Second-order topological superconductors with mixed pairing

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We show that a two-dimensional semiconductor with Rashba spin-orbit coupling could be driven into the second-order topological superconducting phase when a superconductor in proximity exhibits mixed pairing symmetries. The superconducting order we consider involves only even-parity components and meanwhile breaks time-reversal symmetry. As a result, each corner of a square-shaped heterostructure hosts a single Majorana zero mode in the second-order nontrivial phase. Starting from edge physics, we are able to determine the phase boundaries accurately. In the end, a simple criterion for the second-order phase is further established, which concerns the relative position between Fermi surfaces and nodal points of the superconducting order parameter.

Topological superconductors (TSCs) distinguish themselves from trivial ones in the robust mid-gap states—Majorana zero modes (MZMs)—that could form either at local defects or boundaries [1–9]. Among the various proposals for TSCs, semiconducting systems with Rashba spin-orbit coupling (RSOC) [10–13] as well as topologically insulating systems [14] have attracted the most attention. In both of the two platforms, signatures of MZMs have been observed when conventional s-wave pairing is introduced through proximity effect [15–25].

In these conventional, also termed as first-order TSCs, topologically nontrivial bulk in $d$ dimensions is usually accompanied by MZMs confined at $(d-1)$-dimensional boundaries, the so-called bulk-boundary correspondence. Very recently, this correspondence was extended in higher-order topological phases [26–41], where topologically protected gapless modes emerge at $(d-2)$- or even $(d-3)$-dimensional boundaries. Hence second-order TSCs in two dimensions would be characterized by MZMs bound at corners. In Refs. [42–44], the authors demonstrate that a two-dimensional (magnetic) topological insulator could be transformed into a second-order TSC when an unconventional superconductor (SC) with $s_{\pm}$- or $d_{x^2-y^2}$-wave pairing symmetry is in proximity. One may ask then if it is possible for a Rashba semiconductor (RS) to realize this second-order topological superconducting phase simply by proximitizing with a SC alone. In this work, we will show that it is when the SC exhibits mixed pairing symmetries.

Studies of mixed pairing states have continued for quite a long time in cuprate SCs [45], and recently revived in iron-based SCs [46–47]. Representative examples are $s+d$ [48–49], $d_{x^2-y^2}+id_{xy}$ [50–51], $s+id$ [52–55], and $s+is$ pairing [56]. Recent studies in Ref. [57] and [58] suggest that superconducting pairing with mixed parity $(p+id)$ could turn a metallic system into a second-order TSC. Here we propose that a heterostructure of RS and mixed-pairing SC with even-parity components only ($s$ and $d_{x^2-y^2}$ pairing) may also realize the topologically nontrivial phase. In addition, we find that in this setup the emergence of the second-order topological superconducting phase is closely related to the relative position between nodal points of the pairing order parameter and the non-degenerate Fermi surfaces split by RSOC.

The hybrid system we consider consists of a 2D RS in contact with a SC with mixed pairing, as is schematically shown in Fig. 1(a). Due to proximity effect, RS also develops the superconducting order, and could be described by a two-dimensional Bogoliubov de-Gennes (BdG) Hamiltonian, which in the Nambu spinor basis

$$\Psi(k) = \{c_k, c_{-k}^\dagger, c_{k_1}^\dagger, c_{-k_1}^\dagger\}^T$$

has the following form,

$$H = \frac{1}{2} \sum_k \Psi^\dagger(k) \mathcal{H}(k) \Psi(k),$$

$$\mathcal{H}(k) = h(k)\tau_3 + \Delta_s(k)\tau_1 + \Delta_{sd}(k)\tau_2.$$  \hspace{1cm} (1)

In Eq. (1), $h(k) = 2A(\sin k_x\sigma_2 - \sin k_y\sigma_1) - 2t(\cos k_x + \cos k_y) - \mu$, with $t$, $A$ and $\mu$ being hopping amplitude, RSOC strength and chemical potential respectively, and Pauli matrices $\sigma_{1,2,3}$, $\tau_{1,2,3}$ act in spin and Nambu space separately. The superconducting term in this model only contains even-parity components, with

$$\Delta_s(k) = \Delta_0 + 2\Delta_1(\cos k_x + \cos k_y)$$

in Eq. (1), denoting pure $s$-wave pairing, and

$$\Delta_{sd}(k) = -2\Delta_2(\cos k_x + \cos k_y).$$
\[ \delta \cos k_y + \eta \), describing \( s + d \) pairing that in addition exhibits a \( \pi/2 \)-phase shift relative to \( \Delta \). Due to the phase difference, \( \Delta_{sd} \) breaks time-reversal symmetry (TRS). We denote this mixed pairing as \( s + i(s + d) \) for short, which reduces to \( s + id \) pairing when \( \delta = -1, \eta = 0 \), and to \( s + is \) when \( \delta = 1 \). The energy spectrum of Hamiltonian (1) has a simple form,

\[ E(k) = \pm \sqrt{\epsilon_+^2(k) + \Delta_s^2(k) + \Delta_{sd}^2(k)}, \]

where \( \epsilon_\pm(k) = \pm 2A \sqrt{\sin^2 k_x + \sin^2 k_y} - 2t(\cos k_x + \cos k_y) - \mu \), being the kinetic energy.

When \( |\Delta_0| < 4|\Delta_1| \), \( \Delta_s \) becomes \( s_i \)-wave pairing. In the absence of \( \Delta_{sd} \) term, the model is well known to support first-order topological superconducting phase that features TRS-protected helical Majorana modes on the edges, as well as nodal superconducting phase with point nodes [59] (see the phase diagram in Fig. 1(b)). Turning on \( \Delta_{sd} \) is supposed to break TRS and gap out the helical modes. Instead of driving the system into trivial phases, we will demonstrate that this TRS-breaking term may give birth to second-order topological superconducting phases, featuring MZMs bound at corners.

To understand the origin of second-order phases, we may start from gapless edge states in absence of \( \Delta_{sd} \) and then consider effects of this mass term on the gapless modes.

As is known, second-order phases appear when gapless states on intersecting edges acquire mass gaps of opposite signs. To investigate the edge physics, we consider a cylinder geometry, where periodic boundary condition (PBC) is assumed along \( y \) direction (see Fig. 1(a)) and open boundary condition (OBC) in \( x \) direction. Accordingly, Hamiltonian in Eq. 1 needs to be rewritten in a suitable basis that we denote by \( \Psi(k_y) = \oplus_j \psi_j(k_y) \), where \( \psi_j(k_y) = \{c_{j,k_y}^\uparrow, c_{j,-k_y}^\downarrow, c_{j,-k_y}^\uparrow, c_{j,-k_y}^\downarrow\}^T \). For \( j \) stands for lattice site and \( N_x \) is the total number of sites. In the new basis, we would have

\begin{align*}
[\mathcal{H}_{1D}(k_y)]_{j,j} &= M = M_{\alpha\beta} \Gamma_{\alpha\beta}, \\
[\mathcal{H}_{1D}(k_y)]_{j,j+1} &= (\mathcal{H}_{1D}(k_y))_{j+1,j}^T = T = T_{\alpha\beta} \Gamma_{\alpha\beta}.
\end{align*}

In Eq. 3, \( \Gamma_{\alpha\beta} = \tau_\alpha \otimes \sigma_\beta \) with \( \alpha, \beta = 0, 1, 2, 3 \), and the two tensors \( M \) and \( T \) have the following components: \( M^{30} = -\mu - 2t \cos k_y, \ M^{31} = -2A \sin k_y, \ M^{10} = \Delta_0 + 2\Delta_1 \cos k_y, \ M^{20} = -2\Delta_2(\eta + \delta \cos k_y), \ M^{30} = -t, \ M^{32} = -t, \ T^{30} = -A, \ T^{10} = \Delta_1 \) and \( T^{20} = -\Delta_2 \). Energy spectrum and corresponding wave functions in this geometry could be determined from eigenvalue equation \( \mathcal{H}_{1D}(k_y) \phi = E(k_y) \phi \), which leads to

\[ M\phi_j + T\phi_{j-1} + T\phi_{j+1} = E(k_y)\phi_j, \]

for any \( j \), with \( \phi_j \) being a four-component vector that represents the wave function at site \( j \).

In the first-order phase when \( \Delta_{sd} = 0 \), the spectrum \( E(k_y) \) supports doubly degenerate MZMs at \( k_y = \pi \) if \( \Delta_0/\Delta_1 > 0 \) and at \( k_y = 0 \) otherwise [59]. Additionally, the gapless modes are localized on edge AB and CD defined in Fig. 1(a). Without loss of generality, hereafter we will assume \( \Delta_0/\Delta_1 > 0 \), and the edge states could thus be described by massless Dirac Hamiltonian around \( k_y = \pi \). In the nodal phase, zero modes in the spectrum \( E(k_y) \) would appear at the projections of bulk nodes on the edge Brillouin zone (BZ), as is shown in Fig. 2(a) and (c). There are eight nodes in total, which relate to one another through four-fold rotation \( C_4 \), mirror reflections \( M_x \) and \( M_y \) with mirror planes sitting at \( k_x = 0 \) and \( k_y = 0 \), respectively. In the absence of \( \Delta_{sd} \), bulk Hamiltonian (1) is invariant under these operations, i.e.,

\begin{align*}
\mathcal{U}^{-1}_C \mathcal{H}(k_x, k_y) \mathcal{U}_C &= \mathcal{H}(-k_x, k_y), \\
\mathcal{U}^{-1}_{M_x} \mathcal{H}(k_x, k_y) \mathcal{U}_{M_x} &= \mathcal{H}(-k_x, k_y), \\
\mathcal{U}^{-1}_{M_y} \mathcal{H}(k_x, k_y) \mathcal{U}_{M_y} &= \mathcal{H}(k_x, -k_y),
\end{align*}

where \( \mathcal{U}_C = e^{i\pi \sigma_3/4}, \mathcal{U}_{M_x} = \sigma_1, \) and \( \mathcal{U}_{M_y} = \sigma_2 \). Due to these crystalline symmetries, we may denote the eight bulk nodes by \( \pm(k_x, \pm k_y) \) and \( \pm(k_x, \pm k_y) \). Define \( \Delta = \Delta_0/(4\Delta_1) \), and we have

\[ \cos k_y = -\Delta \pm \sqrt{1 - \Delta^2 - (\mu - 4\Delta \Delta_2)^2/(8A^2)}. \]

In contrast to the first-order phase, zero modes at \( \pm k_y \) in the nodal phase are not localized. However, in the regions enclosed by these gapless points, when \( k_y \in (-k_y, -k_y) \cup \),
(k_+, k_-) (0 < k_+ < k_- < π is assumed), we find that two localized states with opposite excitation energy would exist on each edge, as is evidenced in Fig. 2 (c) and (d). It seems that these edge states are not topologically protected, since each gapless point is the projection of two bulk nodes carrying opposite topological charges (see Fig. 2 (a)) which are supposed to cancel with each other. The charge for each bulk node is defined by the winding number \( w \) along a contour surrounding this node, with
\[
w = \frac{1}{2\pi i} \int_c [k] \nabla q(k)], \tag{7}
\]
q(k) in Eq.(7) is the well-known q matrix \( \mathbf{q} \) in the spectrally flattened Hamiltonian written in off-diagonal form and the path \( l \) we take is shown in Fig. 2(a). Possibly, these localized edge states are the remnants of those in the first-order phase. In our specific model defined in Eq.(4), they are robust provided the system is in the nodal phase. Hence we may still describe the low-energy physics of the edges with massless Dirac Hamiltonian in this circumstance, except that the edge Hamiltonian is only defined for \( k_y \in (-k_-, -k_+) \cup (k_+, k_-) \), and that states at Dirac points \( \pm k_\pm \) are not strictly localized.

So we have established that, edge modes emerge both in the first-order topological superconducting phase and in the nodal phase, when \( \Delta_{sd} = 0 \). Edge states in these two phases could be well described by one-dimensional massless Dirac Hamiltonian, with Dirac points being located at \( k_y^c = \pi \) in the first-order phase, and at \( k_y^c = \pm k_\pm \) in the nodal phase. Note that Hamiltonian (4) preserves chiral symmetry \( \Gamma_{20} \) in absence of \( \Delta_{sd} \), which guarantees that, for any state \( \phi \) with finite energy \( E(k_y) \) there would be a state \( \Gamma_{20}\phi \) (shorthand for \( \oplus \Gamma_{20}\phi \)) with opposite energy \( -E(k_y) \). Hence the gapless modes at Dirac points are doubly degenerate on each edge. Instead of going into details of the gapless states, we will attempt to construct an effective edge Hamiltonian with a unified form.

First, multiplying Eq.(4) with \( \phi_j^\dagger \Gamma_{10} \) on both sides, summing over \( j \) and then adding to it with the Hermitian conjugating counterpart, we are then left with
\[
M^{10} = \sum_j E(k_y)\phi_j^\dagger \Gamma_{10} \phi_j - T^{10} \phi_j^\dagger(\phi_{j-1} + \phi_{j+1}), \tag{8}
\]
where the normalization condition \( \phi^\dagger \phi = 1 \) is used. One could also multiply Eq.(4) with \( \phi_j^\dagger \Gamma_{20} \) and follow the same procedure as above, which would lead to
\[
T^{10} \sum_j \phi_j^\dagger \Gamma_{20}(\phi_{j-1} + \phi_{j+1}) = 0, \tag{9}
\]
due to orthogonality condition \( \phi^\dagger \Gamma_{20} \phi = 0 \). At the gapless point \( k_y^c \), Eq.(8) reduces to
\[
M^{10} = -T^{10} \sum_j \phi_j^\dagger(\phi_{j-1} + \phi_{j+1}). \tag{10}
\]
Take the two-fold degenerate zero modes at Dirac points as basis, denoted by \( \{ \phi(k_y^c), \Gamma_{20} \phi(k_y^c) \} \), and we could then project Hamiltonian (4) onto it. Utilizing the two equalities in Eq.(9) and (10), one arrives at the effective low-energy Hamiltonian for edge AB and CD, given by
\[
\mathcal{H}_{Edge}(k_y) = v_2(k_y)s_2 + v_3(k_y)s_3 + m_{sd}(k_y)s_1 \tag{11}
\]
where
\[
v_2(k_y) = \sum_{j,\{\alpha\beta\}} [M^{\alpha\beta}(k_y) - M^{\alpha\beta}(k_y^c)]\phi_j^\dagger \Gamma_{20}\alpha\beta \phi_j,
\]
\[
v_3(k_y) = \sum_{j,\{\alpha\beta\}} [M^{\alpha\beta}(k_y) - M^{\alpha\beta}(k_y^c)]\phi_j^\dagger \Gamma_{20}\alpha\beta \phi_j,
\]
\[
m_{sd}(k_y) = -2\Delta_2(\delta \cos k_y + \eta - \cos k_y^c - 2\Delta), \tag{12}
\]
with indices \( \{\alpha\beta\} \) taking \( \{30, 31, 10\} \) and Pauli matrices \( s_1, 2, 3 \) acting in edge space. It should be pointed out that \( \phi_j \) in Eq.(12), i.e., wave functions at gapless point(s), could be obtained from Eq.(11) in principle, although we don’t have to, given that it is the mass gap that we care foremost. Clearly, \( m_{sd} \) in Eq.(11) plays the role of mass field and would open a finite gap at the gapless point, whose value doesn’t depend on the specific form of \( \phi_j \). Given the edge Hamiltonian Eq.(11), the condition when second-order phases emerge can be determined by comparing signs of mass gaps on intersecting edges, which we shall detail in the following.

Let us consider rotating the basis in Eq.(1) to \( \Psi’(k’) = U_{\mathcal{C}} \Psi(C_{\mathcal{A}}k’) \), where \( k’ \) stands for coordinates in \( O-k_y^c k_y^c k_x \) system defined in Fig. 1(a) and relates to \( k \) through \( C_4 \) rotation \( C_{\mathcal{A}}k’ = k \), namely, \( \{-k_y^c k_y^c k_x\} = (k_x, k_y) \). Rewriting Hamiltonian (1) in this new basis, we would have
\[
H = \frac{1}{2} \sum_{k’} \Psi’^\dagger(k’) \mathcal{H}’(k’) \Psi’(k’), \tag{13}
\]
\[
\mathcal{H}’(k’) = U_{\mathcal{C}} \mathcal{H}(C_{\mathcal{A}}k’) U_{\mathcal{C}}^{-1} = h(k’) + \Delta_2(k’) + \Delta_{sd}(k’),
\]
where \( \Delta_2(k’) = -2\Delta_2(\delta \cos k_y + \delta \cos k_x + \eta) \) and the last equality in Eq.(13) is due to \( C_4 \) symmetry of \( h \) and \( \Delta_2 \) detailed in Eq.(15). Comparing the two Hamiltonian in Eq.(11) and (13), one may immediately conclude that edge Hamiltonian along edge AD and BC could be obtained from Eq.(11) simply by replacing \( k_y \) with \( k_y’ \), followed by modification of the mass term, which yields
\[
\mathcal{H}_{Edge}(k_y’) = v_2(k_y’)s_2 + v_3(k_y’)s_3 + m_{sd}(k_y’)s_1, \tag{14}
\]
with
\[
m_{sd}(k_y’) = -2\Delta_2(\cos k_y’ - \eta - \delta \cos k_y’ - 2\Delta), \tag{15}
\]
and the definitions of \( v_2 \) and \( v_3 \) are given in Eq.(12). It is obvious that Dirac points in the two edge Hamiltonian, \( \mathcal{H}_{Edge}(k_y) \) and \( \mathcal{H}_{Edge}(k_y’) \), both reside at \( k_y’ \). The second-order topological superconducting phase therefore emerges when the two edge Hamiltonian exhibit gaps with opposite signs, i.e., when
\[
m_{sd}(k_y’)m_{sd}(k_y’) < 0. \tag{16}
\]
Substituting the expression of $k^c_\gamma$ into Eq. (16), we arrive at the conditions for second-order phases,

$$|\eta - f_1| < |f_3|,$$

$$|\mu - 4t\tilde{\Delta}| < \frac{2\sqrt{2}A}{1 - \delta}\sqrt{f_2^2 - (\eta - f_1)^2},$$

with $f_1 = (1 + \delta)\tilde{\Delta}$, $f_2 = (1 - \delta)\sqrt{1 - \Delta^2}$ and $f_3 = (1 - \delta)(1 - \Delta)$. Eq. (19) determines which kind of superconducting pairing could possibly induce the second-order phase, while Eq. (20) establishes the relation of Fermi surfaces with the pairing potential in this nontrivial phase. Indeed, we observe that the nodal point $k^n$ ($\Delta_s(k^n) = \Delta_{sd}(k^n) = 0$) of the pairing order parameter, marked by magenta circle in Fig. 3, always lies between the two Fermi surfaces in the second-order phase. This is verified by the fact that Eq. (20) could also be obtained by requiring

$$\epsilon_+ (k^n)\epsilon_-(k^n) < 0,$$  

where $\epsilon_{\pm}$ are the same as those in Eq. (2) and take zero separately on the two Fermi surfaces. In addition, we also note that Eq. (19) actually guarantees the existence of nodal point $k^n$. Therefore, one may determine when the system resides in the second-order phase, either from Eq. (19) and (20), or from Eq. (21), both of which would yield the accurate parameter regime, as illustrated in Fig. 3. Due to mirror symmetries $\mathcal{M}_x$ and $\mathcal{M}_y$ exhibited in Hamiltonian (1), there would be four MZMs in the nontrivial phase, with each of the four corners accommodating one, as shown in the insets of Fig. 3.

With these criteria in mind, let us now consider two specific pairing forms aforementioned, namely, $s + is$ and $s + id$ pairing. In the former case, one may verify that Eq. (19) would never be fulfilled, and hence the system is trivial. In the latter case, however, Eq. (19) is always valid and Eq. (20) simply reduces to Eq. (17), suggesting that $s + id$ pairing favors second-order phases.

In summary, we established that the admixture of $s$- and $d$-wave pairing with broken TRS could drive a RS into the second-order topological superconducting phase, as long as the point node of pairing order parameter lies between the two Fermi surfaces. Several mechanisms [52–55] have been put forward that might give rise to this mixed pairing, especially in those iron-based SCs where the pairing symmetry is expected to evolve between $s$- and $d$-wave form with doping [61] or pressure [62, 63]. $s + id$ pairing could possibly exist in these materials as an intermediate state, and other mixed-pairing forms such as $s + i(s + d)$ may develop further when nematic order exists additionally [64]. One can thus expect that the proximitized RS with these iron-based SCs might realize the second-order TSC and that MZMs bound at the corners therein could be detected.

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