

Supplemental Material for Bogoliubov Fermi Surfaces in Superconductors with Broken Time-Reversal Symmetry

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I. MAPPING TO A GENERAL TWO-ORBITAL MODEL

In this section, we show that the most general model for a normal-state system with a two-valued orbital degree of freedom where the orbitals have the same parity and are chosen to be real can be unitarily transformed into the $j = 3/2$ Hamiltonian given in the main text. We expand the single-particle Hamiltonian in terms of Kronecker products in orbital-spin space,

$$H_N(\mathbf{k}) = \sum_{\mu,\nu=0,x,y,z} c_{\mu,\nu}(\mathbf{k}) \hat{s}_\mu \otimes \hat{\sigma}_\nu, \quad (1)$$

where \hat{s}_μ ($\hat{\sigma}_\nu$) are the Pauli matrices in orbital (spin) space. Hermiticity implies $c_{\mu,\nu}(\mathbf{k}) = c_{\mu,\nu}^*(\mathbf{k})$. Inversion maps $H_N(\mathbf{k})$ onto $U_P H_N(-\mathbf{k}) U_P^\dagger$, where $U_P = 1_4$ ($U_P = -1_4$) if the orbitals are both even (odd). The extra sign for the odd case obviously drops out and can be disregarded. Hence, for the Hamiltonian to be symmetric under inversion, we simply require $c_{\mu,\nu}(\mathbf{k}) = c_{\mu,\nu}(-\mathbf{k})$. Time reversal maps $H_N(\mathbf{k})$ onto $U_T H_N^*(-\mathbf{k}) U_T^\dagger$. $c_{\mu,\nu}(\mathbf{k})$ is thus mapped onto $c_{\mu,\nu}^*(-\mathbf{k}) = c_{\mu,\nu}(\mathbf{k})$. Under the assumption of real-valued orbitals, \hat{s}_y and the spin components $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ are odd under time reversal, whereas the remaining matrices are even. This is achieved by $U_T = \hat{s}_0 \otimes i\hat{\sigma}_y$.

In order for the Hamiltonian $H_N(\mathbf{k})$ to be invariant under time reversal, only those Kronecker products can appear in Eq. (1) that are even, specifically the six products with $\{\mu, \nu\} = \{0, 0\}, \{x, 0\}, \{z, 0\}, \{y, x\}, \{y, y\}, \{y, z\}$. The corresponding $c_{\mu,\nu}(\mathbf{k})$ are real and even functions of \mathbf{k} . Note that the five nontrivial Kronecker products are mutually anticommuting and thus form a representation of the five Dirac matrices.

We now show that the generalized Luttinger-Kohn model [1] adopted in the main text is equivalent to Eq. (1). It is expressed in terms of the angular-momentum $j = 3/2$ matrices

$$J_x = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad (2)$$

$$J_y = \frac{i}{2} \begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad (3)$$

$$J_z = \frac{1}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}. \quad (4)$$

The generalized Luttinger-Kohn model involves five sets of products of the $j = 3/2$ matrices, specifically $(2J_z^2 - J_x^2 - J_y^2)/6$, $(J_x^2 - J_y^2)/(2\sqrt{3})$, $(J_x J_z + J_z J_x)/(2\sqrt{3})$, $(J_x J_y + J_y J_x)/(2\sqrt{3})$, and $(J_y J_z + J_z J_y)/(2\sqrt{3})$. These matrices also form a set of five Dirac matrices and there is a unitary transformation between them and the five allowed nontrivial Kronecker products discussed above. Specifically, we find

$$U^\dagger \frac{2J_z^2 - J_x^2 - J_y^2}{6} U = \hat{s}_z \otimes \hat{\sigma}_0, \quad (5)$$

$$U^\dagger \frac{J_x^2 - J_y^2}{2\sqrt{3}} U = \hat{s}_x \otimes \hat{\sigma}_0, \quad (6)$$

$$U^\dagger \frac{J_x J_z + J_z J_x}{2\sqrt{3}} U = \hat{s}_y \otimes \hat{\sigma}_y, \quad (7)$$

$$U^\dagger \frac{J_x J_y + J_y J_x}{2\sqrt{3}} U = \hat{s}_y \otimes \hat{\sigma}_z, \quad (8)$$

$$U^\dagger \frac{J_y J_z + J_z J_y}{2\sqrt{3}} U = \hat{s}_y \otimes \hat{\sigma}_x, \quad (9)$$

with the unitary matrix

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (10)$$

Note that one can pairwise swap the orbital-spin matrices $\hat{s}_\mu \otimes \hat{\sigma}_\nu$ by an appropriate unitary transformation so that this mapping is entirely general. We hence see that the generalized Luttinger-Kohn model is equivalent to the most general single-particle Hamiltonian of a time- and inversion-symmetric material with two identical-parity orbitals and spin. The generalized Luttinger-Kohn representation is convenient, however, as it allows us to exploit the symmetry properties of the angular-momentum matrices J_i under rotations to gain insight into the underlying physics.

We can obtain six on-site pairing states in the orbital-spin representation by multiplying the six allowed Kronecker products by the unitary part of the time-reversal operator, $U_T = \hat{s}_0 \otimes i\hat{\sigma}_y$. We hence obtain one orbitally trivial spin-singlet gap proportional to $\hat{s}_0 \otimes \hat{\sigma}_y$ and five ‘‘anomalous’’ gaps proportional to $\hat{s}_x \otimes \hat{\sigma}_y$, $\hat{s}_z \otimes \hat{\sigma}_y$, $\hat{s}_y \otimes \hat{\sigma}_z$, $\hat{s}_y \otimes \hat{\sigma}_0$, and $\hat{s}_y \otimes \hat{\sigma}_x$, which are either orbital-triplet spin-singlet or orbital-singlet spin-triplet pairing states. It is straightforward to map these states onto the gap matrices in the equivalent spin-3/2 formulation: the orbitally trivial spin-singlet state maps onto the singlet gap matrix η_s , while the anomalous gaps map onto the quintet gap matrices. Hence, we can describe any even-parity pairing state, without loss of generality, in terms of a linear combination of the six spin-3/2 gap functions with even-parity coefficients $\psi_i(\mathbf{k})$.

II. EXISTENCE AND PROPERTIES OF THE PFAFFIAN

In this section, we provide additional details on constructing the topological invariant protecting the Fermi surfaces. Our starting point is the Hamiltonian in the superconducting state,

$$H(\mathbf{k}) = \begin{pmatrix} H_N(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^\dagger(\mathbf{k}) & -H_N^T(\mathbf{k}) \end{pmatrix}. \quad (11)$$

Recall that $H_N(\mathbf{k})$ is even in \mathbf{k} . We employ the spin-3/2 basis used in the main text. We first show that a \mathbf{k} -independent unitary matrix Ω exists such that $\tilde{H}^T(\mathbf{k}) = -\tilde{H}(\mathbf{k})$ for $\tilde{H}(\mathbf{k}) = \Omega H(\mathbf{k}) \Omega^\dagger$, i.e., the Hamiltonian can be transformed into antisymmetric form.

The proof proceeds as follows: 1. The Hamiltonian $H(\mathbf{k})$ satisfies parity and charge-conjugation symmetries and thus also their product, i.e.,

$$U_{CP} H^T(\mathbf{k}) U_{CP}^\dagger = -H(\mathbf{k}), \quad (12)$$

where $U_{CP} \equiv U_C U_P^* = (\hat{\tau}_x \otimes 1_4)(\hat{\tau}_0 \otimes 1_4) = \hat{\tau}_x \otimes 1_4$. The $\hat{\tau}_i$ denote Pauli matrices in particle-hole (Nambu) space. We find that the CP symmetry squares to +1 since $(CP)^2 = (U_{CP} \mathcal{K})^2 = U_{CP} U_{CP}^* = \hat{\tau}_0 \otimes 1_4 = +1_8$. In the presence of such a symmetry, two-dimensional Fermi surfaces are characterized by a \mathbb{Z}_2 invariant [2, 3].

2. For *any* CP symmetry that squares to unity we have $U_{CP}^* = U_{CP}^{-1} = U_{CP}^\dagger$ and thus $U_{CP} = U_{CP}^T$, hence U_{CP} is symmetric. Any (complex) symmetric matrix can be diagonalized by a unitary *congruence*, i.e., there exist a unitary matrix Q and a diagonal matrix Λ such that (note the transpose)

$$U_{CP} = Q \Lambda Q^T. \quad (13)$$

Inserting this equation into Eq. (12) yields

$$Q \Lambda Q^T H^T(\mathbf{k}) Q^* \Lambda^\dagger Q^\dagger = -H(\mathbf{k}). \quad (14)$$

Since $\Lambda = Q^\dagger U_{CP} Q^*$ is unitary and diagonal, it can be written as $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots)$ with $|\lambda_i| = 1$. Now let

$$\sqrt{\Lambda} \equiv \text{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \dots), \quad (15)$$

where for each i , $\sqrt{\lambda_i}$ is the complex root with arbitrary but fixed sign. Also let

$$\sqrt{\Lambda}^\dagger \equiv \text{diag}(\sqrt{\lambda_1}^*, \sqrt{\lambda_2}^*, \dots), \quad (16)$$

with the same choice of signs as in Eq. (15). It is trivial to show that this is a root of Λ^\dagger . Furthermore, $\sqrt{\Lambda}$ and $\sqrt{\Lambda}^\dagger$ are obviously diagonal, and thus symmetric, and also unitary. We can thus rewrite Eq. (14) as $Q\sqrt{\Lambda}\sqrt{\Lambda}Q^T H^T(\mathbf{k})Q^*\sqrt{\Lambda}^\dagger\sqrt{\Lambda}^\dagger Q^\dagger = -H(\mathbf{k})$ and find that

$$(\sqrt{\Lambda}^\dagger Q^\dagger H(\mathbf{k})Q\sqrt{\Lambda})^T = -\sqrt{\Lambda}^\dagger Q^\dagger H(\mathbf{k})Q\sqrt{\Lambda}. \quad (17)$$

With the unitary matrix $\Omega \equiv \sqrt{\Lambda}^\dagger Q^\dagger$, Eq. (17) can be written as $(\Omega H(\mathbf{k})\Omega^\dagger)^T = -\Omega H(\mathbf{k})\Omega^\dagger$. Hence, $\tilde{H}(\mathbf{k}) \equiv \Omega H(\mathbf{k})\Omega^\dagger$ is indeed antisymmetric.

For the Hamiltonian $H(\mathbf{k})$ given in Eq. (11) above together with Eq. (1) in the main text, a possible choice is

$$\Omega = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \otimes 1_4. \quad (18)$$

This yields

$$\tilde{H}(\mathbf{k}) = \frac{1}{2} \begin{pmatrix} H_N - H_N^T + \Delta + \Delta^\dagger & -i(H_N + H_N^T) + i(\Delta - \Delta^\dagger) \\ i(H_N + H_N^T) + i(\Delta - \Delta^\dagger) & H_N - H_N^T - \Delta - \Delta^\dagger \end{pmatrix}, \quad (19)$$

where we have suppressed the argument \mathbf{k} . The terms involving the normal-state Hamiltonian H_N are obviously antisymmetric. For this, it is crucial that H_N is even in \mathbf{k} . From Eq. (12), one easily finds $\Delta^T = -\Delta$, which implies that also the superconducting terms in $\tilde{H}(\mathbf{k})$ are antisymmetric. Hence, we do find $\tilde{H}^T(\mathbf{k}) = -\tilde{H}(\mathbf{k})$.

Since $\tilde{H}(\mathbf{k})$ is antisymmetric, its Pfaffian $P(\mathbf{k}) \equiv \text{Pf} \tilde{H}(\mathbf{k})$ exists. The Pfaffian is real for any spinful system since (a) the dimension of the Hamiltonian is a multiple of four (2×2 for Nambu and spin space), thus the Pfaffian is a polynomial of even degree of the components of $\tilde{H}(\mathbf{k})$, and (b) $\tilde{H}(\mathbf{k})$ is hermitian and antisymmetric and thus these components are purely imaginary.

Note further that the ambiguity in the signs of the roots in $\sqrt{\Lambda}$ means that Ω can be multiplied on the left by a diagonal matrix D with arbitrary components ± 1 on the diagonal. With $\Omega \rightarrow D\Omega$ we get $\Omega^\dagger \rightarrow \Omega^\dagger D$ and $\tilde{H}(\mathbf{k}) \rightarrow D\tilde{H}(\mathbf{k})D$. This leads to $\text{Pf} \tilde{H}(\mathbf{k}) \rightarrow \det D \text{Pf} \tilde{H}(\mathbf{k})$. Hence, $P(\mathbf{k})$ is only determined up to an overall sign. But this sign is selected by fixing the root $\sqrt{\Lambda}$ once for all \mathbf{k} . Thus sign *changes* in $P(\mathbf{k})$ are meaningful.

Since $\det H(\mathbf{k}) = \det \tilde{H}(\mathbf{k}) = P^2(\mathbf{k})$, the zeros of $P(\mathbf{k})$ give the nodes of the superconducting state. Thus if the Pfaffian changes sign as a function of \mathbf{k} , the surface separating regions with $P(\mathbf{k}) \gtrless 0$ is a two-dimensional Fermi surface. However, $P(\mathbf{k})$ can in addition have zeros of even multiplicity, which do not separate regions with different sign. These *accidental* zeros can form two-dimensional surfaces or line or point nodes.

For the general $k_z(k_x + ik_y)$ state of Eq. (4) in the main text, the Pfaffian is

$$P(\mathbf{k}) = (\epsilon_+ \epsilon_-)^2 + 4\Delta_0^2 (\epsilon_+ \epsilon_- + c_{xz}^2 + c_{yz}^2) + \Delta_1^2 |\psi|^2 (\epsilon_+^2 + \epsilon_-^2) + 8\Delta_0 \Delta_1 c_0 |\psi|^2 + \Delta_1^4 |\psi|^4, \quad (20)$$

where $\epsilon_\pm(\mathbf{k})$ are the normal-state eigenenergies. We have chosen the signs in the root $\sqrt{\Lambda}$ in such a way that $P(\mathbf{k}) > 0$ in the limit of large \mathbf{k} . Equation (20) is correct for arbitrary real and even coefficients $c_i(\mathbf{k})$. Note that when $\Delta_0 = 0$, the equation $P(\mathbf{k}) = 0$ implies the usual relationship for zero-energy states in a spin-singlet superconductor, i.e., $(\epsilon_+^2 + \Delta_1^2 |\psi|^2)(\epsilon_-^2 + \Delta_1^2 |\psi|^2) = 0$, implying nodes when $\epsilon_\pm = 0$ and $\psi = 0$; since $\psi(\mathbf{k}) \propto c_{xz}(\mathbf{k}) + ic_{yz}(\mathbf{k})$ to ensure that the full gap function $\Delta(\mathbf{k})$ transforms under rotations like $Y_{2,1}(\hat{\mathbf{k}})$, we have line nodes in the $k_z = 0$ plane and point nodes along the line $k_x = k_y = 0$. With both $\Delta_0 \neq 0$ and $\Delta_1 \neq 0$, we see that along the nodal directions, for which $\psi \propto c_{xz} + ic_{yz} = 0$, we have zero-energy excitations for $\epsilon_+ \epsilon_- (4\Delta_0^2 + \epsilon_+ \epsilon_-) = 0$. The two solutions for $\epsilon_+ \epsilon_-$ that follow from the latter equation give the two points of the Bogoliubov Fermi surface along these nodal directions. Away from the nodal directions, the other terms in Eq. (20) no longer vanish. However, they are continuous functions of the direction $\hat{\mathbf{k}}$, implying that the Fermi surface still exists at least for a finite range away from the nodal directions. In the main text, we consider the special case of a pure quintet gap, $\Delta_1 = 0$.

Finally, we show that the Pfaffian can be chosen non-negative if the system is also time-reversal symmetric and the combined inversion and time-reversal symmetry squares to -1 , i.e., if there exists a unitary matrix U_{PT} so that $U_{PT} H^T(\mathbf{k}) U_{PT}^\dagger = H(\mathbf{k})$ and $U_{PT} U_{PT}^* = -1$. Hence, if both symmetries are present, the \mathbb{Z}_2 invariant exists but is necessarily trivial. This has essentially been shown using the method of Clifford algebra extensions in [2]. In the following, we give a more elementary proof.

1. Kramers' theorem shows that under the last two conditions all eigenvalues of $H(\mathbf{k})$ have even degeneracy. Furthermore, condition (12) above implies that the eigenvalues come in pairs $\{E_i(\mathbf{k}), -E_i(\mathbf{k})\}$. Since the dimension of $H(\mathbf{k})$ is a multiple of four, the spectrum thus consists of quadruplets $\{E_i(\mathbf{k}), E_i(\mathbf{k}), -E_i(\mathbf{k}), -E_i(\mathbf{k})\}$.

2. $P(\mathbf{k})$ is a polynomial of the components of $\tilde{H}(\mathbf{k})$, which are linear combinations of the components of $H(\mathbf{k})$. Hence, $P(\mathbf{k})$ is a polynomial of the components of $\mathcal{H}(\mathbf{k})$. The coefficients are independent of \mathbf{k} .

3. We have $P^2(\mathbf{k}) = \det \tilde{H}(\mathbf{k}) = \det H(\mathbf{k}) = \prod_i E_i^4(\mathbf{k})$ so that $P(\mathbf{k}) = \pi(\mathbf{k}) \prod_i E_i^2(\mathbf{k})$ with $\pi(\mathbf{k}) = \pm 1$.

4. Consider the eigenenergies $E_i(\mathbf{k})$ as functions of a real parameter h , which can be any real or imaginary part of a component of the hermitian, finite-dimensional matrix $H(\mathbf{k})$. Theorem 7.6 of Alekseevsky *et al.* [4] shows under the weak additional condition that no two eigenvalues meet of infinite order for any real h unless they are equal for all h that the $E_i(\mathbf{k})$ can be chosen as smooth functions of h . Then $\prod_i E_i^2(\mathbf{k})$ is a smooth function of h .

5. We have already shown that $P(\mathbf{k})$ is a polynomial in h , that $\prod_i E_i^2(\mathbf{k}) = \pi(\mathbf{k}) P(\mathbf{k})$ is a smooth function of h , and that $\pi(\mathbf{k}) = \pm 1$. Then $\pi(\mathbf{k})$ is constant.

6. Noting the ambiguity in choosing Ω and thus the overall sign of the Pfaffian, we can choose $\pi(\mathbf{k}) = +1$ at some \mathbf{k} and consequently at all \mathbf{k} . Thus we indeed obtain $P(\mathbf{k}) = \prod_i E_i^2(\mathbf{k}) \geq 0$.

III. STABILITY OF STATES WITH BROKEN TIME-REVERSAL SYMMETRY

In this section, we provide additional details on the free-energy expansion. We show that states with broken time-reversal symmetry featuring Bogoliubov Fermi surfaces can be energetically stable. The relative stability of spin-singlet broken-time-reversal states over time-reversal-invariant states with the same transition temperature has been attributed to the gapping of nodes that appear in the time-reversal-symmetric state by breaking this symmetry [5]. A common example is the chiral d -wave state with line nodes, for which the usual spin-singlet gap function takes the form $\psi(\mathbf{k}) = \psi_0 k_z(\nu_x k_x + \nu_y k_y)$. In the broken-time-reversal state, we have $(\nu_x, \nu_y) = (1, i)/\sqrt{2}$, which leads to line nodes for $k_z = 0$ and point nodes at $k_x = k_y = 0$. In the nodal time-reversal-invariant state, we instead have $(\nu_x, \nu_y) = (1, 0)$, which also leads to line nodes for $k_z = 0$ and additional line nodes for $k_x = 0$. In this case, the broken-time-reversal state is believed to be stable because it gaps the $k_x = 0$ line node so that only two point nodes remain, gaining condensation energy. However, we have found that these point nodes become inflated \mathbb{Z}_2 -protected Fermi surfaces, and it is reasonable to ask if the broken-time-reversal state is still stable.

We consider the spherically symmetric normal-state Hamiltonian $H_N(\mathbf{k}) = \alpha k^2 + \beta(\mathbf{k} \cdot \mathbf{J})^2 - \mu$ and an on-site gap function that is a linear combination of η_{xz} and η_{yz} . For this gap function, it is known that there are two essentially different possible ground states [5]: a time-reversal-invariant state $\Delta_r = (\bar{\Delta}/2)\eta_{xz}$ with $k_z k_x$ symmetry and a broken-time-reversal state $\Delta_a = (\bar{\Delta}/2\sqrt{2})(\eta_{xz} + i\eta_{yz})$ with $k_z(k_x + ik_y)$ symmetry. The time-reversal-invariant state $(\bar{\Delta}/2)\eta_{yz}$ is degenerate with Δ_r . For these two states, the off-diagonal block in the Hamiltonian $H(\mathbf{k})$ reads

$$\Delta_r = \frac{\bar{\Delta}}{2} \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad (21)$$

and

$$\Delta_a = \frac{\bar{\Delta}}{\sqrt{2}} \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (22)$$

respectively. These two matrices have been normalized such that $\text{Tr} \Delta^\dagger \Delta = \bar{\Delta}^2$ ($\bar{\Delta}$ is assumed real).

Near T_c , the mean-field free energy can be expressed as a power series in Δ . The expression is standard [6, 8],

$$F = \frac{1}{2V} \text{Tr} \Delta^\dagger \Delta + \frac{k_B T}{2} \sum_{\mathbf{k}, \omega_n} \sum_{l=1}^{\infty} \frac{1}{l} \text{Tr} [\Delta \tilde{G}(\mathbf{k}, \omega_n) \Delta^\dagger G(\mathbf{k}, \omega_n)]^l, \quad (23)$$

where the constant V is the BCS pairing interaction (which is the same for Δ_a and Δ_r), ω_n are the Matsubara frequencies, T is the temperature, and the normal-state Green's functions G and \tilde{G} satisfy $[i\omega_n - H_N(\mathbf{k})]G(\mathbf{k}, \omega_n) = 1$ and $[i\omega_n + H_N^T(\mathbf{k})]\tilde{G}(\mathbf{k}, \omega_n) = 1$. To find G and \tilde{G} , we note that $H_N^T(k_x, k_y, k_z) = H_N(k_x, -k_y, k_z)$ so that \tilde{G} is given once we know G . Some algebra then gives

$$G(\mathbf{k}, \omega_n) = G_+(\mathbf{k}, \omega_n) + \left[(\hat{\mathbf{k}} \cdot \mathbf{J})^2 - \frac{5}{4} \right] G_-(\mathbf{k}, \omega_n), \quad (24)$$

$$\tilde{G}(\mathbf{k}, \omega_n) = \tilde{G}_+(\mathbf{k}, \omega_n) + \left[(\hat{\mathbf{k}} \cdot \mathbf{J}^T)^2 - \frac{5}{4} \right] \tilde{G}_-(\mathbf{k}, \omega_n), \quad (25)$$

with

$$G_{\pm}(\mathbf{k}, \omega_n) = \frac{1}{2} \left(\frac{1}{i\omega_n - \epsilon_1} \pm \frac{1}{i\omega_n - \epsilon_2} \right), \quad (26)$$

$$\tilde{G}_{\pm}(\mathbf{k}, \omega_n) = \frac{1}{2} \left(\frac{1}{i\omega_n + \epsilon_1} \pm \frac{1}{i\omega_n + \epsilon_2} \right), \quad (27)$$

$\epsilon_1 = (\alpha + 9\beta/4)k^2 - \mu$, and $\epsilon_2 = (\alpha + \beta/4)k^2 - \mu$. Denoting the free energies for Δ_r and Δ_a by F_r and F_a , respectively, we find, to fourth order in Δ ,

$$F_a - F_r \cong \frac{\bar{\Delta}^4 k_B T}{16} \sum_{\mathbf{k}, \omega_n} \left\{ \tilde{G}_+^2 G_+^2 + (1 - 2l_1 l_{-1}) \left(\tilde{G}_-^2 G_+^2 + \tilde{G}_+^2 G_-^2 \right) + 4(l_1 l_{-1} - 1) \tilde{G}_- G_- \tilde{G}_+ G_+ + (1 - l_1^2 l_{-1}^2) \tilde{G}_-^2 G_-^2 \right\}, \quad (28)$$

where $l_{\pm 1} = \sqrt{3} \cos \theta \sin \theta e^{\pm i\phi}$ and θ and ϕ are the spherical angles denoting the direction of \mathbf{k} . Note that the term of order Δ^2 drops out of the free-energy difference under the integral over ϕ . The analysis of the above expression reveals that either Δ_r or Δ_a can be stable, depending on the parameters. In particular, first consider the case of vanishing spin-orbit coupling, $\beta = 0$. In this limit, we find $\tilde{G}_- = G_- = 0$ so that only the first term in the sum in Eq. (28) survives, and we have $F_a > F_r$ so that Δ_r has lower free energy. This limit has also been considered in the context of $j = 3/2$ pairing in cold atoms [6, 7] and the results agree with what we find. Consequently, the broken-time-reversal state is not stable for $\beta = 0$.

Now consider the single-band limit, which can be reached, for example, by taking a large $|\beta|$, such that $\alpha + 9\beta/4$ and $\alpha + \beta/4$ have opposite sign, and a large chemical potential. If only ϵ_1 crosses the Fermi surface, for sufficiently small $k_B T/\mu \ll 1$ we can safely take the limit $|\epsilon_2|/k_B T \rightarrow \infty$ to find the asymptotic expression

$$F_a - F_r \cong \frac{\bar{\Delta}^4}{1024 k_B T} \sum_{\mathbf{k}} l_1^2 l_{-1}^2 \left(\frac{1 - k_B T \sinh(\epsilon_1/k_B T)/\epsilon_1}{\epsilon_1^2 (1 + \cosh(\epsilon_1/k_B T))} \right) < 0. \quad (29)$$

This is the result expected from single-band weak-coupling theory, and demonstrates that the broken time-reversal state is stable in this limit.

The above analysis implies that for fixed α and μ there will be a transition from Δ_a to Δ_r as a function of spin-orbit coupling β . It is straightforward to show that the momentum and Matsubara sum in Eq. (28) only depends on the dimensionless ratios β/α and $\mu/k_B T$, apart from prefactors that do not affect its sign. Numerical evaluation indicates that transitions exist for any value of $\mu/k_B T$. We consider explicitly the case of $|\beta| \ll \alpha$, in which the two spherical Fermi surfaces have nearly identical k_F . We then find by expanding in β/α that this transition takes place at $x \equiv |\beta|\mu/\alpha k_B T = |\beta|k_F^2/k_B T \approx 9.324$. For $x \lesssim 9.324$, we find that the time-reversal-invariant state Δ_r is the ground state, while for $x \gtrsim 9.324$, Δ_r is unstable towards Δ_a . This indicates that the broken-time-reversal state is stabilized by modest spin-orbit coupling.

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