A crib-shaped triplet pairing gap function for an orthogonal pair of quasi-one dimensional Fermi surfaces in \( \text{Sr}_2\text{RuO}_4 \)

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The competition between spin-triplet and singlet pairings is studied theoretically for the tight-binding \( \alpha\beta \) bands in \( \text{Sr}_2\text{RuO}_4 \), which arise from two sets of quasi-one dimensional Fermi surfaces. Using multiband FLEX approximation, where we incorporate an anisotropy in the spin fluctuations as suggested from experiments, we show that (i) the triplet can dominate over the singlet (which turns out to be extended), and (ii) the triplet gap function optimized in the Eliashberg equation has an unusual, very non-sinusoidal form, whose time-reversal-broken combination exhibits a crib-shaped amplitude with dips.

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Spin-triplet superconductivity is of great conceptual importance. It is interesting to ask how the spins in a Cooper pair can align, since usually the singlet pairing is favored so that some special mechanism should be envisaged to account for a triplet superconductivity. The \( p \)-wave pairing in superfluid \(^3\text{He}\) is an outstanding example, where a clear picture of the hard-core interaction favoring the triplet exists.

In the past several years, \( \text{Sr}_2\text{RuO}_4 \) has attracted much attention as a strong candidate for triplet superconductivity. In a seminal paper, Rice and Sigrist suggested a mechanism for triplet pairing in this material, which they call an ‘electronic version of \(^3\text{He}\)’. In their scenario the orbital degeneracy causes ferromagnetic spin fluctuations, which is considered to favor the triplet pairing. Subsequent experiments indeed suggested triplet pairing. However, a new puzzle arose when the spin fluctuation in \( \text{Sr}_2\text{RuO}_4 \) was found to be antiferromagnetic rather than ferromagnetic in a neutron scattering experiment. Usual wisdom dictates that antiferromagnetic spin fluctuations lead to singlet \( d \)-wave pairing.

Recently, Kuwabara and one of the present authors have proposed that anisotropy in the spin fluctuation, observed in NMR experiments for \( \text{Sr}_2\text{RuO}_4 \), may lead to triplet \( p \)-wave pairing. However, simple functional forms for triplet and singlet gap functions were assumed in ref. 7, i.e.,

\[
\text{pairing.}
\]

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In ref. 7, the form of the gap function turns out to have unexpected, non-sinusoidal forms, which are in sharp contrast with the \( k_x \) or sin \( k_x \) gap functions assumed previously. As a result, the amplitude of the gap has a shape of a crib along the Fermi surface, which may resolve the controversial experiments. The origin of the peculiar behavior of the gap function is traced back to the singular \( k \)-dependence in the spin susceptibility due to a nesting of two sets of quasi-one dimensional Fermi surfaces.

The ruthenate is essentially a three-band system, which arises from \( d_{xz} \) orbitals aligned linearly along the \( x \) axis, \( d_{yz} \) along the \( y \), and \( d_{2g} \) in the \( xy \) plane. The former two give rise to the \( \alpha, \beta \) bands, which are well nested due to the quasi-one dimensionality and causes antiferromagnetic spin fluctuations. In this paper, we concentrate on the \( \alpha, \beta \) bands, namely, we consider a tight-binding model,

\[
H = -t \sum_{\sigma} \sum_{m=xz,yz} \sum_{(i,i')} c_{i\sigma}^m c_{i'\sigma}^m + \text{H.c.}
\]

\[
- t' \sum_{\sigma} \sum_{(i,j)} \left( c_{i\sigma}^{xz} c_{j\sigma}^{yz} + \text{H.c.} \right) + U \sum_{m=xz,yz} n_{i\sigma}^m n_{i\overline{\sigma}}^m.
\]

on a square lattice. Here \( c_{i\sigma}^m \) creates an electron at \( d_m (m = \text{xz or yz}) \) orbital, the nearest-neighbor hopping integral \( t \) is along the \( x(y) \) direction for \( d_{xz}(d_{yz}) \) orbitals. We take \( t = 1 \) as a unit of energy.

We have also included the next nearest-neighbor hopping \( t' \) which corresponds to a weak hybridization. When \( t' \neq 0 \) the two sets of quasi-one-dimensional bands anticross, and two two-dimensional (rounded-square) bands result, which are the \( \alpha \) and \( \beta \) bands. The on-site repulsive interaction, \( U \), is considered within each orbitals, and in-
terorbital interactions are neglected for simplicity. The band filling is \( n = 4/3 \) electrons per orbital in \( \text{Sr}_2\text{RuO}_4 \).

In treating the interaction, we employ the FLEX approximation. This method is a kind of self-consistent random-phase approximation (RPA) where the dressed Green’s function is used in the RPA diagrams. In the multiband version of FLEX the Green’s function \( G \), the susceptibility \( \chi \), the self-energy \( \Sigma \), and the superconducting gap function \( \phi \) all become \( 2 \times 2 \) matrices, e.g., \( G_{lm}(\mathbf{k}, i\epsilon_n) \), where \( l, m \) denote \( dx^2-\delta \) or \( dxz \) orbitals. The orbital-indexed matrices for Green’s function and the gap functions can be converted into band-indexed ones with a unitary transformation. As for the spin susceptibility, we diagonalize the \( 2 \times 2 \) matrix \( \chi_{\text{zz}}^{\text{irr}} \) and concentrate on the larger eigenvalue, denoted as \( \chi_{\text{zz}} \).

The actual calculation proceeds as follows:

(i) Dyson’s equation is solved to obtain the renormalized susceptibility \( \chi \) in terms of the irreducible susceptibility \( \chi_{\text{irr}} \). Then brings about the self-energy, \( \Sigma(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{k}'} G(\mathbf{k} + \mathbf{q})G(\mathbf{k}) \) (N-number of \( k \)-point meshes). Here we have taken account of the anisotropy in the spin susceptibility, \( \alpha \) à la Kuwabara-Ogata. From the NMR experiments, \( \chi_{\text{zz}}^{\text{irr}}(q) = -\frac{1}{2\pi} \sum_{\mathbf{k}} G(\mathbf{k} + \mathbf{q})G(\mathbf{k}) \) (\( N \)-number of \( k \)-point meshes).

(ii) The fluctuation-exchange interaction \( V^{(1)}(q) \) is given as

\[
V^{(1)}(q) = \frac{1}{2} V_{\text{sp}}^{zz}(q) + V_{\text{sp}}^{+-}(q) + \frac{1}{2} V_{\text{ch}}(q). \tag{2}
\]

The effective interactions due to longitudinal (zz) and transverse (+−) spin fluctuations (sp) and that due to charge fluctuations (ch) have the forms

\[
V_{\text{sp}}^{zz}(q) = U^2 \chi_{\text{sp}}^{zz}(q), \quad V_{\text{sp}}^{+-}(q) = U^2 \chi_{\text{sp}}^{+-}(q), \quad \text{and} \quad V_{\text{ch}} = U^2 \chi_{\text{ch}},
\]

respectively, where the spin and the charge susceptibility are

\[
\chi_{sp}^{zz}(q) = \chi_{\text{irr}}^{zz}[1 - U \chi_{\text{irr}}^{zz} - q]^{-1}, \quad \chi_{sp}^{+-}(q) = \alpha \chi_{\text{irr}}^{zz}[1 - U \alpha \chi_{\text{irr}}^{zz}(q)]^{-1}, \quad \chi_{ch}(q) = \chi_{\text{irr}}^{zz}(q)[1 + U \chi_{\text{irr}}^{zz}(q)]^{-1}, \tag{3-5}
\]

in terms of the irreducible susceptibility \( \chi_{\text{irr}}^{zz}(q) = \frac{1}{2\pi} \sum_{\mathbf{k}} G(\mathbf{k} + \mathbf{q})G(\mathbf{k}) \) (\( N \)-number of \( k \)-point meshes).

(iii) \( V^{(1)}(q) \) then brings about the self-energy, \( \Sigma(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{k}'} G(\mathbf{k} - \mathbf{q})V^{(1)}(q) \), which is fed back to Dyson’s equation, and the self-consistent iterations are repeated until convergence is attained. We take \( 64 \times 64 \) \( k \)-point meshes and up to 16384 Matsubara frequencies in order to ensure convergence at low temperatures.

We determine \( T_c \) as the temperature at which the eigenvalue \( \lambda \) of the Eliashberg equation,

\[
\lambda_{m} \phi_{\mu m}(\mathbf{k}) = -\frac{T}{N} \sum_{\mathbf{k}'} \sum_{\mathbf{k}'} V^{(2)}_{\mu m}(\mathbf{k} - \mathbf{k}') G_{\mu}(\mathbf{k}') G_{\mu n}(\mathbf{k}) \phi_{\mu m}(\mathbf{k}'), \tag{6}
\]

reaches unity. Here the pairing interaction \( V^{(2)}_{\mu}(\mathbf{k} - \mathbf{k}') \) is given by

\[
V^{(2)}_{\mu}(\mathbf{k} - \mathbf{k}') = \frac{1}{2} V_{\text{sp}}^{zz} + V_{\text{sp}}^{+-} - \frac{1}{2} V_{\text{ch}} \tag{7}
\]

for singlet pairing,

\[
V_{t\perp}^{(2)} = -\frac{1}{2} V_{\text{sp}}^{zz} - \frac{1}{2} V_{\text{ch}} \tag{8}
\]

for triplet pairing with \( S_z = \pm 1 \) \((\hat{a} \perp \hat{z})\), and

\[
V_{t\parallel}^{(2)} = \frac{1}{2} V_{\text{sp}}^{zz} - V_{\text{sp}}^{+-} - \frac{1}{2} V_{\text{ch}} \tag{9}
\]

for triplet pairing with \( S_z = 0 \) \((\hat{d} \parallel \hat{z})\). Here \( \hat{d} \) is the \( d \)-vector characterizing the triplet pairing gap function.

When the electron-electron repulsion, which causes fluctuations, is short-ranged (as for the Hubbard \( U \) interaction) the spin fluctuations are much stronger than the charge fluctuations, i.e., \( (V_{\text{sp}} \gg V_{\text{ch}}) \). When fluctuations for a certain (‘nesting’) wave vector \( \mathbf{Q} \) are pronounced, the main contribution in the summation in eq.(6) comes from those satisfying \( k - k' \equiv \mathbf{Q} \), which should be the case when the Fermi surface is nested. The present Fermi surface is indeed well nested due to the quasi-one-dimensionality.

Now turn to the results summarized in Fig.1 for \( t' = 0.3 \) and \( U = 5 \). In Fig.1(a), the ridges in \( |G|^2 \) delineate \( \alpha \) and \( \beta \) Fermi surfaces. These quasi-1D surfaces are strongly nested at \( q \equiv (2\pi/3, q_y) \) and \( q \equiv (q_x, 2\pi/3) \) (mod 2\( \pi \), so that the spin susceptibility is ridged in a crible shape as shown in Fig.1(b), with peaks at the corners, \( q \equiv (\pm 2\pi/3, \pm 2\pi/3) \). This is consistent with neutron scattering experiments.

The triplet and singlet gap functions obtained by solving the Eliashberg equation are shown in Fig.1(c) and (d), respectively. Remarkably, the triplet gap function takes a strange shape: although the symmetry is consistent with wave, its form is far from \( \sin k_y \), along the rounded-square Fermi surface. Rather, it has an almost constant amplitude on a pair of parallel sides, \( k_x \equiv \pm 2\pi/3 \) (mod 2\( \pi \)), of the square with a vanishing amplitude on the other pair \( (k_y = \pm 2\pi/3) \) of parallel sides. This applies to each of the \( \alpha \) and \( \beta \) bands. Of course the symmetry dictates that the other solution \( (p_y) \), rotated by 90 degrees from what is described here \( (p_x) \), enters on an equal footing as we shall discuss below.

Why do we have this peculiar behavior for the FLEX+Eliashberg optimized gap function? To begin with, superconductivity arises due to pair scattering from \( (k, -k) \) to \( (k', -k') \) mediated by the pairing interaction \( V^{(2)}(q) \), where \( q = k - k' \) is the momentum transfer. From the BCS gap equation we can see that superconductivity arises if the quantity

\[
V_\phi = -\frac{\sum_{\mathbf{k}, \mathbf{k}' \in \text{FS}} V_{\mu}^{(2)}(\mathbf{k} - \mathbf{k}') \phi_{\mu}(\mathbf{k}) \phi_{\mu}(\mathbf{k}')}{\sum_{\mathbf{k} \in \text{FS}} |\phi(\mathbf{k})|^2} \tag{10}
\]

is positive and large, where we denote the gap function as \( \phi_{\mu} \) (\( \mu = s \) for singlet and \( t \) for triplet pairing).
As discussed by Kuwabara and Ogata, and independently by Sato and Kohmoto, the $p$-wave pairing, with $\phi_t(k)\phi_t(k+Q) < 0$, is favored when spin anisotropy is so strong as to realize $V^{zz}_{sp}(Q) > 2V^{+}_{sp}(Q)$, i.e., $V_{\parallel}(Q) > 0$. However, the present self-consistent calculation shows that the situation is a little more involved. A key factor is the spin fluctuation that is enhanced along a line $q = (q_x, 2\pi/3)$. For a given nodal line (vertical for $p_x$ pairing), the pair scatterings across one pair of parallel sides of the Fermi surface become all favorable as indicated by $\bigcirc$ in Fig. 2(a). This gives rise to the near-constant gap function on that pair of sides of the Fermi surface. By contrast, the pair scatterings across the other pair of parallel sides ($\times$ in Fig. 2(a)) lead to

$$-V^{(2)}_t(k_x, k'_x, Q) < 0$$

in eq. (11) when $k_x, k'_x$ have the same sign. Since $-V^{(2)}_t$ is negative, the $p_x$-wave gap functions on these sides of the Fermi surface is unfavored. This explains the gap function shown in Fig. 1(c).

Now, let us move on to the competing superconducting state in the singlet channel. Although Kuwabara and Ogata discussed a competition between the triplet $p_x$-wave and a singlet $d_{x^2-y^2}$-wave, we find here that the real competitor (the most stable singlet state) is unexpectedly an extended $s$-wave rather than $d_{x^2-y^2}$-wave. This is understood as follows. Since $V_s(Q) > 0$ is repulsive, $\phi_s(k)\phi_s(k+Q) < 0$ has to be satisfied. For the $d_{x^2-y^2}$-wave, the $k, k' = k + Q$ on the Fermi surface that

![FIG. 1. The contour plot of the FLEX result for Green’s function $|G|^2$; (a), spin susceptibility (b), optimized gap function for the spin triplet (c) or singlet (d) pairing for $U = 5, t' = 0.3, \alpha = 0.8$, and $T = 0.02$. The left(right) panel for the $a(b)$ band, and white(black) corresponds to positive(negative) amplitude in (c,d).](image1)

![FIG. 2. Pair scatterings across the Fermi surface which favor (\bigcirc) or unfavor (\times) $p_x$-wave pairing (a), those contributing to $d_{x^2-y^2}$ (b) or to extended $s$ pairings (c). The white(grey) areas represent positive(negative) $\phi$.](image2)
seen that for the value of $\alpha$ shown in Fig. 3 as functions of temperature. Quantified by the eigenvalues of the Eliashberg equation, tribute to the extended s-wave pairing (Fig. 2(c)).

Why this pairing is weaker. If we extrapolate extended-s, although having a greater magnitude of the triplet does dominate at low temperatures. The singlet $k_s$ with $k$ is maximized for that combination.

The competition between the triplet and singlet is suggested.

The absolute value of the gap function for that linear combination on the Fermi surface is displayed in Fig. 4, which has a crib shape with dips at the corners around $k \equiv (\pm 2\pi/3, \pm 2\pi/3)$. The dip arises because $\phi_\alpha$ in each of the $p_x$ and $p_y$ channels has already sharp drops at the corner of the Fermi surface. Thus, in phase-insensitive experiments, the gap function obtained here may look like a two-dimensional $f$-wave pairing with nodes along $k_x = \pm k_y$, since a dip and a node are indistinguishable when the temperature is greater than the dip. Further study on this point is under way.

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In eqs. (2), (7) − (9) we have omitted the first- and second-order terms, $U$ and $-U^2 \chi_0$ (in eq. 2), which are negligible when spin and/or charge fluctuations are strong, although we have taken those terms into account in the actual calculation.

The simultaneous enhancement of the triplet pairing and the spin fluctuations is reminiscent of the Tomonaga-Luttinger theory for purely 1D systems, where one can show that the susceptibilities for the triplet pairing and the SDW may diverge simultaneously for $T \to 0$ when the SU(2) symmetry in the interaction is broken. However, in the Tomonaga-Luttinger case, the triplet pairing dominates over the SDW only when the electron-electron interaction is attractive, in sharp contrast with the present case where the interaction is repulsive. The difference comes from a different origin of the broken SU(2) here, which is the anisotropy in the irreducible susceptibility (which arises at a single electron level) rather than the anisotropic electron-electron interaction.

We note that, while the qualitative result does not depend crucially on $t' (= 0.3$ in this paper), the quantitative shape of the dip does.