First and second-order topological superconductivity and temperature-driven topological phase transitions in the extended Hubbard model with spin-orbit coupling

Majid Kheirkhah,1 Zhongbo Yan,2 Yuki Nagai,3, 4 and Frank Marsiglio1

1Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2E1
2School of Physics, Sun Yat-Sen University, Guangzhou 510275, China
3CCSE, Japan Atomic Energy Agency, 178-4-4, Kashiwa, Chiba, 277-0871, Japan
4Mathematical Science Team, RIKEN Center for Advanced Intelligence Project (AIP), 1-4-1 Nihonbashi, Chuo-ku, Tokyo 103-0027, Japan

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The combination of spin-orbit coupling with interactions results in many exotic phases of matter. In this paper we investigate the superconducting pairing instability of the two-dimensional extended Hubbard model with both Rashba and Dresselhaus spin-orbit coupling within the mean-field level at both zero and finite temperature. We find that both first and second-order time-reversal symmetry breaking topological gapped phases can be achieved under appropriate parameters and temperature regimes due to the presence of a favored even-parity $s + id$-wave pairing even in the absence of an external magnetic field or intrinsic magnetism. This results in two branches of chiral Majorana edge states on each edge and a single zero-energy Majorana corner state at each corner of the sample. Interestingly, we also find that not only tuning the doping level leads to a direct topological phase transition between these two distinct topological gapped phases, but also using the temperature as a highly controllable and reversible tuning knob leads to different direct temperature-driven topological phase transitions between gapped and gapless topological superconducting phases. Our findings suggest new possibilities in interacting spin-orbit coupled systems by unifying both first-order and higher-order topological superconductors in a simple but realistic microscopic model.

Introduction — Spin-orbit coupling (SOC) is ubiquitous in condensed matter systems and responsible for many remarkable phenomena [1–15]. In recent years, a surge of research interest in SOC was stimulated by the discovery that SOC plays a critical role in realizing various topological phases, ranging from non-interacting or weakly correlated topological insulators (TIs) and topological superconductors (TSCs) to strongly correlated topological phases [16–19]. Among them, TSCs are noticeable as they harbor Majorana modes which are believed to be a possibility for the building blocks of topological quantum computation [20–24]. While odd-parity superconductors generally provide a natural realization of TSCs [25–30], their scarcity in nature turns out to be a serious obstacle from an experimental point of view. Fortunately, SOC enables the realization of effective odd-parity superconductivity (SC) on the basis of abundant even-parity SC, providing a more readily accessible route for the realization of TSCs [31–38]. Over the past decade, remarkable progress along this route has been witnessed [39–47].

Very recently, a new class of topological phases, named higher-order TIs and TSCs, have emerged and attracted a great deal of attention first because of the enrichment due to boundary physics, but also of the occurrence of new possibilities for topological phase transitions [48–63]. The word “order” in this context gives the co-dimension of the gapless boundary modes, namely, an $n$-th order TI or TSC has gapless boundary modes with co-dimension $n$. As the gapless boundary modes of all conventional TIs and TSCs have $n = 1$, they thus belong to the first-order topological phases in this language.

Because higher-order TSCs provide new platforms of Majorana modes, their potential application in topological quantum computation has triggered quite a few theoretical proposals on their experimental realizations [64–88]. However, the superconducting pairings in previous works were mostly introduced phenomenologically, and realistic microscopic models for higher-order TSCs are still generally lacking. Over the past decade, the Hubbard model with SOC and on-site interaction, as one of the simplest microscopic models for first-order TSCs, has been extensively studied in both condensed matter and in the cold atom communities [89–95]. In this work, we extend the Hubbard model in two dimensions to include both on-site (repulsive) and inter-site (attractive) interactions and investigate its even-parity superconducting pairing instability at the mean-field level [96].

Our study reveals that depending on the temperature and the parameters of the model, the leading pairing channel can be $d$-wave, $s$-wave, or $s + id$-wave [97, 98]. Remarkably, we find when the $s + id$-wave is favored, a first-order TSC with two branches of chiral edge states and a second-order TSC with four Majorana corner modes, as well as a direct topological phase transition between them, can be realized by tuning the Fermi surface (FS) structure, even in the absence of a magnetic field or magnetism. Furthermore, we show that the temperature itself is a highly controllable and reversible tuning knob to drive topological phase transitions in this system.

Theoretical formalism — The two-dimensional extended Hubbard model, which provides a simple descrip-
tion for short-ranged interacting systems [96], reads as

\[
H = -t \sum_{\langle i,j \rangle, \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} + \text{h.c.} - \mu \sum_{i,\alpha} c_{i,\alpha}^\dagger c_{i,\alpha} + \lambda_R \sum_{i,\alpha,\beta} i(c_{i,\alpha}^\dagger s_{i,\beta} c_{i+\hat{x},\beta} - c_{i,\alpha}^\dagger s_{\bar{i},\beta} c_{\bar{i}+\hat{y},\beta}) + \text{h.c.}
\]

\[
+ \lambda_D \sum_{i,\alpha,\beta} i(c_{i,\alpha}^\dagger s_{i,\beta} c_{i+\hat{y},\beta} - c_{i,\alpha}^\dagger s_{\bar{i},\beta} c_{\bar{i}+\hat{x},\beta}) + \text{h.c.}
\]

\[
+ U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \frac{V}{2} \sum_{i,j,\alpha} \hat{n}_{i,\alpha} \hat{n}_{j,\alpha},
\]

(1)

where \( \langle i,j \rangle \) denotes summation over nearest-neighbor sites, \( c_{i,\alpha}^\dagger \) denotes the creation (annihilation) operator at site \( i \) with spin \( \alpha = (\uparrow, \downarrow) \), \( \hat{n}_{i,\alpha} = c_{i,\alpha}^\dagger c_{i,\alpha} \), \( t \) the nearest-neighbor hopping amplitude, \( \mu \) the chemical potential, \( \lambda_R \) (\( \lambda_D \)) is the Rashba (Dresselhaus) SOC amplitude, \( U \) is the on-site repulsive (\( U > 0 \)) interaction strength, and \( V \) is the nearest-neighbor attractive (\( V < 0 \)) interaction strength. The unit vector along the \( x \) (\( y \))-direction is represented by \( \hat{x} \) (\( \hat{y} \)), and \( s_{x,y} \) are Pauli matrices in spin space, the abbreviation \( \text{h.c.} \) stands for Hermitian conjugation, and the symbol \( i \) is taken to denote the pure imaginary number in order to avoid confusion with the site-index \( i \) appearing in the subscript.

Although in the presence of SOC, odd-parity and even-parity pairings can generally coexist, we restrict ourselves to even-parity pairing for the sake of clarity and simplicity. Accordingly, the Bogoliubov-de Gennes (BdG) Hamiltonian at the mean-field level in momentum space [99] can be rewritten as

\[
\mathcal{H}(k) = \tau_z \{ \xi(k)s_0 + l_x(k)s_x + l_y(k)s_y \} + \Delta(k)\tau_x s_0,
\]

(2)

where \( \tau_x, y, z \) are Pauli matrices in particle-hole space, and \( \xi_k = -2t(\cos k_x + \cos k_y) - \mu \) is the kinetic energy measured from the Fermi energy; \( l(k) = (l_x(k), l_y(k)) \) is the SOC vector, with \( l(k) = l_R(k) + l_D(k) \), where \( l_R(k) = 2\lambda_R(\sin k_y, -\sin k_x) \) and \( l_D(k) = 2\lambda_D(\sin k_x, -\sin k_y) \) represents the Rashba and Dresselhaus SOC, respectively; the superconducting order-parameter is given by

\[
\Delta(k) = \Delta_0^s + \Delta_0^d \eta_s(k) + \Delta_0^d \eta_d(k),
\]

(3)

where \( \Delta_0^s, \Delta_0^d \), and \( \Delta_0^d \) are momentum-independent complex numbers that represent on-site s-wave, extended s-wave, and d-wave SC, respectively. The three pairing amplitudes satisfy the following self-consistent superconducting gap equations,

\[
\Delta_0^s = -\frac{U}{4N} \sum_{k,\sigma} \Delta(k) F_{\sigma}(k),
\]

(4)

\[
\Delta_0^d = -\frac{V}{N} \sum_{k,\sigma} \Delta(k) \eta_s(k) F_{\sigma}(k),
\]

(5)

\[
\Delta_0^d = -\frac{V}{N} \sum_{k,\sigma} \Delta(k) \eta_d(k) F_{\sigma}(k),
\]

(6)

where \( N \) denotes the number of sites, \( \sigma = \pm 1 \), \( \eta_s(k) = (\cos k_x + \cos k_y)/2 \), \( \eta_d(k) = (\cos k_x - \cos k_y)/2 \) and

\[
F_{\sigma}(k) = \frac{1}{E_k^\sigma} \tanh \left( \frac{\beta E_k^\sigma}{2} \right).
\]

(7)

Here \( \beta \) is the inverse of temperature, and

\[
E_k^\sigma = \sqrt{\xi_k^2(\sigma) + |\Delta(k)|^2},
\]

(8)

are the two excitation spectra of the BdG Hamiltonian, where \( \xi_s(k) = \xi(k) + \sigma l(k) \) refers to the normal-state spectra with \( l(k) \) the magnitude of the \( l(k) \) vector.

To capture the phases of the three pairings, we define \( \Delta_0^s, \xi_\alpha^s \) for \( \alpha = \{0, s, d\} \), with \( \Delta_0 \) and \( \phi_\alpha \) being real numbers. Accordingly, the three complex self-consistent equations given by Eq. (4) to Eq. (6) can be separated into six real equations. By solving the self-consistent equations numerically, we find that when both s-wave and d-wave superconducting order-parameter are nonvanishing, their phases favor \( \phi_s = \phi_0 \) and \( \phi_d = \phi_0 \pm \pi/2 \) (“±” are degenerate in energy). Therefore, the superconducting order-parameter can be written explicitly as

\[
\Delta(k) = \Delta_0 + \Delta_s \eta_s(k) + i\Delta_d \eta_d(k),
\]

(9)

and accordingly, the six real self-consistent superconducting gap equations are reduced to

\[
\Delta_0 = -\frac{U}{4N} \sum_{k,\sigma} \{ \Delta_0 + \Delta_s \eta_s(k) \} F_{\sigma}(k),
\]

(10)

\[
\Delta_s = -\frac{V}{N} \sum_{k,\sigma} \eta_s(k) \{ \Delta_0 + \Delta_s \eta_s(k) \} F_{\sigma}(k),
\]

(11)

\[
1 = -\frac{V}{N} \sum_{k,\sigma} \eta_d^2(k) F_{\sigma}(k).
\]

(12)

It should be noted that when s-wave and d-wave pairing coexist, the last term of the BdG Hamiltonian (Eq. 2) should be rewritten as \( \{ \Delta_0 + \Delta_s \eta_s(k) \} \tau_x - \Delta_d \eta_d(k) \tau_y \) \( s_0 \). Throughout this work, we set the hopping amplitude \( t = 1 \) to be the energy unit, and other choices of parameters, \( \{ \lambda_R, U, V \} = \{0.3, 2, -5\} \) are set, unless we clearly mention otherwise.

Results — We first perform the self-consistent calculations at zero-temperature. For definiteness, we consider that only \( \lambda_D \) and \( \mu \) are tunable parameters. We restrict
FIG. 1. (Color online) Zero-temperature phase diagram for $\{t, \lambda R, U, V\} = \{1, 0.3, 2, -5\}$. The phase diagram contains $d$, $s$-wave SC (red color region), $s+id$-wave SC (blue color region), and $s$-wave SC (green color region). The time-reversal symmetry breaking $s+id$-wave SC phase consists of three topologically distinct phases, including first-order and second-order TSC, and topologically trivial SC.

Odd-parity superconductor is determined by the relative configuration of the FS and the pairing nodes, and there exists a simple relation between the Chern number $C$ and the number of FSs $(N_F)$ enclosing one time-reversal invariant point, which is $(-1)^C = (-1)^{N_F}$ [25]. Another important point is that if the normal state of a superconductor does not have a FS, the underlying topology must be trivial since such a phase can continuously transform to the limit $|\mu| \to \infty$ without the closing of either the bulk or the boundary gap. As the constant-energy contour satisfying $[\xi_{\mathbf{k}}] + l(\mathbf{k}) = 0$ represents the FS of $\mathcal{H}_+(\mathbf{k})$, the semi-positive characteristic of $[\xi_{\mathbf{k}}] + l(\mathbf{k})$ implies the absence of a FS when the energy spectra of $\mathcal{H}_+(\mathbf{k})$ are gapped. In other words, $\mathcal{H}_+(\mathbf{k})$ is always trivial in topological and we only need to focus on $\mathcal{H}_-(\mathbf{k})$.

Interestingly, we notice that $\mathcal{H}_-(\mathbf{k})$ takes a form similar to the toy model realizing second-order TSC proposed in Ref. [75]. Since the normal state has TRS, the number of FSs determined by $[\xi_{\mathbf{k}}] - l(\mathbf{k}) = 0$ must be even. Then, from the formula $(-1)^C = (-1)^{N_F}$, we know that $C$ must be an even integer. Then $C$ is a nonzero even integer, the system corresponds to a first-order TSC with $C$ branches of chiral edge states. When $C = 0$, the system is either a trivial superconductor or a second-order TSC, depending on whether the even-number of FSs $(N_F = 2$ for this Hamiltonian) can be continously deformed to annihilate with each other without crossing any removable Dirac pairing nodes (not at TRI points) or not. As shown in Ref. [75], when there are four removable Dirac pairing nodes whose net sum of winding number (defined as $\omega = (1/2\pi i) \oint \Delta^{-1}_+ \partial_{\mathbf{k}} \Delta_+ d\mathbf{k}$, with the closed integration contour enclosing only the interested pairing node) is zero lying between the two FSs, the system realizes a second-order TSC. Another way to understand this picture is via the edge theory. To be specific, when the four removable Dirac pairing nodes of $\mathcal{H}_-(\mathbf{k})$ lie between the two FSs, it means that if we neglect the $d$-wave pairing, the line nodes of $s$-wave pairing (satisfying $\Delta_0 + \Delta_s \eta_0 = 0$) can be chosen to lie between the two FSs. Since without the $d$-wave pairing, the full Hamiltonian restores the TRS, then according to the formula $\nu = \prod_i [sgn(\Delta_i)]^{m_i}$, we have $\nu = -1$, indicating the realization of a first-order TRI TSC which hosts a pair of helical Majorana edge states. Bringing back the $d$-wave pairing, the helical edge states are gapped out due to the breaking of TRS. However, as the $d$-wave pairing itself has line nodes along the directions $k_x = \pm k_y$, four Majorana zero-modes will be left at the four corners when we use open boundary conditions in both $x$ and $y$ directions [66, 68].

Based on the above analysis, we find that within the $s + id$-wave pairing regime, the change of topology only takes place when the FSs cross the removable Dirac pairing nodes at which $\Delta_0 + \Delta_s \eta_0 = 0$ and $\Delta_0 \eta_0 = 0$ are simultaneously fulfilled. As for the parameters considered we find $\Delta_0 \ll \Delta_s$; these nodes are almost fixed at the four points $Q_{\pm, \pm} = (\pm \pi/2, \pm \pi/2)$. There-
fore, the condition for topological phase transitions can be very accurately described by the normal state condition $|Q_{\pm \pm} - l(Q_{\pm \pm})| = 0$. It is straightforward to find that the solutions give two straight lines satisfying $|\mu - 2\sqrt{2}|_{\lambda_R \pm \lambda_D}| = 0$ [99], which correspond to the two dashed lines in Fig. 1.

To support the above analysis, we further diagonalize the mean-field BdG Hamiltonian in real space [99]. To be specific, we fix $\lambda_D = 0.6$ and study the evolution of boundary modes with $\mu$. The results are presented in Fig. 2. In accordance with the phase diagram in Fig. 1, we know that $\mu_{c, 1} \approx 3\sqrt{2}/5 \approx 0.85$ and $\mu_{c, 2} \approx 9\sqrt{2}/5 \approx 2.55$ are two critical points in the regime with $s + id$-wave pairing [99]. Within each phase, we show one representative configuration of FSs and pairing nodes (Fig. 2(b-e)). Fig. 2(b) shows that within the regime $0 < \mu < \mu_{c, 1}$, the four pairing nodes at $(\pm \pi/2, \pm \pi/2)$ remain to be located between the two concentric FSs, as shown in Fig. 2(c). As one pair-
ing node takes the same winding number as its inversion partner, the transition from the configuration in Fig. 2(b) to that in Fig. 2(c) suggests a change of Chern number by 2. In other words, a first-order TSC with $C = 2$ is realized in the regime $\mu > \mu_c$. To demonstrate this phase, we consider a cylinder geometry with open-boundary conditions only along the $x$-direction. The numerical result confirms the existence of two chiral Majorana modes on each edge (see Fig. 2(g)), and therefore the realization of a first-order TSC with $C = 2$. Remarkably, the above results suggest that a topological phase transition between second-order and first-order TSCs takes place at $\mu_c$. Numerical calculations reveal the absence of gapless boundary modes (Fig. 2(h),(i)) in the regime $\mu > \mu_c$, indicating that the Hamiltonian is trivial in topology in this regime.

So far, we have restricted the results to the zero-temperature limit. By performing self-consistent calculations at finite temperature, we find that for a given configuration of FSs, different pairing types exhibit different temperature dependence. As a result, the favored pairing can undergo a dramatic change at some critical temperature. To be specific, Fig. 3 shows two examples whose ground states at zero-temperature are second-order and first-order $s + id$-wave TSCs. From this figure, it is readily seen that the increase of temperature leads to a change of the favored pairing from gapped $s + id$-wave TSC to $d$-wave gapless SC at a parameter-dependent critical temperature. Since the $d$-wave pairing leads to the realization of nodal or Dirac SC, it indicates that the temperature itself provides a way to tune the underlying topological properties.

**Conclusions** — In this paper we showed that both first-order and second-order time-reversal symmetry breaking topological superconductivity as well as the topological phase transition between them can emerge in the extended Hubbard model with both Rashba and Dresselhaus SOC, even in the absence of an external magnetic field or magnetic order. Moreover, we demonstrated that with appropriate FS structure, tuning only the temperature can result in interesting topological phase transitions in this system. Our findings are relevant to many systems; for instance, oxide interfaces (like LaAlO$_3$/SrTiO$_3$) and cold atom systems are two typical classes in which both SOC and interactions are tunable [103, 104].

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Supplemental Material for “First and second-order topological superconductivity and temperature-driven topological phase transitions in the extended Hubbard model with spin-orbit coupling”

Majid Kheirkhah,1 Zhongbo Yan,2 Yuki Nagai,3,4 and Frank Marsiglio1

1Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2E1
2School of Physics, Sun Yat-Sen University, Guangzhou 510275, China
3CCSE, Japan Atomic Energy Agency, 178-4-4, Wakashiba, Kashiwa, Chiba, 277-0871, Japan
4Mathematical Science Team, RIKEN Center for Advanced Intelligence Project (AIP), 1-4-1 Nihonbashi, Chuo-ku, Tokyo 103-0027, Japan

This supplemental material provides the details of the derivations of some important equations presented in the main text. It consists of four sections: (I) The gap equations in momentum space, (II) the Bogoliubov-de Gennes Hamiltonian in real space, (III) effective realization of odd-parity superconductivity, and (IV) phase boundaries in the $s + id$-wave pairing regime.

1. THE GAP EQUATIONS IN MOMENTUM SPACE

As the normal state has time-reversal symmetry and we are interested in the superconducting pairing instability, the last line of the real-space Hamiltonian in the main text can be written in momentum space as,

$$H_{int} = \frac{1}{N} \sum_{k,q} (U + V(\zeta_{k-q})c_{k,q}^\dagger c_{-k,q} + \text{h.c.}),$$

(S1)

where $\zeta_{k-q} = \sum_\delta e^{-i(k-q)\cdot \delta} = 2\{\cos(k_x - q_x) + \cos(k_y - q_y)\}$ and $\delta$ is the coordinates of the four nearest-neighbours of a given site in a square lattice with unit lattice constant. Note that we have dropped terms corresponding to pairing with non-zero center-of-mass momentum. Performing mean-field decoupling by considering only the even-parity superconducting order-parameter and ignoring constant terms leads to the following quadratic Hamiltonian,

$$H_{MF}^{int} = \frac{1}{2} \sum_k \Delta_{\alpha\beta}(k)c_{k,\alpha}^\dagger c_{-k,\beta}^\dagger c_{-k,\beta} + \text{h.c.},$$

(S2)

where the even-parity superconducting order-parameter can be written as $\Delta_{\alpha\beta}(k) = i\Delta(k)\eta^\alpha_{\beta}$ and

$$\Delta(k) = -\frac{1}{N} \sum_q \left\{U + \frac{V}{2}(\zeta_{k+q} + \zeta_{k-q})\right\} \langle c_q^\dagger c_{-q}\rangle.$$  

(S3)

It is obvious that $\Delta(-k) = \Delta(k)$ by using of the fact that $\zeta_k$ is an even function of $k$, i.e. $\zeta_k = \zeta_{-k}$. It can be shown that,

$$\zeta_{k+q} + \zeta_{k-q} = 8\{\eta_s(k)\eta_s(q) + \eta_d(k)\eta_d(q)\},$$

(S4)

where $\eta_s(k) = (\cos k_x + \cos k_y)/2$, and $\eta_d(k) = (\cos k_x - \cos k_y)/2$. This leads to the following superconducting gap functions,

$$\Delta(k) = \Delta^0 + \Delta^s_\alpha \eta_s(k) + \Delta^d_\alpha \eta_d(k).$$

(S5)

where $\Delta^0_{s,d}$ are some complex numbers and are given by Eq. (4) to Eq. (6) of the main paper. If we define $\Delta^\alpha_\alpha = \Delta^\alpha e^{i\phi_\alpha}$ for $\alpha \in \{0, s, d\}$ where all the $\Delta_\alpha$ and $\phi_\alpha$ are real numbers, those three complex equations are separated into six real equations. We restrict ourselves to the even-parity $s + id$-wave pairing which is more favorable in energy by setting $\phi_s = \phi_0$ and $\phi_d - \phi_0 = \pm\pi/2$. Therefore, the resulting $s + id$-wave pairing order-parameter reads as,

$$\Delta(k) = \Delta_0 + \Delta_s \eta_s(k) + i\Delta_d \eta_d(k).$$

(S6)
Finally, the total Hamiltonian in the Nambu space can be written as,

\[ H = \frac{1}{2} \sum_{k} (c_{k}^\dagger \ c_{-k}) \mathcal{H}(k) \begin{pmatrix} c_{k} \\ c_{-k}^\dagger \end{pmatrix}, \]

where \( c_{k} = (c_{k^\uparrow}, c_{k^\downarrow}) \) and \( c_{-k} = (c_{-k^\uparrow}, c_{-k^\downarrow}) \), as well as

\[ \mathcal{H}(k) = \xi(k) \tau_z s_0 + l_x(k) \tau_0 s_x + l_y(k) \tau_2 s_y - (\Delta_0 + \Delta_s \eta^s_k) \tau_y s_y - \Delta_d \eta^d_k \tau_z s_y, \]

where \( \xi(k) = -2t(\cos k_x + \cos k_y) - \mu \), \( l_x(k) = 2(\lambda_R \sin k_x + \lambda_D \sin k_z) \), and \( l_y(k) = -2(\lambda_R \sin k_x + \lambda_D \sin k_y) \). The Pauli matrices in spin and particle-hole spaces are denoted by \( s_0, s_\tau \), respectively. Note that in the main paper a different Nambu basis was used.

2. THE BOGOLIUBOV-DE GENNES HAMILTONIAN IN REAL-SPACE

The mean-field real-space Hamiltonian can be rewritten as,

\[ H = \frac{1}{2} \sum_{ij} (c_{i}^\dagger \ c_{j}) \begin{pmatrix} A_{ij} & B_{ij} \\ -B_{ij}^\dagger & -A_{ij}^\dagger \end{pmatrix} \begin{pmatrix} c_{j} \\ c_{i}^\dagger \end{pmatrix}, \]

where \( c_{i} = (c_{i^\uparrow}, c_{i^\downarrow}) \) and \( c_{j} = (c_{j^\uparrow}, c_{j^\downarrow}) \) for \( i = (i_x, i_y) \). The hermitian property of \( H \), and the canonical anti-commutation relation \( \{c_{i}, c_{j}^\dagger\} = \delta_{ij} \) imply that the \( 2N \times 2N \) complex matrix \( A \) and \( B \) satisfy \( A^\dagger = A \) and \( B^T = -B \) relations, respectively, where \( N \) is the number of sites and \( T \) stands for transpose. The components of \( A \) and \( B \) matrices are given by,

\[ A_{ij} = s_0 A_{ij}^0 + s_x A_{ij}^x + s_y A_{ij}^y, \]

\[ B_{ij} = s_y (i \Delta^s_{ij} - \Delta^d_{ij}), \]

where

\[ A_{ij}^0 = -t (\delta_{j,i-x} + \delta_{j,i-z} + \delta_{j,i+y} + \delta_{j,i-y}) - \mu \delta_{ij}, \]

\[ A_{ij}^x = -i \lambda_R (\delta_{j,i+y} - \delta_{j,i-y}) - i \lambda_D (\delta_{j,i+z} - \delta_{j,i-z}), \]

\[ A_{ij}^y = +i \lambda_R (\delta_{j,i+z} - \delta_{j,i-z}) + i \lambda_D (\delta_{j,i+y} - \delta_{j,i-y}), \]

\[ \Delta^s_{ij} = \Delta_0 \delta_{ij} + \frac{\Delta_d}{4} (\delta_{j,i+x} + \delta_{j,i-z} + \delta_{j,i+y} + \delta_{j,i-y}), \]

\[ \Delta^d_{ij} = \frac{\Delta_d}{4} (\delta_{j,i+x} + \delta_{j,i-z} - \delta_{j,i+y} - \delta_{j,i-y}). \]

In this section and the main paper, the symbol \( i \) denoting pure imaginary number should not be confused with the site-index that generally occurs subscripted.

3. EFFECTIVE REALIZATION OF ODD-PARITY SUPERCONDUCTIVITY

For generality, here we further include an out-of-plane Zeeman field. Accordingly, the normal state Hamiltonian is

\[ H_0 = \sum_{k} (c_{k^\uparrow}^\dagger, c_{k^\downarrow}^\dagger) \begin{pmatrix} \xi_k + h_z & l_z - i l_y \\ l_x + i l_y & \xi_k - h_z \end{pmatrix} \begin{pmatrix} c_{k^\uparrow} \\ c_{k^\downarrow} \end{pmatrix}, \]

The spin singlet-pairing superconductivity is described by

\[ H_{SC} = \sum_{k} (\Delta_s(k) + i \Delta_d(k)) c_{k^\uparrow} c_{-k^\downarrow}^\dagger + h.c., \]
where $\Delta_s(k) = \Delta_0 + \Delta_s \eta_s(k)$ and $\Delta_d(k) = \Delta_d \eta_d(k)$. We first follow Ref. [S1] and do the following transformation
\[ c_{k,\uparrow} = (\cos \frac{\theta_k}{2} c_{k,+} + e^{-i\phi_k} \sin \frac{\theta_k}{2} c_{k,-}), \] (S19)
\[ c_{k,\downarrow} = (e^{i\phi_k} \sin \frac{\theta_k}{2} c_{k,+} - \cos \frac{\theta_k}{2} c_{k,-}), \] (S20)
where $\theta_k$ satisfies $\cos \theta_k = h_z/\Lambda_k$ with $\Lambda_k = \sqrt{h_x^2 + l_x^2 + l_y^2}$, and $\phi_k$ satisfy $e^{i\phi_k} = (l_x + il_y)/\sqrt{l_x^2 + l_y^2}$. Substituting Eq. (S19) and Eq. (S20) into Eq. (S17), we have
\[ H_0 = \sum_k (\xi_k + \Lambda_k) c_{k,\uparrow}^\dagger c_{k,+} + (\xi_k - \Lambda_k) c_{k,-}^\dagger c_{k,-} \] (S21)
for the superconducting part,
\[ H_{SC} = \sum_k \left( -\frac{h_z (\Delta_s(k) + i\Delta_d(k))}{\Lambda_k} c_{k,\uparrow}^\dagger c_{k,-} + h.c. \right) + \frac{1}{2} \sum_k \left( -\frac{(\Delta_s(k) + i\Delta_d(k))(l_x - il_y)}{\Lambda_k} c_{k,\uparrow}^\dagger c_{k,-} + h.c. \right) + \frac{1}{2} \sum_k \left( -\frac{(\Delta_s(k) + i\Delta_d(k))(l_x + il_y)}{\Lambda_k} c_{k,-}^\dagger c_{k,-} + h.c. \right) \] (S22)
Below we go beyond Ref. [S1] and do a band-dependent gauge transformation, $c_{k,+} = -\tilde{c}_{k,+} e^{i\varphi_k}$, $c_{k,-} = \tilde{c}_{k,-}$, with $e^{i\varphi_k} = (\Delta_s(k)+i\Delta_d(k))/\sqrt{\Delta_s^2(k)+\Delta_d^2(k)}$. Accordingly, we have
\[ H_0 = \sum_k (\xi_k + \Lambda_k) \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,+} + (\xi_k - \Lambda_k) \tilde{c}_{k,-}^\dagger \tilde{c}_{k,-}, \] (S23)
\[ H_{SC} = \sum_k \left( \frac{h_z \sqrt{\Delta_s^2(k)+\Delta_d^2(k)}}{\Lambda_k} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,-} + h.c. \right) + \frac{1}{2} \sum_k \left( -\frac{(\Delta_s(k) - i\Delta_d(k))(l_x - il_y)}{\Lambda_k} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,+} + h.c. \right) + \frac{1}{2} \sum_k \left( -\frac{(\Delta_s(k) + i\Delta_d(k))(l_x + il_y)}{\Lambda_k} \tilde{c}_{k,-}^\dagger \tilde{c}_{k,-} + h.c. \right) \] (S24)
By further doing the following transformation
\[ \tilde{c}_{k,\uparrow} = \cos \frac{\gamma_k}{2} \tilde{c}_{k,+} + \sin \frac{\gamma_k}{2} \tilde{c}_{k,-}, \] (S25)
\[ \tilde{c}_{k,-} = \sin \frac{\gamma_k}{2} \tilde{c}_{k,+} - \cos \frac{\gamma_k}{2} \tilde{c}_{k,-}, \] (S26)
where $\gamma_k = \arctan \frac{h_z \sqrt{\Delta_s^2(k)+\Delta_d^2(k)}}{\Lambda_k \xi_k}$, the Hamiltonian can be further transformed into the below form
\[ H = \sum_{k,\sigma} \epsilon_{k,\sigma} \tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma} - \frac{1}{2} \left( \frac{(\Delta_s(k) - i\Lambda_d(k))(l_x - i\Lambda_y)}{\Lambda_k} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,-,\uparrow} + h.c. \right), \] (S27)
where $\epsilon_{k,\pm} = \sqrt{\epsilon_{k,\pm}^2 + \frac{\Delta_s^2(k)+\Delta_d^2(k)}{\Lambda_k^2} h_z^2} \pm \Lambda_k$. It is readily seen that the Hamiltonian can be decoupled into two independent parts, i.e., $H = H_+ + H_-$.\[ \text{with}\]
\[ H_+ = \sum_k \epsilon_{k,\uparrow} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,\uparrow} - \frac{1}{2} \left( \frac{(\Delta_s(k) - i\Lambda_d(k))(l_x - i\Lambda_y)}{\Lambda_k} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,-,\uparrow} + h.c. \right), \] (S28)
\[ H_- = \sum_k \epsilon_{k,-} \tilde{c}_{k,-}^\dagger \tilde{c}_{k,-} - \frac{1}{2} \left( \frac{(\Delta_s(k) + i\Lambda_d(k))(l_x + i\Lambda_y)}{\Lambda_k} \tilde{c}_{k,-}^\dagger \tilde{c}_{k,-,\downarrow} + h.c. \right). \] (S29)
It is obvious that both $H_+$ and $H_-$ describe odd-parity superconductors. It is worthy pointing out the pairing forms in $H_+$ and $H_-$ are similar to that in the toy model for second-order topological odd-parity superconductors proposed in Ref. [S2]. In the limit $h_z = 0$, we obtain Eq. (13) in the main paper.
4. PHASE BOUNDARIES IN THE $s + id$-WAVE PAIRING REGIME

As shown in the Fig. 1 of the main paper, the $s + id$-wave superconducting regime consists of three time-reversal symmetry breaking topologically distinct phases. The boundaries between these phases are two straight lines with the same slope but different intercepts. In this section, we are going to derive the equations of those two lines.

The nodes of $s + id$-wave pairing are located where both $\Delta_0 + \Delta_s \eta_s(k) = 0$ and $\eta_d(k) = 0$ are simultaneously satisfied in the first Brillouin zone (FBZ) while the Fermi surfaces of the normal state are determined by the equation $\varepsilon_\sigma(k) = \xi(k) + \sigma l(k) = 0$. As explained in the main paper, a topological phase transition happens in the $s + id$-wave regime when the Fermi surface cross these pairing nodes. It can be shown that the four pairing nodes in the FBZ satisfy,

$$\frac{4\Delta_0 t}{\Delta_s} + \sigma l(k) = \mu,$$

or

$$\frac{4\Delta_0 t}{\Delta_s} \pm 2\sqrt{(\lambda_R \sin k_y + \lambda_D \sin k_x)^2 + (\lambda_R \sin k_x + \lambda_D \sin k_y)^2} = \mu.$$  

(S30)

(S31)

Since $\eta_d(k) = 0$ are satisfied on the two lines $k_x = \pm k_y$, using the fact that $\sin k_x = \pm \sin k_y$ on these two lines leads to

$$\sin^2 k_x (\lambda_R \pm \lambda_D)^2 = \frac{1}{2} \mu^2 - \frac{2\Delta_0 t}{\Delta_s}.$$  

(S32)

At the pairing nodes, we also have $\cos k_x = -\frac{\Delta_0}{\Delta_s}$, so,

$$\{1 - \frac{(\Delta_0)}{\Delta_s}^2\} (\lambda_R \pm \lambda_D)^2 = \frac{1}{2} \mu^2 - \frac{2\Delta_0 t}{\Delta_s}.$$  

(S33)

For $\Delta_0 \ll \Delta_s$, we have

$$(\lambda_R \pm \lambda_D)^2 \simeq \frac{\mu^2}{8}. $$  

(S34)

If we restrict ourselves to the lines with positive slope in $\lambda_D - \mu$ plane, we will have

$$\lambda_D \simeq \frac{\sqrt{2}}{4} \mu \pm \lambda_R,$$

(S35)

which are the equations of two lines with the slope $\sqrt{2}/4$ and intercept $\lambda_R$ (the boundary between first and second-order TSC phases) and intercept $-\lambda_R$ (the boundary between first-order TSC and the topologically trivial phase).

[S1] Jason Alicea, “Majorana fermions in a tunable semiconductor device,” Phys. Rev. B 81, 125318 (2010).
[S2] Zhongbo Yan, “Higher-order topological odd-parity superconductors,” Phys. Rev. Lett. 123, 177001 (2019).