. \quad (49a)
\]

A low-lying state is gotten by operating on \( |\Omega\rangle \) with \( a^\dagger_\epsilon \)

\[
a^\dagger_\epsilon |\Omega\rangle = |f\rangle, \quad (49b)
\]

\[
a_\epsilon |f\rangle = |\Omega\rangle. \quad (49c)
\]

The remaining states, created by \( a^\dagger_\epsilon \) can be built either on the vacuum \( |\Omega\rangle : a^\dagger_\epsilon a^\dagger|\Omega\rangle = \ldots |\Omega\rangle \) or on the low-lying state \( |f\rangle : a^\dagger_\epsilon |\Omega\rangle = a^\dagger_\epsilon a^\dagger|\Omega\rangle \).

Now let us remove the antivortex by passing \( R \) to infinity. Both \( \Psi_{\pm\epsilon}^\pm \) collapse to their zero-mode limit, \( \Psi_{\epsilon}^\pm \rightarrow \Psi_\epsilon^0 \), and the expansion in Eq. (42) becomes

\[
\hat{\Psi} = \hat{\Psi}_{\text{cont}} + \left( a_\epsilon + a^\dagger_\epsilon \right) \sqrt{2} |\Psi_\epsilon^0\rangle = \hat{\Psi}_{\text{cont}} + A \sqrt{2} |\Psi_\epsilon^0\rangle. \quad (50)
\]

Moreover the action of \( A = \frac{1}{\sqrt{2}}(a_\epsilon + a^\dagger_\epsilon) = A^\dagger \) may be read off Eq. (49). Renaming \( |\Omega\rangle \) as \( |b\rangle \), we find

\[
\{A,A\} = 1,
\]

\[
A|b\rangle = \frac{1}{\sqrt{2}} |f\rangle,
\]

\[
A|f\rangle = \frac{1}{\sqrt{2}}|b\rangle. \quad (51)
\]

and two towers of states are built upon \( |b\rangle \) and \( |f\rangle \).

In this way we justify the two-dimensional, fermion parity preserving realization of the zero-mode algebra in a superconducting/topological insulator system. [Note the occurrence of the factor \( \sqrt{2} \) modifying \( \Psi_\epsilon^0 \). This explains its first appearance in Eq. (40). This factor compensates in the completeness sum for the loss of the antivortex wave function].

Because no explicit solutions in a vortex/antivortex background are available, the argument in this section is qualitative, without explicit formulas. However, one may consider a one-dimensional example with Majorana fermions in the presence of a kink and/or a kink antikink pair. In that model one can solve equations explicitly and verify the behavior described here for the two-dimensional vortex case. In this way one also establishes that even in one spatial dimension (in the absence of rotation and spin to enforce fermion parity) the two-dimensional realization of the zero-mode algebra is appropriate.

In Appendix B we present an approximate determination of the low-energy eigenvalues in the presence of a vortex/antivortex pair. The result supports the above qualitative argument: an exponentially small splitting of the zero-energy mode is established. Also in the appendix, we study the two vortex background, and find, within the same approximation that no energy splitting occurs; rather two zero modes persist as anticipated by index theorems.

VII. QUANTIZING MAJORANAS FERMIONS IN GENERIC SUPERCONDUCTORS

In the preceding sections we showed that Majorana’s quantization prescription of the Dirac equation directly applies to the full quantum field describing the proximity effect of an s-wave superconductor to surface states of a topologi-
cal insulator. Below we shall show that Majorana’s quantization prescription of real neutral fermions is rather generic in superconductors with or without Dirac-type dispersions. The construction below is possible for any half-integer spin (fermionic) particle. The reality conditions on the fermionic fields follow from symmetries of the BdG Hamiltonian for superconductors constructed in the Nambu basis.

Let us consider a system with fermionic degrees of freedom $\psi_{r,n,s}$ and $\tilde{\psi}_{r,n,s}$, where $r$ labels position, $n$ the possible flavors (bands, for instance), and $s$ the spin (half-integer) along a chosen quantization axis. For simplicity, we shall define an index $\alpha=(r,n,s)$ that encodes all these degrees of freedom. The Hamiltonian describing superconductivity in such a system can be written as

$$\mathcal{H} = \sum_{\alpha=0}^{1} \left[ \psi^\dagger_{\alpha} H_{\alpha} \psi_{\alpha} + \frac{1}{2} \psi^\dagger_{\alpha} \Delta \psi_{\alpha} + \frac{1}{2} \psi^\dagger_{\alpha} \Delta^* \psi_{\alpha} \right].$$

We stress that fermionic statistics underlies this result, as it is the reason for the minus signs and the complex conjugation in both terms in the second row of Eq. (55).

It follows from this symmetry that positive and negative eigenmodes of $h$ are paired

$$h\Phi_E = E\Phi_E \Rightarrow h(C\Phi_E^\dagger) = -E(C\Phi_E^\dagger)$$

or equivalently

$$C\Phi_{+E} = \Phi_{-E}.$$  

B. Generic Majorana basis and its real equation of motion

Consider a unitary transformation $V$, under which

$$h \rightarrow \tilde{h} = VhV^\dagger.$$  

It follows that

$$\tilde{h}^* = V^\dagger h^* V = V^\dagger C^\dagger VhV^\dagger V.$$  

so the transformation law of $C$ is

$$C \rightarrow \tilde{C} = VCV^\dagger.$$  

(Notice that $\tilde{C}C^* = VCV^\dagger C^\dagger V^\dagger = I$ so $\tilde{C}^{-1} = \tilde{C}^*$ still.)

We will construct below a unitary matrix $V$ such that $\tilde{C} = I$. This basis is the appropriate Majorana representation for the generic superconducting system of half-integer spin particles (for any number of flavors). In this basis, one has $\tilde{h} = -h^*$ so that $\tilde{h}$ is imaginary or equivalently $i\tilde{h}$ is real. It follows from Schrödinger’s equation that

$$\left(\partial_t + i\tilde{h}\right)\Psi = 0$$

so the equation of motion for the field is purely real and thus admits purely real solutions. Notice that this path mirrors Majorana’s formulation of the Dirac equation for spin 1/2 particles (he constructed a purely imaginary representation of the Dirac matrices, obtaining an equation of motion that was real).

Notice that in this basis the commutation relations become

$$\{\Psi_a, \Psi_b\} = C_{ab} = C^\dagger = C^{-1}.$$  

A. Conjugation symmetry

One can easily check that any BdG-type $h$ as in Eq. (55) possesses the following conjugation symmetry

$$-h^* = C^* h C.$$
with $S'$ the $y$ component of the angular-momentum operator (in a representation such that $S'$ is a purely imaginary matrix). $T$ is a real antisymmetric matrix ($T=T^*$ and $T^T=-T$) with $T^2=-i_s^\text{spin\times flavor}$ when spin is half-integer. For instance, for spin 1/2 particles $T=\text{i}a^3$.

Consider the following transformation:

$$V = \begin{pmatrix} Q_- & -iQ_+ \\ iQ_+ & Q_- \end{pmatrix} e^{i\pi/4}, \quad Q_\pm = \frac{1}{2}(1 \mp iT)$$

(compare with Eq. (26).) Notice that $Q_\pm$ are projectors ($Q_+^2=Q_+$), that $Q_+^2=Q_-$, and that $Q_+^2 + Q_-^2 = i_s^\text{spin\times flavor}$ and $Q_-Q_+ = 0$. Also notice that $Q_-^2 = Q_+^2 = Q_-^2$. One can then easily check that the above defined $V$ is such that

$$C = VCV^T = I.$$

**VIII. SUMMARY**

In this paper we studied mainly three issues regarding the quantization of Majorana fermions in superconductors, following closely Majorana’s original definitions, and looked beyond just the Majorana zero-energy modes that are bound to topological defects such as vortices. We started by analyzing the specific case of Dirac-type systems describing $s$-wave-induced superconductivity on the surface of topological insulators. We showed that the entire $\psi$ field of the superconductor model (and not merely particular modes) obeys equations that are analogous to the Majorana equations of particle physics.

We then analyzed the quantization of the theory in the presence of vortices. We showed that fermion parity can be preserved even with a single zero-energy state. This quantization scheme shows that one can obtain a two-dimensional Hilbert in the presence of a single vortex in an infinite plane, presenting a case where each Majorana fermion can be, when present in odd numbers, more than half a qubit.

Finally, we showed that the Majorana quantization procedure that we discussed for the Dirac-type equations describing $s$-wave-induced superconductivity on the surface of topological insulators does extend, more broadly, to any superconductor. The constraints imposed by fermionic statistics on the symmetries of Bogoliubov-de Gennes Hamiltonians are sufficient to allow real-field solutions in the constrained doubled Nambu space that can then be quantized as Majorana fields. This results follows simply from fermionic statistics plus superconductivity, irrespectively of the presence or absence of any other symmetries in the problem, such as spin-rotation invariance or time-reversal symmetry.

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**APPENDIX A**

We present the four-component, positive energy solutions to Eq. (11). The eigenvalues

$$E_\pm = \sqrt{(\ell + \mu)^2 + |\Delta|^2}$$

are associated with the eigenvectors

$$\Phi_+(k) = \frac{1}{\sqrt{E_+}} \left( \begin{array}{c} \Delta \\ \sqrt{E_+ - k + \mu} \end{array} \right),$$

$$\Phi_-(k) = \frac{1}{\sqrt{E_-}} \left( \begin{array}{c} \Delta \\ -\sqrt{E_- + k + \mu} \end{array} \right).$$

The negative-energy spinors are given by $\Phi^*_+(\mathbf{k})|\pm\rangle$ are defined in the text.

**APPENDIX B**

We study the low-lying energy levels of the Dirac-type Hamiltonian $h$ in Eq. (9) with $\mu$ set to zero and $\Delta$ chosen first in an approximate vortex/antivortex profile

$$\Delta_{\text{v,v}} = m e^{i\Omega(r-R/2)} e^{-i\Omega(r+R/2)}$$

and then similarly with two vortices,

$$\Delta_{\text{v,v}} = m e^{i\Omega(r-R/2)} e^{i\Omega(r+R/2)}$$

Here $\Omega$ is the argument of the appropriate vector

$$e^{i\Omega(r)} = \frac{x + iy}{r} = e^{i\theta},$$

$$e^{i\Omega(\pm R)} = \pm \frac{(X + iY)}{R} = \pm e^{i\theta}$$

with $x=r \cos \theta$, $y=r \sin \theta$, $X=R \cos \Theta$, $Y=R \sin \Theta$. One vertex is located at $r=R/2$, the antivortex or the second vortex at $r=-R/2$.

1. Vortex/antivortex

Near the vortex at $r=R/2$ the order parameter $\Delta_{\text{v,v}}$ is approximated by

$$\Delta_{\text{v,v}} \rightarrow \Delta_0 = m e^{i\Omega(r-R/2)} e^{-i\Omega(R)} = m e^{i\Omega(r-R/2)} e^{-i\theta}.$$ (B3)

The zero mode in the presence of $\Delta_0$ differs from Eq. (47a) by a phase due to the additional phase $e^{i\theta}$ in $\Delta_0$. Also the location is shifted by $R/2$.

$$\psi_0^v = \left( \begin{array}{c} v \\ 0 \\ 0 \\ -v^* \end{array} \right), \quad v = \frac{m}{\sqrt{\pi}} e^{-i(\pi/4+i\theta/2)} e^{-m|r-R/2|}.$$ (B4)

Similarly, with the order parameter near the antivortex at $r=-R/2$ taken as
\[ \Delta \psi_{0} \rightarrow \Delta_{0} = me^{i \Omega(r)} e^{-i \Omega(r) \pi / 2} = -me^{i \theta} e^{-i \Omega(r) \pi / 2} \]

the zero mode solution replacing Eq. (47b) reads

\[ \psi_{0}^{\mu} = \begin{pmatrix} 0 \\ \bar{v} \\ 0 \end{pmatrix}, \quad \bar{v} = \frac{m}{\sqrt{\pi}} e^{i(3 \pi / 4 + \theta / 2)} e^{-m [r + R / 2]} \]  

(B6)

Next we evaluate the matrix element between \( \bar{v} \) in Eq. (9), with \( \mu = 0 \) and order parameters as in Eq. (B1). We find that the diagonal matrix elements vanish \( \langle \bar{v} | h | v \rangle = 0 \). The energy shift \( \Delta E \), determined by the off-diagonal elements of \( h \), is

\[ \Delta E = \pm | \langle \bar{v} | h | v \rangle | \].  

(B7)

The evaluation of the first integrand proceeds by recalling that \( p_{r} v = \Delta_{0} (r - R / 2) v \) and yields, after a shift of integration variable by \( R / 2 \)

\[ \int d^{2} r \bar{v}^{*} p_{r} v = -i \frac{m^{3}}{\pi} \int_{0}^{\infty} r d \theta e^{-m r} \int_{-\pi}^{\pi} d \theta_{0} e^{i(\theta - \theta_{0})} \exp - m r^{2} + R^{2} + 2 r R \cos (\theta - \Theta) \]  

(B9a)

A further shift of \( \theta \) by \( \Theta \) leaves

\[ \int d^{2} r \bar{v}^{*} p_{r} v = -i \frac{2m^{3}}{\pi} \int_{0}^{\infty} r d \theta e^{-m r} \int_{0}^{\pi} d \theta \cos \theta e^{-m R} \]  

(B9b)

For the second integrand, a similar shift, first by \( R / 2 \) and then by \( \Theta \) gives

\[ \int d^{2} r \bar{v}^{*} \Delta_{0} e^{i \bar{v} v} = i \frac{2m^{2}}{\pi} \int_{0}^{\infty} d \theta e^{-m r / 2} e^{-m r} \int_{0}^{\pi} r \int_{0}^{\pi} d \theta R \cos \theta \]  

(B10a)

We notice that the \( \theta \) integrand may also be presented as \(-i \frac{2m}{\pi} e^{-m R} \), thereby transforming Eq. (B10a) after an integration by parts into

\[ \int d^{2} r \bar{v}^{*} \Delta_{0} e^{i \bar{v} v} = i \frac{2m^{2}}{\pi} \int_{0}^{\infty} d r (1 - rm) e^{-mr} \int_{0}^{\pi} d \theta e^{-m R} \]  

(B10b)

Thus we find that

\[ \langle \bar{v} | h | v \rangle = i \epsilon, \]

\[ \epsilon = 4m^{2} \int_{0}^{\infty} d r e^{-mr} \frac{1}{\pi} \int_{0}^{\pi} d \theta [1 - rm(1 + \cos \theta)] e^{-mR} \]  

(B11)

and the energy is shifted from zero by \( \pm \epsilon \).

Numerical integration of Eq. (B11) at large \( R \) yields a result consistent with

\[ \epsilon = -\frac{8}{\pi} \sqrt{m(mR)^{1 / 2} e^{-mR}} \]  

(B12)

This may be derived analytically with the following argument. We replace the upper limit \( (\infty) \) of the \( r \) integral by \( R \) and approximate \( D \) by \( R + r \cos \theta \). The \( \theta \) integral now leads to modified Bessel functions \( I_{0} \) and \( I_{1} \), and we keep only their large argument, exponential asymptote. The remaining \( r \) integral yields Eq. (B12).

2. Two vortices

The order parameter in Eq. (B2) describing two vortices located at \( r \approx \pm R / 2 \) reduces at \( R \approx R / 2 \) to

\[ \Delta_{v} - \Delta_{w} = me^{i \Omega(r - R / 2)} e^{i \Omega(r)} = me^{i \Omega(r - R / 2)} e^{i \theta} \]  

(B13a)

while the one at \( r = -R / 2 \) becomes

\[ \Delta_{v} - \Delta_{w} = me^{i \Omega(r - R / 2)} e^{i \Omega(r + R / 2)} = -me^{i \theta} e^{i \Omega(r + R / 2)} \]  

(B13b)

The corresponding zero modes differ by phases from the vortex solution in Eq. (47a) or (B4) but they retain their spinor structure.

\[ \psi_{0}^{\mu} = \begin{pmatrix} v_{+} \\ 0 \\ 0 \end{pmatrix}, \quad \psi_{0}^{\mu*} = \begin{pmatrix} v_{+}^{*} \\ 0 \\ 0 \end{pmatrix} \]  

(B14)

The explicit expressions for \( v_{+} \) and \( v_{-} \) are not needed because the above form of the spinors guarantees that all matrix elements of \( h \) vanish. Thus, within our approximation, the two-vortex background retains its two zero modes. This is to be expected because asymptotically such a configuration is indistinguishable from a double vortex

\[ \Delta_{w} \rightarrow me^{i \Omega(r)} e^{i \Omega(r)} = me^{i \theta} \]  

(B15)

and a double vortex possesses two zero modes.1
The same zero-energy mode with damped Bessel function oscillations occurs also in descriptions of bilayer graphene with the condensate $\Delta$ arising from states bound by interlayer Coulomb forces and the role of the chemical potential $\mu$ taken by an external constant biasing voltage (Refs. 15 and 16).