Collective Order Parameter Modes and Spin Fluctuations for Spin-Triplet Superconducting State in Sr_2RuO_4

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We calculate the collective order parameter modes for possible spin-triplet p-wave pairing states in Sr_2RuO_4. The modes are classified in terms of pairing states corresponding to the irreducible representations of D_{4h} for the layered perovskite structure. Besides the phase and amplitude modes, we obtain spin modes which couple to external fields parallel to the basal plane. Observation of the frequencies of the modes can yield information about the nature of the pairing state. We derive also the strong-coupling theory for spin-triplet pairing mediated by exchange of spin fluctuations and make comparison with the corresponding fluctuation exchange approximation for spin-singlet pairing.

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Convincing experimental evidence has been collected that the superconducting state in the new oxide superconductor Sr_2RuO_4 [1] is formed by spin-triplet p-wave Cooper pairs [2,3] in analogy to suprafluid ^{3}He [4]. The possible Cooper pairing states have been classified according to the irreducible representations of the tetragonal point group D_{4h} corresponding to the layered perovskite structure of Sr_2RuO_4 [3]. It has been shown that the odd-parity pairing state which is compatible with all the present data is the two-dimensional analog of the ABM (Anderson-Brinkman-Morel) state in suprafluid ^{3}He [4].

The presence of ferromagnetism in related compounds such as $SrRuO_3$ suggests that the pairing interaction in Sr_2RuO_4 arises from exchange of ferromagnetic spin fluctuations (paramagnons) [5]. Local density approximation shows that in Sr_2RuO_4 ferromagnetic and antiferromagnetic spin fluctuations coexist which can lead to a competition between p-wave and d-wave superconducting symmetries in Sr_2RuO_4 [6]. In the first part of this Letter, we address this question of spin-triplet versus spin-singlet pairing by comparing the self-consistent FLEX (fluctuation exchange) approximations for the two-dimensional (2D) Hubbard Hamiltonian for spin-triplet [7] and for spin-singlet [8] pairing. The latter theory can describe qualitatively many properties of d-wave superconductivity in high-T_c cuprates. It turns out that the spin-fluctuation pairing interaction for the spin-triplet state is only one-third of that for the spin-singlet state. Thus, one might conclude that, at least within the framework of the 2D Hubbard model, d-wave pairing is favored. However, it may be that the actual 2D character of the band structure of Sr_2RuO_4 [6], combined with the self-consistent calculation of the spin-fluctuation spectrum within the FLEX approximation, leads to a dominant ferromagnetic component of the spin fluctuations and thus to a stabilization of the p-wave pairing state in comparison to the d-wave pairing state.

Suprafluid ^{3}He exhibits an amazing richness of collective order parameter modes in the ABM and Balian-Werthamer states [9] which have been observed by NMR and ultrasound attenuation techniques. Therefore one might hope that also in the superconducting state of Sr_2RuO_4 there exist many nontrivial collective modes whose observation can yield more information about the nature of the superconducting state. We calculate here the collective modes in analogy to those in cubic crystals [10] by making a decomposition of the pairing interaction and the order parameter fluctuations in terms of the six pairing states $\vec{d}_j$ corresponding to the irreducible representations of D_{4h} [3]. We find fluctuations of the pairing state $\vec{d}$ (perpendicular to the basal plane) which have frequencies $\omega = 2\Delta_0$ and $\omega = \sqrt{3}\,\Delta_0$ (Δ_0 is the amplitude of the gap) for the states without and with nodes [3]. The latter mode corresponds to the amplitude mode which has been found for d-wave pairing [11]. These amplitude modes couple to charge density by particle-hole asymmetry at the Fermi surface. New modes in comparison to those for d-wave pairing consist in fluctuations $\delta\vec{d}$ parallel to the basal plane. These modes have finite frequencies if the coupling constants for in-plane pairing states $\vec{d}_j$ are smaller than those for pairing states $\vec{d}_j$ perpendicular to the plane. If the coupling constants become equal, these mode frequencies tend to zero which corresponds to the Goldstone modes for broken rotational symmetry. These modes can be excited by external fields which couple to spin density and are polarized parallel to the basal plane. The new modes corresponding to fluctuations of the spin degrees of the spin-triplet order parameter might yield valuable information about the nature of the pairing state in Sr_2RuO_4. However, the number of nontrivial modes is far less than the modes for the ABM state in suprafluid ^{3}He, such as the clapping and flapping modes [9]. If there exist also antiferromagnetic spin fluctuations in Sr_2RuO_4, one expects to observe a spin-density mode in the dynamical spin susceptibility such as in the case of d-wave pairing in the high-T_c cuprates [11].

First, we present the FLEX equations for the normal self-energy Σ and the three components d_μ of the spin-triplet pairing state for the one-band 2D Hubbard Hamiltonian with one-site Coulomb repulsion U:

$$\Sigma(k) = T \sum_{k'} \left[t_{00}(k - k') + \sum_{\nu} t_{\nu\nu}(k - k') \right] G(k'); \qquad (k \equiv \vec{k}, i\omega_n), \tag{1}$$

$$d_\mu(k) = -T \sum_{k'} \left[t_{00}(k - k') + \sum_{\nu} t_{\nu\nu}(k - k') - 2t_{\mu\mu}(k - k') \right] F_\mu(k'); \qquad (\mu, \nu \equiv x, y, z). \tag{2}$$

Here, G and F_μ are the normal and anomalous Green's functions [10], and $t_{\mu\mu}$ are the components of the particle-hole T matrix [7]:

$$t_{00}(q) = \frac{1}{2} U^2 \frac{\chi_{00}(q)}{1 + U\chi_{00}(q)}; \qquad t_{\mu\mu}(q) = \frac{1}{2} U^2 \frac{\chi_{\mu\mu}(q)}{1 - U\chi_{\mu\mu}(q)}; \qquad (q \equiv \vec{q}, i\nu_m), \tag{3}$$

$$\chi_{00}(q) = -T \sum_{k} \left[G(k + q)G(k) - \sum_{\nu} F_\nu(k + q)F^*_\nu(q) \right]; \qquad (\mu, \nu = x, y, z), \tag{4}$$

$$\chi_{\mu\mu}(q) = -T \sum_{k} \left[G(k + q)G(k) - \sum_{\nu} F_\nu(k + q)F^*_\nu(k) + 2F_\mu(k + q)F^*_\mu(k) \right]. \tag{5}$$

Comparison of Eqs. (1) and (2) with the FLEX equations for d-wave pairing [8] shows that the overall pairing interaction for $d_\mu(k)$ is attractive [see minus sign in front of the right-hand side of Eq. (2)] instead of repulsive for d-wave pairing, that the charge-fluctuation interaction t_{00} in Eq. (2) has opposite sign in comparison to d-wave pairing, and that the spin-fluctuation interaction above T_c, $(\sum_\nu t_{\nu\nu} - 2t_{\mu\mu})$ in Eq. (2), is only one-third of that for d-wave pairing. Below T_c, the irreducible susceptibilities $\chi_{\mu\mu}$ in Eq. (5) are quite different from the irreducible spin susceptibility for d-wave pairing [8]. One recognizes that the feedback effect of the anomalous Green's functions F_μ on the susceptibilities $\chi_{\mu\mu}$ in Eq. (5) gives rise to an enhancement of the $t_{\mu\mu}$ in Eq. (3) and thus to an enhancement of the overall pairing interaction in Eq. (2) below T_c.

Second, we present the main equations which are needed to calculate the order parameter collective modes in analogy to those for p-wave pairing in cubic crystals [10]. The p-wave spin-triplet pairing states $\vec{d}_j$ corresponding to the irreducible representations of the tetragonal point group D_{4h} for the layered perovskite structures are the following [3]:

$$\begin{aligned} &A_{1u}\colon \vec{d}_1 = \hat{x}k_x + \hat{y}k_y; \qquad A_{2u}\colon \vec{d}_2 = \hat{x}k_y - \hat{y}k_x, \\ &B_{1u}\colon \vec{d}_3 = \hat{x}k_x - \hat{y}k_y; \qquad B_{2u}\colon \vec{d}_4 = \hat{x}k_y + \hat{y}k_x, \\ &E_u\colon \vec{d}_5 = \sqrt{2}\,\hat{z}k_x; \qquad \vec{d}_6 = \sqrt{2}\,\hat{z}k_y. \end{aligned} \tag{6}$$

For simplicity, we take the orbital basis set $k_x = \cos\phi$ and $k_y = \sin\phi$ on a cylindrical Fermi surface. The weak-coupling pairing interaction can be written as a sum of projection operators [10] onto the basis states $\vec{d}_j$ in Eq. (6) with eigenvalues v_j $(v_5 = v_6)$:

$$V(\vec{k}, \vec{k}') = -\sum_{j=1}^{6} v_j\, \vec{d}_j(\vec{k})\, \vec{d}^\dagger_j(\vec{k}'). \tag{7}$$

The fluctuations $\delta\vec{d}$ of the equilibrium pairing state $\vec{d}$ are decomposed in terms of the basis vectors in Eq. (6):

$$\delta\vec{d}(\vec{k}; \vec{q}, i\nu_m) = \sum_j \delta\Delta_j(\vec{q}, i\nu_m)\, \vec{d}_j(\vec{k}). \tag{8}$$

Then the coupled Bethe-Salpeter equations for the order parameter fluctuations in the particle-particle and hole-hole channels can be decomposed with the help of Eqs. (7) and (8) in terms of coupled equations for the fluctuation components $\delta\Delta_j$ and $\delta\Delta^*_j$ [see Eq. (33) in Ref. [10]]. The charge- and spin-fluctuation contributions in the particle-hole channels yield coupling terms proportional to external fields U_s and $\vec{U}_a$.

We consider first the a-phase equilibrium state,

$$\vec{d} = \Delta_0 \hat{z}(k_x + ik_y), \tag{9}$$

which corresponds to the ABM state of suprafluid ^{3}He and is compatible with all the present experiments [3]. From now on, we specialize to eigenvalues $v_1 = v_2$ and $v_3 = v_4$ in Eq. (7). Then the orbital part of the pairing interaction in Eq. (7) having factors $(v_1 + v_3)$ and v_5 is proportional to $(\vec{k} \cdot \vec{k}')$, and the orbital part of the interaction with factor $(v_3 - v_1)$ is proportional to $(k_x k'_y - k_y k'_x)$. The latter orbital part is the term which corresponds to spin-orbit coupling [3]. For the equilibrium state in Eq. (9) and this specification of the eigenvalues, we find with the help of the orthonormality of the basis states in Eq. (6) with respect to angle integration that for wave vector $\vec{q} = 0$ the twelve equations for the fluctuation component decouple into three sets of four equations each. The first two sets of equations yield fluctuations being proportional to $(\vec{d}_1 + \vec{d}_3)$ and $(\vec{d}_2 - \vec{d}_4)$, respectively, which are excited to external fields $\vec{U}_a$ coupling to spin density and lying parallel to the basal xy plane. The resulting contributions to the irreducible spin susceptibility $\chi^{\mu\nu}$, the so-called fluctuation susceptibilities [9] $\chi_{\rm fl}^{\mu\nu}$, are the following:

$$\chi_{\rm fl}^{xx}(0,\omega) = \chi_{\rm fl}^{yy}(0,\omega) = N(0)\,\frac{\Delta_0^2\omega^2F^2(\omega)}{[\omega^2F(\omega) - (x_1 + x_3)]}, \tag{10}$$

$$x_j = \ln(T_c/T_{cj});$$
$$F(\omega) = \int_{-\infty}^{+\infty} d\varepsilon[E(4E^2 - \omega^2)]^{-1}\tanh(E/2T); \tag{11}$$
$$E^2 = \varepsilon^2 + \Delta_0^2.$$

Here, T_{cj} is the superconducting transition temperature corresponding to the in-plane coupling constant v_1 or v_3, and T_c is the largest transition temperature corresponding to the coupling constant $v_5 = v_6$ [10]. For $T_{cj} \to T_c$, the mode frequency $\omega \to 0$ for $\vec{q} = 0$ which corresponds to the Goldstone mode for broken rotational symmetry. The third set of equations yields, on the one hand, fluctuations of the phase of $\vec{d}$ with frequency $\omega = 0$ corresponding to the Goldstone mode for broken gauge invariance. This frequency is renormalized to that of the 2D plasmon frequency by the long-range Coulomb interaction. On the other hand, one obtains fluctuations of the amplitude of $\vec{d}$ which can be excited by external fields U_s which couple to charge density. This mode yields the following fluctuation contribution to the charge susceptibility χ^{00}:

$$\chi_{\rm fl}^{00}(0,\omega) = 16N(0)\,\frac{\Delta_0^2(\langle\varepsilon_k\rangle)^2}{\langle\omega^2 - 4|\vec{d}(\vec{k})|^2\rangle}. \tag{12}$$

Here, the brackets $\langle\cdots\rangle$ mean the average taken with the integrand of the function $F(\omega)$ in Eq. (11). Thus, the mode frequency is $\omega = 2\Delta_0$. We remark that the irreducible spin and charge susceptibilities $\chi^{\mu\nu}(\vec{q},\omega)$ for the ABM state have been calculated for finite $\vec{q}$ and finite magnetic fields in Ref. [9].

We have calculated also the collective modes for the b-phase state $\vec{d} = (\Delta_0/\sqrt{2})\hat{z}(k_x - k_y)$ [3] which has nodes at angles $\phi = \pi/4$ and $3\pi/4$. The main difference of the collective modes in comparison to those of the a-phase state in Eq. (9) is that the averages $\langle\cdots\rangle$ in Eq. (12) are taken with the integrand of $F(\omega)$ times the angle dependent function $(k_x - k_y)^2$. This yields a frequency of the amplitude mode of about $\omega = \sqrt{3}\,\Delta_0$ which lies well below the pair-breaking edge $2\Delta_0$. However, the coupling strength $(\langle\varepsilon_k\rangle)^2$ of the amplitude mode in Eq. (12) is rather small because $\langle\varepsilon_k\rangle$ is of the order $dN(\varepsilon)/d\varepsilon$ where $N(\varepsilon)$ is the density of states. It was speculated that the amplitude mode with frequency $\omega = \sqrt{3}\,\Delta_0$ for d-wave pairing might yield a contribution to the B_{1g} Raman spectrum in the high-T_c cuprates [11].

In summary, we have calculated quite generally the collective order parameter modes for spin-triplet p-wave pairing states in layered perovskite structures such as Sr_2RuO_4. Our method is based on a decomposition of the weak-coupling pairing interaction and the equations for the order parameter fluctuations in terms of the spin-triplet pairing states $\vec{d}_j$ ($j = 1,\ldots,6$) corresponding to the irreducible representations of the tetragonal point group D_{4h} [3]. For the a-phase and b-phase pairing states $\vec{d} = \Delta_0\hat{z}(k_x + ik_y)$ and $\vec{d} = (\Delta_0/\sqrt{2})\hat{z}(k_x + k_y)$, we obtain amplitude fluctuations with frequencies $\omega = 2\Delta_0$ and $\omega = \sqrt{3}\,\Delta_0$, respectively. These modes couple to charge density fluctuations, however, their coupling strength is rather small of the order of $dN(\varepsilon)/d\varepsilon$ which is a measure of the electron-hole asymmetry at the Fermi surface. Most interesting are the modes involving the spin degrees of the order parameter $\vec{d}$. These modes consist of fluctuations $\delta\vec{d}$ parallel to the basal xy plane and yield contributions to the in-plane spin susceptibility. The resonance frequencies ω of these modes scale with $(\omega/\Delta_0)^2 = \ln(T_c/T_{cj})$, where $T_{cj} \le T_c$ is the superconducting transition temperature corresponding to the in-plane pairing strength. These modes can be observable because their coupling strength to the spin susceptibility is of order $\omega^2\Delta_0^2$. Observation of these modes would yield information about the asymmetry of the pairing interaction.

We have also derived the strong-coupling equations for the self-energy and spin-triplet $\vec{d}$ vector mediated by exchange of spin and charge fluctuations within the framework of the 2D Hubbard Hamiltonian. Comparison with the corresponding FLEX equations for spin-singlet pairing shows that, in the former case, the pairing interaction is attractive and its magnitude is above T_c only one-third of the latter. However, only a self-consistent calculation of the spin-fluctuation spectrum based on the actual band structure of Sr_2RuO_4 can tell whether the spin-fluctuation interaction is peaked at $\vec{q} = 0$ yielding spin-triplet pairing, or around $\vec{q} = (\pi,\pi)$ yielding spin-singlet pairing. Recently T. Imai *et al.* [12] have reported NMR relaxation rate measurements on this material which show that the spin-fluctuation spectrum is not peaked near the latter q but that the NMR results favor a maximum at small q.

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