The Resonance Peak in Sr$_2$RuO$_4$: Signature of Spin Triplet Pairing

Dirk K. Morr$^1$, Peter F. Trautman$^{1,2}$, and Matthias J. Graf$^2$

$^1$ Theoretical Division, MS B262, Los Alamos National Laboratory, Los Alamos, NM 87545
$^2$ Baylor University, Waco, TX 76798

We study the dynamical spin susceptibility, $\chi(\mathbf{q}, \omega)$, in the normal and superconducting state of Sr$_2$RuO$_4$. In the normal state, we find a peak in the vicinity of $\mathbf{Q}$, $\approx (0.72\pi, 0.72\pi)$, in agreement with recent inelastic neutron scattering (INS) experiments. We predict that for spin triplet pairing in the superconducting state a resonance peak appears in the out-of-plane component of $\chi$, but is absent in the in-plane component. In contrast, no resonance peak is expected for spin singlet pairing.

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The superconducting (SC) state of Sr$_2$RuO$_4$ has been the focus of intense experimental and theoretical research over the last few years. Sr$_2$RuO$_4$ is isosstructural with the high-temperature superconductor (HTSC) La$_2$−xSr$_x$CuO$_4$ and is the only known layered perovskite which is superconducting in the absence of Cu [1]. Understanding the pairing mechanism in Sr$_2$RuO$_4$ could therefore provide important insight into the origin of unconventional superconductivity in general, and that of the HTSC in particular. Since a related compound, SrRuO$_3$, is a ferromagnet, it was suggested [2] that Sr$_2$RuO$_4$ is a triplet superconductor in which the pairing is mediated by ferromagnetic paramagnons. Experimental support for spin triplet pairing comes from Knight shift (KS) reversal symmetry in the SC state. However, the momentum dependence of the superconducting gap is still unclear. While originally a $p$-wave symmetry, belonging to the $E_u$ representation of the $D_{4h}$ point group, was proposed for the superconducting gap [3], recent specific heat [4], thermal conductivity [5], penetration depth [6], and magnetic nuclear resonance [7] experiments suggest the presence of line nodes in $\Delta(\mathbf{k})$ and thus pairing with higher orbital momentum.

The spin susceptibility, $\chi(\mathbf{q}, \omega)$, is an important input parameter for any theory ascribing the pairing mechanism in Sr$_2$RuO$_4$ to the exchange of spin fluctuations. In this letter we present a scenario for the momentum and frequency dependence of $\chi(\mathbf{q}, \omega)$, both in the normal and superconducting state. In the normal state, we find a peak in Im $\chi$ whose momentum position is close to that reported by Sidis et al. [2] in inelastic neutron scattering (INS) experiments. Our results for Re $\chi$ agree with the prediction by Mazin and Singh [13] of a peak in the normal-state static susceptibility, $\chi(\mathbf{q}, \omega = 0)$, around $\mathbf{q} = (2\pi/3, 2\pi/3)$. We show that for triplet pairing in the superconducting state the in-plane, $\chi_{\perp} = (\chi_{xx} + \chi_{yy})/2$, and out-of-plane, $\chi_{zz}$, components of the dynamic spin susceptibility are qualitatively different. In particular, we predict that a resonance peak, similar to the one observed in the HTSC [8], appears in $\chi_{zz}$, but is absent in $\chi_{\perp}$. Since no resonance peak exists for spin singlet pairing, it is an important signature of spin triplet superconductivity.

Contributions to the dynamic spin susceptibility in Sr$_2$RuO$_4$ come from three electronic bands which are derived from the Ru 4$d$ $xy$, $xz$, and $yz$-orbitals. A comparison of angle-resolved photoemission (ARPES) [15] and de Haas-van Alphen (dHvA) [16] experiments with band-structure calculations [17] shows a substantial hybridization only between the $xz$- and $yz$-orbitals, with a resulting hole-like ($\alpha$-band) and electron-like Fermi surface ($\beta$-band), while the decoupled $xy$-orbitals give rise to the electron-like $\gamma$-band [18]. Thus the electronic structure of Sr$_2$RuO$_4$ can be described by the tight-binding Hamiltonian

$$
\mathcal{H} = \sum_{\mathbf{k}, \sigma} e_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \sum_{\mathbf{k}, \sigma} e_{\mathbf{k}} a_{\mathbf{k}, \sigma}^\dagger a_{\mathbf{k}, \sigma} + \sum_{\mathbf{k}, \sigma} e_{\mathbf{k}} b_{\mathbf{k}, \sigma}^\dagger b_{\mathbf{k}, \sigma} - \sum_{\mathbf{k}, \sigma} (t_{\perp} a_{\mathbf{k}, \sigma}^\dagger b_{\mathbf{k}, \sigma} + h.c.),
$$

where $c_{\mathbf{k}}^\dagger, a_{\mathbf{k}}^\dagger, b_{\mathbf{k}}^\dagger$ are the fermionic creation operators in the $\alpha$, $\beta$ and $\gamma$-bands, respectively, and $t_{\perp}$ reflects the hybridization between the $xz$ and $yz$-bands [19]. After diagonalizing the Hamiltonian, Eq. (1), we obtain the energy dispersions for the $\gamma$ and hybridized $\alpha$ and $\beta$-bands

$$
\epsilon_{\alpha, \beta}(\mathbf{k}) = \epsilon_{\mathbf{k}}^c \pm \sqrt{(\epsilon_{\mathbf{k}}^c)^2 + t_{\perp}^2}, \quad \epsilon_{\gamma}(\mathbf{k}) = \epsilon_{\mathbf{k}}^{\gamma},
$$

with $\epsilon_{\mathbf{k}}^c = (\epsilon_{\mathbf{k}}^{xx} + \epsilon_{\mathbf{k}}^{yy})/2$. By fitting the area and shape of the $\alpha$ and $\beta$-FS to those observed by ARPES [15] and dHvA experiments [16], we obtain $t_{\perp} \approx 0.1$ eV; the Fermi surfaces for all three bands are shown in Fig. [1].

The superconducting gap for unitary spin triplet pairing can be written as

$$
\Delta_{\xi\eta}(\mathbf{k}) = |\mathbf{d}(\mathbf{k}) \cdot \sigma i \sigma_2| \xi\eta
type{4}
$$

where $\sigma$ are the Pauli matrices. We assume that spin-orbit coupling locks the $\mathbf{d}$ vector along the crystal $c$ axis,
where the upper (lower) sign applies to

d_{z}(k) = \Delta(k) = \Delta_{0} \sin k_{x} \sin k_{y} \sin(k_{x} + i k_{y}), \quad \text{(5)}

which was shown to be consistent with the low temperature power laws observed in specific heat and thermal conductivity experiments. Our conclusions are, however, insensitive to the detailed form of the gap function for triplet pairing. We take $\Delta_{0} \approx 1 \text{ meV}$ as reported by Andreev point-contact spectroscopy.

For spin triplet pairing, and isotropic spin fluctuations, the unrenormalized band susceptibility, $\chi$, is given by

$$
\chi_{ij}^{\text{hyb}}(p) = -\frac{1}{2} \sum_{\mathbf{k},m} A_{k,q}^{\text{hyb}} \left\{ G_{r\eta}(1) G_{\eta\delta}^{\text{hyb}}(1 + p) \right\},
$$

where $r, s = \alpha, \beta, \gamma$ are band indices, $p = (\mathbf{q}, i\omega_{n})$, $l = (k, \nu_{m})$ are four-vectors, and

$$
G_{r\eta}(1) = -\frac{i\nu_{m} + \epsilon_{r}(k)}{\nu_{m}^{2} + E_{r}^{2}(k)}, \quad F_{\eta\delta}(1) = \frac{\Delta_{\eta\delta}(k)}{\nu_{m}^{2} + E_{\eta}^{2}(k)},
$$

are the normal and anomalous Greens functions, respectively, with $E_{r}(k) = \sqrt{\epsilon_{r}^{2}(k) + |\Delta_{k}|^{2}}$ [23]. The hybridization between the bands is reflected in

$$
A_{k,q}^{\text{hyb}} = \frac{1}{2} \pm \frac{\epsilon_{k}^{-} \epsilon_{k+q}^{-} + t_{1}^{2}}{2\sqrt{(\epsilon_{k}^{-})^{2} + t_{1}^{2}}} \frac{\epsilon_{k+q}^{-} + t_{2}^{2}}{\sqrt{(\epsilon_{k+q}^{-})^{2} + t_{2}^{2}}}, \quad \text{(8)}
$$

where the upper (lower) sign applies to $rs = \alpha\alpha, \beta\beta$ ($rs = \alpha\beta, \beta\alpha$), $A_{\gamma\gamma} = 1$, and $A_{rs} = 0$ otherwise. In what follows we distinguish between $\chi_{ij}^{\text{hyb}} = \chi_{ij}^{\alpha\alpha} + \chi_{ij}^{\beta\beta} + 2\chi_{ij}^{\alpha\beta}$, which arises from intra- and interband quasiparticle transitions in the $\alpha$ and $\beta$-bands, and $\chi_{ij}^{\alpha\beta}$ due to quasiparticle excitations in the $\gamma$-band. Note that the out-of-plane, $\chi_{zz}(p)$, and in-plane susceptibility, $\chi_{\perp}(p)$, differ in the form of their superconducting coherence factors, which as we show below, gives rise to their qualitatively different frequency and momentum dependence. Finally, the bare susceptibility, Eq.(4), in correlated electron systems is renormalized by an effective quasiparticle interaction, $U$, and one has in random-phase approximation (RPA), neglecting vertex corrections

$$
\chi_{ij}^{\text{hyb},\gamma} = \chi_{ij}^{\text{hyb},\gamma} \left(1 - U \chi_{ij}^{\text{hyb},\gamma}\right)^{-1}. \quad \text{(9)}
$$

In Fig. 3 we present the normal state susceptibility, $\chi_\text{NS} = (\chi_{zz} + 2\chi_{xy})/3$, obtained from Eq.(4) with $\Delta_{0} = 0$ for $\omega = 6.0 \text{ meV}$ along the momentum path shown in the inset. In the vicinity of $(\pi, \pi)$, $\chi_{\text{NS}}^{\text{hyb}}$ exhibits peaks at $Q_{i}$ and $P_{i}$, arising from the nesting properties of the $\alpha$ and $\beta$-bands, while $\chi_{zz}\text{NS}$ provides only a weakly $q$-dependent background [24]. Moreover, for $q \to 0$ the form of $\text{Im} \chi_{\text{NS}}^{\text{hyb}} \sim q^{-1}$ reflects the predominantly one-dimensional (1D) character of the $xz, yz$-bands, while $\text{Im} \chi_{\text{NS}}^{\text{hyb}} \sim \omega/q$ arises from the cylindrical nature of the $xy$-band.

In Fig. 3 we present the RPA susceptibility, $\tau_{\text{NS}}$, in the normal state. A fit of our results, Eq.(10), to the measured $\omega$-dependence of $\text{Im} \chi_{\text{NS}}^{\text{hyb}}$ at $Q_{i}$ (see inset) yields $U = 0.175 \text{ eV}$[24] in agreement with Ref. [13]. Due to the $q$-structure of $\text{Re} \chi_{\text{NS}}^{\text{hyb}}$ (Fig. 3b), and the weak $q$-dependence of $U$, Im $\chi_{\text{NS}}^{\text{hyb}}$ is reduced from its bare...
yields Im $\chi$ in the low frequency limit, which are excited in the low frequency limit, which yields Im $\chi_{NS}$ is strongly suppressed for all $q$. Thus, the experimentally observed peak close to $Q_1$ arises primarily from Im $\chi_{NS}^{hyb}$ and the strongest SC pairing most likely occurs between electrons in the $\beta$-band.

In Fig. 4b we present the frequency dependence of Im $\chi_{NS}^{hyb}$ at $Q_1$ in the normal and superconducting state. There exist three channels for quasiparticle excitations with wavevector $Q_i$, which contribute to Im $\chi_{NS}^{hyb}$, as indicated by arrows in Fig. 4b. In the normal state all three channels are excited in the low frequency limit, which yields Im $\chi_{NS}^{hyb}$ $\sim$ $\omega$, in agreement with our numerical results in Fig. 4a. The dominant contribution to Im $\chi_{NS}^{hyb}$, both in the normal and superconducting state, arises from excitations of type (3), since (a) they are intraband $xz$ (or $yz$) transitions and thus independent of $t_\perp$, and (b) the FS exhibits the largest nesting in this region of momentum space.

In the superconducting state excitations (1-3) possess nonzero threshold energies, $\omega_n$, with $n = 1, 2, 3$, that are determined by the momentum dependence of the order parameter and the shape of the Fermi surface. Specifically, $\omega_n = |\Delta_k| + |\Delta_{k+Q_1}|$, where $k$ and $k + Q_1$ both lie on the Fermi surface, as shown in Fig. 4b. For the band parameters chosen, we obtain $\omega_1 \approx 0.15\Delta_0$, $\omega_2 \approx 0.8\Delta_0$, and $\omega_3 \approx 2.1\Delta_0$. Since excitations (1-3) are well separated in frequency, we can identify their relative contribution to Im $\chi_{NS}^{hyb}$. While $\omega_1$ cannot be observed in the frequency dependence of Im $\chi_{NS}^{hyb}$, due to the negligible spectral weight of excitation (1), $\omega_2$ and $\omega_3$ can clearly be identified. The large spectral weight of excitation (3) likely makes $\omega_3$ the experimentally observable spin gap. Moreover, due to the superconducting coherence factors which appear in the calculation of $\chi_{NS}^{hyb}$, the overall frequency dependence of the in-plane and out-of-plane component of Im $\chi_{NS}^{hyb}$ are qualitatively different. Specifically, since Re($\Delta_k \Delta_{k+q}$) is negative for transition (3), but positive for transition (2), Im $\chi_{zz}^{hyb}$ (Im $\chi_{xz}^{hyb}$) exhibits a sharp jump at $\omega_{c1}$ ($\omega_{c2}$) and increases continuously at $\omega_{c2}$ ($\omega_{c3}$). Consequently, Re $\chi_{zz}^{hyb}$ (Re $\chi_{xz}^{hyb}$) possesses a logarithmic divergence at $\omega_{c3}$ ($\omega_{c2}$).

In Fig. 4b we present the RPA susceptibility, Im $\chi_{NS}^{hyb}$, in the superconducting state, assuming that $U$ remains unchanged below $T_c$. Due to the logarithmic divergence of Re $\chi_{zz}^{hyb}$ at $\omega_{c3}$, Im $\chi_{NS}^{hyb}$ exhibits a resonance peak at a frequency slightly below $\omega_{c3}$. In contrast, Im $\chi_{xz}^{hyb}$ increases continuously above $\omega_{c3}$. The logarithmic divergence of Re $\chi_{zz}^{hyb}$ at $\omega_{c2}$ is rapidly smoothed out for finite quasiparticle damping due to its small prefactor and is likely experimentally not observable. Thus, we predict that for triplet pairing Im $\chi_{NS}^{hyb}$ and Im $\chi_{xz}^{hyb}$ possess qualitatively different frequency dependencies at $Q_1$, with only Im $\chi_{NS}^{hyb}$ exhibiting a resonance peak below $\omega_{c3}$. In con-
trast, a resonance peak was predicted in Refs. [27,28] for the in-plane component $\text{Im} \chi_{zz}$, but not for $\text{Im} \chi_{xy}$. A comparison of our results for $\chi_{zz,\pm}$ with those in [27,28] suggests that the SC coherence factors for $\chi_{zz,\pm}$ have been interchanged in Refs. [27,28]. We obtain the correct $\omega, q \to 0$ limit only for the SC coherence factors which appear in our results for $\chi_{zz,\pm}$ in Eq. (8). In this case, we find that $\text{Re} \chi_{zz}$ decreases below $T_c$ when a SC gap opens, while $\text{Re} \chi_{\pm}$ remains unchanged. As shown by Leggett [30], this result is a general property of any unitary state if $d || c$.

We find that our results are insensitive to details of the electronic band structure or the symmetry of the gap function for spin triplet pairing. In particular, for a nodeless superconducting gap with ‘$p$-wave’ symmetry [3], $\Delta(k) = \Delta_0 (\cos k_x - \cos k_y)/2$, and $d_{xy}$-symmetry, $\Delta(k) = \Delta_0 \sin k_x \sin k_y$, with $\Delta_0 = 1$ meV. In both cases, $\text{Im} \chi^{hyb}_{zz}$ increases continuously above $\omega_{c3}$, since $\Delta(k)$ does not change sign for excitation (3) and no logarithmic singularity occurs in $\text{Re} \chi^{hyb}_{zz}$. In contrast, for spin singlet pairing the in-plane and out-of-plane susceptibilities are identical and our calculations (analogous to singlet pairing the in-plane and out-of-plane susceptibilities) are qualitatively different since no resonance peak exists in $\text{Im} \chi^{hyb}_{zz}$. In the inset of Fig. 3 we plot $\text{Im} \chi^{hyb}_{zz}$ at $Q$, as a function of frequency for SC gaps with $d_{x^2-y^2}$ symmetry, $\Delta(k) = \Delta_0 (\cos k_x - \cos k_y)/2$, and $d_{xy}$-symmetry, $\Delta(k) = \Delta_0 \sin k_x \sin k_y$, with $\Delta_0 = 1$ meV. In both cases, $\text{Im} \chi^{hyb}_{zz}$ increases continuously above $\omega_{c3}$, since $\Delta(k)$ does not change sign for excitation (3) and no logarithmic singularity occurs in $\text{Re} \chi^{hyb}_{zz}$. In contrast, for the FS geometry of the HTSC and a SC gap with $d_{x^2-y^2}$ symmetry, one finds $\Delta_k \Delta_{k+Q} Q < 0$, which as described above leads to a resonance peak at $Q = (\pi, \pi)$ [29]. A resonance peak is thus not an intrinsic property of singlet or triplet superconductivity, but arises from the interplay of FS topology and symmetry of the SC gap.

An additional contribution to $\chi_{\pm}$ in the SC state can in principle come from a coupling of the spin density to in-plane fluctuations of $d$. However, for the $q$-independent coupling assumed in Ref. [27], we find that these fluctuation contributions (FC) are three orders of magnitude smaller than those coming from Eq. (6). Moreover, the spin-orbit coupling present in Sr$_2$RuO$_4$ introduces a gap for in-plane fluctuations of $d$ which further suppresses the FC to $\chi_{\alpha}$ and renders them irrelevant.

In summary, we present a scenario for the spin susceptibility in the normal and SC state of Sr$_2$RuO$_4$. In the normal state we find a peak close to the experimentally observed position at $Q_4$. For spin triplet pairing in the superconducting state we show that the momentum and frequency dependence of $\text{Im} \chi_{xx}$ and $\text{Im} \chi_{\pm}$ are qualitatively different. We predict the appearance of a resonance peak in $\text{Im} \chi_{zz}$, similar to the one observed in the HTSC, and its absence in $\text{Im} \chi_{\pm}$. Finally, we show that no resonance peak exists for spin singlet pairing.

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