Mixed-parity superconductivity near Lifshitz transitions in strongly spin-orbit-coupled metals

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We consider a strongly spin-orbit-coupled metal, one of whose Fermi surfaces is close to a Lifshitz (topological) transition. Via a renormalization group analysis of the square-lattice Hubbard model with strong Rashba spin-orbit coupling, we show that such a metal is generically unstable to the formation of mixed-parity superconductivity with a helical triplet component.

I. INTRODUCTION

Topological superconductivity is at the forefront of modern investigations in materials physics due in part to its potential for realizing topological quantum computation via localized Majorana zero modes [1]. In order to obtain non-trivial topology the superconductivity must be of an unconventional form, with spin-triplet Cooper pairs carrying non-zero angular momentum [2]. Such unconventional superconductivity is thought to arise from spin-fluctuation-mediated pairing, distinct from the conventional pairing is the square-lattice Hubbard model

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II. MODEL AND METHODS

We consider a square lattice tight-binding model,

\[ H_0 = -t \sum_{\langle i,j \rangle, s} c_{i,s}^\dagger c_{j,s} - t' \sum_{\langle\langle i,j \rangle \rangle, s,s'} c_{i,s}^\dagger c_{j,s'} - \mu \sum_{i,s} c_{i,s}^\dagger c_{i,s} + iv \sum_{\langle i,j \rangle, s,s'} \left[ (\sigma \times a_{ij}) \cdot \vec{z} \right]_{s,s'} c_{i,s}^\dagger c_{j,s'}, \]

(1)

where \( \langle i,j \rangle \) and \( \langle\langle i,j \rangle \rangle \) denote nearest-neighbor and next-nearest-neighbor hopping with hopping strengths \( t \) and \( t' \) respectively. The spin orientations are denoted \( s,s' \in \{\uparrow, \downarrow\} \), \( v \) is the Rashba spin-orbit coupling strength, \( \sigma = (\sigma_x, \sigma_y, \sigma_z)^T \) the vector of Pauli matrices, and \( a_{ij} \) denotes the unit vectors between nearest-neighbor sites.

The Hubbard interaction term is

\[ V_{\text{int}} = \frac{U}{2} \sum_{s,s', k_1,k_2,k_3,k_4} \delta_{k_1+k_2-k_3-k_4} c_{k_1,s}^\dagger c_{k_2,s}^\dagger c_{k_3,s'} c_{k_4,s}, \]

(2)

describing a contact interaction which is repulsive for \( U > 0 \) and attractive for \( U < 0 \). The interacting Hamiltonian \( H \) is given by \( H_0 + V_{\text{int}} \).

Spin-orbit coupling breaks the spin degeneracy of the non-interacting bands and splits them into two with opposite helicities. After a unitary transformation to the helicity basis the non-interacting Hamiltonian (1) becomes \( H_0 = \sum_{k,\alpha} \xi_k^\alpha c_{k,\alpha}^\dagger c_{k,\alpha} \), with the two helicities denoted by Greek indices \( \alpha \in \{+,-\} \).

\[ \xi_{k,\alpha} = \epsilon_k - \mu + 2v \sqrt{\sin^2 k_x + \sin^2 k_y} \]

(3)

with \( \epsilon_k \) the next-nearest-neighbor Hubbard model dispersion

\[ \epsilon_k = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y. \]

(4)

Here and henceforth we set the lattice spacing to unity. The eigenvectors for the helicity bands are

\[ |\eta_\pm(k)\rangle = \frac{1}{\sqrt{2}} \left( \pm e^{i\theta(k)} \right) \]

(5)

with

\[ e^{i\theta(k)} = \frac{\sin k_y - iv \sin k_x}{\sqrt{\sin^2 k_x + \sin^2 k_y}}. \]

(6)

The spin orientations along the helicity bands are shown in Fig. 1. The operator mapping to the helicity basis is given by

\[ c_{k,\pm} = \frac{1}{\sqrt{2}} (c_{k,\uparrow} \pm e^{-i\theta(k)} c_{k,\downarrow}). \]

(7)

The bare anti-symmetrized Hubbard interaction term \( V_{\text{int}} \) in the helicity basis becomes [26]

\[ V_{\text{int}} = \frac{U}{16} \sum_{\alpha\beta\gamma\delta} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2-k_3-k_4} (\alpha e^{-i\theta(k_1)} - \beta e^{-i\theta(k_2)}) \]

\[ \times (\delta e^{i\theta(k_4)} - \gamma e^{i\theta(k_3)}) c_{k_1,\alpha}^\dagger c_{k_2,\beta}^\dagger c_{k_3,\gamma} c_{k_4,\delta}. \]

(8)

The two van Hove fillings are located at chemical potentials \( \mu_+ \) and \( \mu_- \), given by

\[ \mu_\pm = \pm 2 \left( -t + \frac{(t \pm 2t')^2}{\sqrt{(t \pm 2t')^2 + v^2}} \right) \]

\[ + v \sqrt{1 - \frac{(t \pm 2t')^2}{(t \pm 2t')^2 + v^2}}. \]

(9)

At each van Hove filling there are four van Hove points in the Brillouin zone, as shown in Fig. 1. The filling \( \mu_+ \) is reminiscent of the scenario proposed by Yao and Yang [23], denoted a type-II van Hove singularity, with saddle points located away from the Brillouin zone edge. In the \( \mu_- \) case the type-I van Hove point [20–22] splits into two along the Brillouin zone edge. We call this the edge van Hove scenario. The van Hove points lie at \( K_{1,2} = (\mp \Pi^+, 0) \), \( K_{3,4} = (0, \mp \Pi^+) \) for filling \( \mu_+ \) and \( K_{1,2} = (\mp \Pi^-, \mp \Pi^-) \), \( K_{3,4} = (-\Pi^-, \mp \Pi^-) \) for filling \( \mu_- \), where

\[ \Pi^\pm = \arccos \left( \mp \frac{t \pm 2t'}{\sqrt{(t \pm 2t')^2 + v^2}} \right). \]

(10)

The low energy model that applies close to these van Hove fillings is given by the following imaginary time Lagrangian of spinless fermions,

\[ \mathcal{L}_\pm = \frac{4}{a=1} \sum_{\alpha=1}^{4} \psi_{\alpha}^\dagger (\partial_\tau + \xi_{\pm}^{\alpha} (-i\partial_x, -i\partial_y)) \psi_{\alpha} - \frac{g_1}{2} \psi_{\alpha}^\dagger \psi_{\alpha}^\dagger \psi_{\beta} \psi_{\alpha} \]

\[ - \sum_{a=1}^{4} \sum_{b=3}^{2} g_2 \psi_{\alpha}^\dagger \psi_{\beta}^\dagger \psi_{\beta} \psi_{\alpha} - \left[ i g_3 \psi_{\alpha}^\dagger \psi_{\beta} \psi_{\beta} \psi_{\alpha} + \text{H.c.} \right]. \]

(11)
To determine the possible Fermi surface instabilities, the particle-particle and particle-hole susceptibilities are required. The susceptibilities that can have a double logarithmic divergence are [23]

\[ \chi_{0}^{pp}(\omega) \approx \lambda^{\pm} \ln^{2} \left( \frac{\Lambda}{\omega} \right), \quad \chi_{0}^{ph}(\omega) \approx 2\beta^{\pm} \lambda^{\pm} \ln \left( \frac{\Lambda}{\omega} \right), \]

(15)

with

\[ \beta^{\pm} = \frac{2\sqrt{\kappa^{\pm}}}{1 + \kappa^{\pm}} \ln \left| \frac{\kappa^{\pm} + 1}{\kappa^{\pm} - 1} \right|. \]

(16)

The ratio \( \kappa^{\pm} = m_{y}^{\pm}/m_{x}^{\pm} \) plays the role of a nesting parameter with the logarithm in \( \beta^{\pm} \) diverging as \( \kappa \to 1 \) at perfect nesting. The complete set of relevant susceptibilities, including susceptibilities with single logarithmic divergences, are given in appendix A.

III. RESULTS

We perform an RG analysis using \( y = \ln^{2}(\Lambda/\omega) \) as a flow parameter with \( \Lambda \) a decreasing energy cutoff [27, 28]. The flow equations for the dimensionless couplings \( g_{i} \to \lambda^{\pm} g_{i} \) are

\[ \dot{g}_{1} = -g_{1}^{2} - 2g_{2}^{2}; \quad \dot{g}_{2} = d(g_{2}^{2} + g_{3}^{2}); \quad \dot{g}_{3} = -2g_{1}g_{3} + 4dg_{2}g_{3}. \]

(17)

The \( y \)-dependence of the \( g_{i} \) has been suppressed for brevity. \( \dot{g}_{i} \) denotes the derivative \( dg_{i}/dy \). We have discarded contributions with single logarithmic divergences in this picture; the full flow equations are given in appendix B. \( d \approx d\chi_{0}^{ph}(y)/d\chi_{0}^{pp}(y) \) is approximated as a constant nesting parameter \( 0 \leq d \leq 1 \) to account for the additional logarithmic divergence at perfect nesting. At the beginning of the flow \( g_{i}(y = 0) = \lambda^{\pm} U \) with all couplings equal.

For \( d = 0 \) the differential equations can be solved analytically with the critical value \( y_{c} = (1 + \sqrt{2})/\lambda U \) for which the couplings diverge to strong coupling. We therefore use this as the cutoff for the phase transition. For \( d \neq 0 \) the critical value decreases and the \( g_{3} \) coupling is enhanced. The solutions to the RG equations for \( d = 0 \) and \( d = 1 \) are shown in Fig. 3. \( g_{3} \) retains the sign of \( g_{3}(0) \) due to the \( \beta \)-function vanishing as the coupling goes to zero. \( g_{3} \) decreases under the RG and eventually becomes negative, leading to superconductivity.

The coupling constants \( g_{i} \) flow to strong coupling as \( y \to y_{c} \), therefore our one-loop RG can only provide a qualitative picture of the phase diagram. We introduce the asymptotic form

\[ g_{i} \approx \frac{G_{i}}{y_{c} - y}. \]

(18)
to describe the divergence of the couplings [22].

To analyze the nature of the Fermi surface instabilities, we introduce infinitesimal test vertices for several possible types of order: superconductivity, $q_1$ and $q_2$ density waves, and Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconductivity with finite momentum Cooper pairs. The resulting addition to the Lagrangian is

$$
\delta \mathcal{L} = \sum_{a=1}^{4} \left[ \Delta_{a\bar{a}} \psi_{a}^\dagger \psi_{\bar{a}}^\dagger + \phi_{a\bar{a}} \psi_{a}^\dagger \psi_{\bar{a}} \right] + \sum_{a=1}^{2} \sum_{b=3}^{4} \left[ \phi_{a\bar{b}} \psi_{a}^\dagger \psi_{\bar{b}} + \Delta_{ab} \psi_{a}^\dagger \psi_{b}^\dagger \right] + \text{H.c.}
$$

Spatially uniform ($q = 0$) charge and magnetic orderings are suppressed due to the irrelevance of the intra-patch density-density interaction.

We find for the superconducting channel

$$
\begin{pmatrix}
\Delta_{12} \\
\Delta_{21} \\
\Delta_{34} \\
\Delta_{43}
\end{pmatrix} =
\begin{pmatrix}
-g_1 & g_1 & 2ig_3 & -2ig_3 \\
g_1 & -g_1 & -2ig_3 & 2ig_3 \\
-2ig_3 & 2ig_3 & -g_1 & g_1 \\
2ig_3 & -2ig_3 & g_1 & -g_1
\end{pmatrix}
\begin{pmatrix}
\Delta_{12} \\
\Delta_{21} \\
\Delta_{34} \\
\Delta_{43}
\end{pmatrix}.
$$

The dot again denotes a derivative with respect to $y$. The two possible nonzero eigenvalues of this matrix are $\varepsilon_1 = -2(g_1 - 2g_3)$ and $\varepsilon_2 = -2(g_1 + 2g_3)$ with corresponding eigenvectors $v_1 = (-i, i, -1, 1)^T/\sqrt{4}$, $v_2 = (i, -i, -1, 1)^T/\sqrt{4}$. The superconductivity in the helicity basis is chiral/anti-chiral depending on the sign of $g_3$. We repeat the analysis in the FFLO and the $q_1$ and $q_2$ density wave channels to find all possible orders. The order parameters obey $\Delta_{ij} = \varepsilon_j \Delta_i$; the susceptibilities of the possible orders are $\chi_j(y) \sim (y_c - y)^{\varepsilon_j}$. [22]

The exponents for superconductivity and $q_2$ density wave orders are given by $G_{SC_1} = 2(G_1 - 2G_3)$, $G_{SC_2} = 2(G_1 + 2G_3)$, $G_{\text{DW}_1} = -d(G_2 \pm 2G_3)$. The FFLO superconductivity and $q_1$ density wave order are suppressed and the $q_2$ density wave order is also suppressed away from perfect nesting. The exponents for FFLO and $q_1$ density wave order are $G_{\text{FFLO}} = 2d_y(y_c)G_2$, $G_{\text{DW}} = -d_y(y_c)G_1$ with $d_y$ and $d_y$ defined in appendix B.

In order to obtain a picture of the RG flow to strong coupling we use the monotonically increasing $g_2$ as a flow parameter and redefine the remaining couplings $g_1 = x_1 g_2$ and $g_3 = x_3 g_2$ [24]. The flow equations in terms of these redefined couplings are

$$
\frac{d x_1}{d \ln g_2} = -x_1 - \frac{x_1^2 + 2x_3^2}{d(1 + x_3^2)},
\frac{d x_3}{d \ln g_2} = -x_3 - \frac{2x_3(x_1 - 2d)}{d(1 + x_3^2)}.
$$

The fixed points of these equations describe four trajectories of the RG flow. The flow diagram is plotted in Fig. 4a with $d = 1$. For the metallic fixed point $g_2$ does not flow. The density wave phase exists for $g_3 \to 0$; in this case $g_1 \to 0$ and only $g_2$ diverges. For the superconducting trajectories all couplings diverge with ratios that depend on $d$. As $d \to 0$, the density wave and metal trajectories merge and only the metallic phase survives.

We now consider the superconducting order parameter in the original $\{\uparrow, \downarrow\}$ spin basis. We name the discrete order parameter in analogy to the continuum angular momentum channels. The even-parity order parameters are the isotropic $s$-wave channel $\Delta_s = \Delta(1, 1, 1, 1)$ and nodal $d$-wave $\Delta_d = \Delta(1, 1, -1, -1)$, where these four-
component vectors give the phase of the superconducting order parameter at each of the four van Hove points, \((K_1, K_2, K_3, K_4)\). The odd-parity order parameters correspond to chiral \(p\)-wave \(\Delta_{p_x,ip_y} = \Delta(-i, i, -1, 1)\), and anti-chiral \(p\)-wave \(\Delta_{p_x,-ip_y} = \Delta(i, i, -1, 1)\) in the Yao-Yang van Hove scenario but can represent higher order angular momentum channels for the edge van Hove scenario. The continuum order parameter can be written as \(\Delta(\mathbf{k}) = (\Psi_s(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \mathbf{\sigma})i\sigma_0\). In the Yao-Yang scenario the singlet component of the superconducting \(\Psi_s(\mathbf{k})\) corresponds to an \(s\)-wave form for \(G_{SC_1}\) and a \(d\)-wave form for \(G_{SC_2}\). The triplet component is helical and forms with chiral \(p_x + ip_y\) superconductivity for one spin polarization and anti-chiral \(p_x - ip_y\) superconductivity for the other, with \(\mathbf{d}(\mathbf{k}) = (\sin k_x, \sin k_y, 0)^T\).

In the edge van Hove scenario the form factor is more complicated. If the van Hove points lie at \((\pm \pi/2, \pi), (\pi, \pm \pi/2)\) along the Brillouin zone edge, \(G_{SC_1}\) corresponds to a superposition of singlet \(d\)-wave superconductivity with form factor \(\Psi_s(\mathbf{k}) = \cos 2k_x - \cos 2k_y\) and triplet \(f\)-wave superconductivity with the form factor \(\mathbf{d}(\mathbf{k}) = (\cos k_x - \cos k_y)(\sin k_x, \sin k_y, 0)^T\). The singlet component of \(G_{SC_2}\) is \(s\)-wave instead of \(d\)-wave. For van Hove points lying at different positions along the Brillouin zone edge the form factor requires higher harmonics, up to infinite order as the van Hove points approach the \((0, \pi)\) limit.

Additionally there exists a narrow window of density wave order for \(g_3 \to 0\). The competition between unconventional superconductivity and density-wave order has been seen to arise theoretically in similar spin-orbit split systems such as at oxide interfaces [11]. A schematic phase diagram is given in Fig. 4b.

**IV. SUMMARY AND DISCUSSION**

When the Fermi surface passes through saddle points in the band structure, the density of states is enhanced within the region of the saddle. This allows for an analytical treatment of the RG flow equations and an unbiased analysis of competing phases.

We have shown that mixed-parity superconductivity arises naturally in systems with antisymmetric spin-orbit coupling. The direction of the triplet \(\mathbf{d}(\mathbf{k})\) vector is determined by the local spin quantization axis. Thus the triplet component of the superconducting order parameter forms a helical state, analogous to the quantum spin Hall insulator [29]. The helical superconductivity preserves time-reversal symmetry. The mixed-parity superconducting state is topologically non-trivial if the triplet component is greater than the singlet component [30, 31]. Our case, where both components are equal, lies on the boundary between the topologically trivial and non-trivial phases. Our results suggest the superconductor can be tuned to a topological state, and could be useful for device applications and topological quantum computing.

Recently we became aware of a related study on the hexagonal lattice [32].

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**Appendix A: Full particle-hole and particle-particle susceptibilities**

To compute the full RG flow equations including terms of single logarithmic divergence, all particle-particle and particle-hole susceptibilities are required.

The complete expressions, including susceptibilities reproduced from (15), are [23]:

\[
\begin{align*}
\chi_0^{pp}(\omega) &\approx \lambda^\pm \ln \left(\frac{\Lambda}{\omega}\right), \\
\chi_0^{ph}(\omega) &\approx 2\lambda^\pm \ln \left(\frac{\Lambda}{\omega}\right), \\
\chi_{q_1}^{ph}(\omega) &\approx 2\gamma^\pm \lambda^\pm \ln \left(\frac{\Lambda}{\omega}\right), \\
\chi_{q_2}^{pp}(\omega) &\approx 2\alpha^\pm \lambda^\pm \ln \left(\frac{\Lambda}{\omega}\right).
\end{align*}
\]

The vectors \(q_1\) and \(q_2\) are given by \(2K_1\) and \(K_3 - K_1\) respectively. The \(\pm\) signs of susceptibilities have been suppressed. \(\gamma\) denotes an additional nesting parameter introduced by hand to suppress or enhance \(q_1\) scattering processes relative to the zero-momentum particle-hole processes [24].

**Appendix B: Full RG flow equations**

The complete flow equations including all single and quadratic logarithmic terms are

\[
\begin{align*}
\dot{g}_1 &= -g_1^2 - 2g_3^2 - 2g_2^2d_1 + g_1^2d_3; \\
\dot{g}_2 &= -2g_1g_2d_1 + (g_1^2 + g_3^2)d_3 - g_2^2d_3; \\
\dot{g}_3 &= -2g_1g_3 + 4g_2g_3d_3. 
\end{align*}
\]

The derivative \(\dot{g}_i = dg_i/dy\). The \(d_\alpha(y)\) parameters are defined as \(d_\alpha(y) = d\chi_0^{ph}(y)/d\chi_0^{pp}(y), d_\gamma(y) = d\chi_{q_1}^{ph}(y)/d\chi_0^{pp}(y), d_\delta(y) = d\chi_{q_2}^{pp}(y)/d\chi_0^{pp}(y), d_\beta(y) = d\chi_{q_2}^{pp}(y)/d\chi_0^{ph}(y). \)
The functions \(d_x(y)\), \(x = 1, \alpha, \beta, \gamma\), have the asymptotic forms \(d_x(y) \to 1\) as \(y \to 0\) and \(d_x(y) \to x/\sqrt{y}\), for \(y \to \infty\).

When solving the system of differential equations numerically we approximate the functions \(d_x(y)\) by \(d_x(y) = x/\sqrt{x^2+y}\) to interpolate between small-\(y\) and large-\(y\) asymptotic forms \([23, 24]\).

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