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Spin Density Wave Fluctuations and p-Wave Pairing in Sr$_2$RuO$_4$

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Sr$_2$RuO$_4$ is generally believed to be a chiral p-wave superconductor, in analogy to the superfluidity of $^3$He. The field has attracted a lot of attention for its novel superconductivity [1–4]. The normal state electronic structure is well established. Near the Fermi level there are three Ru 4$d$ bands, a two-dimensional (2D) $\gamma$ band, mainly a $d_{xy}$ orbital, and a pair of quasi-1D ($\alpha$, $\beta$) bands, mainly $d_{xz}$ and $d_{yz}$ orbitals, as illustrated in Fig. 1. There is also a general consensus that the pairing is likely of electronic origin. The recent debate is over which of the bands is the active source of the superconductivity, which is important to our basic understanding of the superconductivity in this material. The debate has been triggered by the failure to observe the persistent edge currents associated with the chirality, though this issue is also controversial [3,5,6]. Early theories propose the pairing predominantly arising from the 2D $\gamma$ band. The 2D scenario predicts a chiral p-wave pairing and an edge current. Microscopic derivations of a chiral p-wave pairing state in the 2D scenario have been proposed based on a 2D Hubbard model by a $T$-matrix approach [7], third-order perturbation theory [8], and functional renormalization group (RG) calculations [9]. Very recently, Raghu et al. [5,10] have argued the quasi-1D scenario as more compatible with the missing edge currents and have provided a microscopic justification for it by using an RG theory, but only in the limit of weak interactions.

A closely related and competing phenomenon in Sr$_2$RuO$_4$ is the strong spin density wave (SDW) fluctuations at an incommensurate nesting wave vector spanning the Fermi surfaces of the 4/3 filled ($\alpha$, $\beta$) bands [11]. SDW fluctuations at this wave vector $\vec{Q} = (2\pi/3, 2\pi/3)$ [12] were recently reported at room temperature and at energies as high as 80 meV [13]. The SDW peaks at $\vec{Q}$, which combine nesting in both nearly 1D Fermi surfaces, grow as the temperature ($T$) is reduced and saturate at the crossover to 3D Fermi liquid behavior at $T_{3D} = 60$ K [11] when the resistivity starts to show a $T^2$ behavior [14]. Smaller peaks were observed at the wave vectors ($\pi$, $2\pi/3$) and ($2\pi/3$, $\pi$). To date, these have been discussed within a random phase approximation (RPA) scheme [15–18]. Because of the highly nesting character of the ($\alpha$, $\beta$) Fermi surface, it is necessary to choose a very weak interaction in RPA with a value typically an order of magnitude smaller than standard estimates [19,20].

In this Letter, we show that treating the 1D character of the ($\alpha$, $\beta$) bands in an RG scheme can explain the strong SDW fluctuation and reconcile the absence of the SDW long-range order at $T > T_{3D}$ using a standard value for the interaction as observed in Sr$_2$RuO$_4$. Furthermore, our RG scheme shows mutual exclusion of p-wave pairing and...
SDW fluctuations in repulsive Hubbard chains and a sharp
suppression of the SDW fluctuations at low frequency in
the $p$-wave superconducting (SC) state. Such suppression
has not been observed in early neutron scattering experi-
ments, and its absence in more complete experiments
would be a challenge to explain within the quasi-1D
scenario.

We start with a single chain Hamiltonian for ($\alpha$, $\beta$)
bands by neglecting the $\gamma$ band,

\[ H_0 = H_0^{\alpha} + H_U, \]

\[ H_0^{\alpha} = \sum_{m,\alpha} E_m c_{\alpha m}^\dagger c_{\alpha m}, \]

\[ H_U = U \sum_{n,\alpha} n_{\alpha n} n_{\alpha n}. \]  

In the above equations, $E_{\alpha m}$ is the Fermi velocity and $k_F$ the Fermi wave vector, $c_{\alpha m,\sigma}$ is the
electron annihilation operator with orbital $m = d_{xz}, d_{yz}$
and momentum $\vec{k}$ and spin $\sigma$. $H_U$ is the Hubbard term for
the on-site intraorbital interaction and $n_{\alpha m} = c_{\alpha m,\sigma}^\dagger c_{\alpha m,\sigma}$.
The properties of single chains in a one-loop RG were
derived in an early application of RG to condensed-matter
systems [21]. This includes the important cancellation
between particle-hole and particle-particle graphs, which is
absent in RPA. With repulsive interactions, the SDW and
triplet superconductivity (TS) response functions have a
power-law form with divergences to infinity or zero, as
$T \to 0$. The phases with enhanced SDW and suppressed TS
and vice versa are separated by a quantum critical point
where the exponent $\theta$ changes sign. In the one-loop ap-
proximation, $\theta = g_2 - g_1/2$, where $g_1$ ($g_2$) is the dimen-
sionless scattering coefficient for backward (forward)
processes. For the model Hamiltonian $H_0$ in Eq. (1), $\theta = U/2\pi v_F > 0$ so that the SDW response function for each
of the orbitals $d_{xz}$ and $d_{yz}$ has the form divergent at $T \to 0$
and is given by

\[ \chi_{\text{RG}}^{\alpha}(\vec{q}, T) = \frac{1}{\pi v_F \theta} \left( \frac{E_0}{T} \right)^{\theta}. \]

with $E_0 = 4t$ the bandwidth. The 1D RG result is very
different from that in RPA, which gives a finite scale
divergence in the SDW response. This RPA scale corre-
spends to a large temperature (up to $10^5$ K) in Sr$_2$RuO$_4$ if
we use typical values of the intrachain hopping $t = 0.3$ eV [2]
and $U = 2.2$ eV [19,20]. To deal with the case of such strong on-site interactions, we compared our results with
the $T$ dependence of spin susceptibility from the
Monte Carlo method [22,23] to extend the one-loop RG
calculations to stronger interactions and found that $\theta$
is screened to be 0.69, which we denote as $\theta^* = 0.69$ from now on.

To have a better modeling for Sr$_2$RuO$_4$, we examine the effects on the SDW fluctuations arising from (1) the hy-
bridization and spin-orbit coupling between the two orbit-
als $d_{xz}$ and $d_{yz}$, which give rise to coupled perpendicular
chains and (2) the on-site interorbital interactions. As we
shall see below, the former introduces a low-energy cutoff
on the response function in Eq. (2), and the latter enhances
SDW fluctuations at the wave vector $(2k_F, 2k_F)$. The effect
of the hybridization and spin-orbit coupling among the two
orbitals can be described by the following perturbed
Hamiltonian to $H_0^{\alpha}$ [5]

\[ \delta H = \sum_{\vec{k},\sigma} \left( -2t'' \sin k_x \sin k_y \epsilon_{\vec{k},x_{yz},\sigma} c_{\vec{k},x_{yz},\sigma} + H.c. \right) \]

\[ + \eta \sum_{m,n,\sigma\sigma'} \sum_{\vec{k}} \left( \epsilon_{\vec{k},m,\sigma}^\dagger c_{\vec{k},n,\sigma'} \vec{t}_{mn} \cdot \vec{\sigma}_{\sigma\sigma'} \right). \]

The angular momentum operators and spin operators are
represented in terms of the totally antisymmetric tensor
$\epsilon_{mn} = i \epsilon_{ann}$ and Pauli matrices $\vec{\sigma}$, respectively. For the
system we are interested in, the strengths of the mixing
and spin-orbit coupling are $t'' = 0.1t$ and $\eta = 0.1t$, respec-
tively [24,25].

When the above perturbation $\delta H$ is taken into account,
the kinetic energy term becomes $H_{\text{kin}}^\alpha = H_0^{\alpha} + \delta H$, and the quasiparticle spectrum opens a gap $2\Delta$ near ($\pm k_F, \pm k_F$) with $\lambda = \sqrt{3(t''/2)^2 + \eta^2}$. Therefore, the dispersion
for the $d_{xz}$ orbital is modified to

\[ \epsilon_{\vec{k},x_z} = v_F |k_z| - k_F \mp \text{sgn}(k_z) L(|k_z|) \lambda, \]

with $L(x)$ the Lorentzian function centered at $k_F$. The bare
spin susceptibility or the SDW response function of $H_{\text{kin}}^{\alpha}$
for both $d_{xz}$ and $d_{yz}$ orbitals is found to be

\[ \chi_{\text{bare}}^\alpha(\vec{q}, T) = \frac{1}{\pi v_F} \left[ \ln \frac{4T}{E_0 + 2\lambda} + \int_0^\infty \ln \left( \frac{x + \lambda}{2\lambda} \right) \text{sech}^2 x dx \right]. \]

with $\vec{q} = (2k_F, q_y)$ and $(q_x, 2k_F)$ for $d_{xz}$ and $d_{yz}$ orbitals,
respectively, where we have set $h = 1$ and the lattice
spacing as the length unit. At low $T$ and in the limit $\lambda \ll E_0$, we have

\[ \chi_{\text{bare}}^\alpha(\vec{q}, T) \approx \frac{1}{\pi v_F} \ln \frac{T + 2\lambda}{E_0}. \]

A standard RG calculation, including particle-particle and
particle-hole graphs, gives the dressed susceptibility when
intraorbital interactions $H_U$ are included,

\[ \chi_{\text{RG}}^\alpha(\vec{q}, T) = \frac{1}{\pi v_F \theta^*} \left( \frac{E_0}{T + 2\lambda} \right)^{\theta^*}. \]

From the expression above, one can see that due to the
hopping between the two orbitals, a finite low-energy
cutoff $\lambda$ appears, killing the divergence as $T \to 0$.

Next, we introduce the interorbital interactions between
the two $4d$ orbitals [19]
\[ H_I = \sum_{i,m<n,\sigma} \{ [U' n_{im\sigma} n_{i'n\sigma}] + (U' - J_H) n_{im\sigma} n_{i'n\sigma} \] 
\[ - J_{Hc} c_{im\sigma}^\dagger c_{i'n\sigma}^\dagger c_{in\sigma} c_{i'm\sigma} \} - J_H [c_{im}^\dagger c_{i'n\sigma}^\dagger n_{i'm\sigma}^\dagger + H.c.], \] (8)

with \( U' \) the interorbital Coulomb repulsion and \( J_H \) the Hund’s rule coupling.

To incorporate the interorbital interactions, we define the joint SDW response function by including the orbital indices \( m \),

\[ \chi_H(\vec{q}, i\Omega) = -i \int_0^\beta e^{i\Omega\tau} \langle T_\tau \mathcal{O}(\vec{q}, \tau) \mathcal{O}^\dagger(\vec{q}, 0) \rangle dt, \] (9)

where

\[ \mathcal{O}(\vec{q}, \tau) = \frac{1}{N} \sum_{k,m} [c_{k,m\uparrow}(\tau) c_{k+\vec{q},m\downarrow}(\tau) - c_{k,m\downarrow}(\tau) c_{k+\vec{q},m\uparrow}(\tau)], \] (10)

with \( N \) the total number of sites and \( \vec{q} = (2k_F, q_y) \) and \( (q_x, 2k_F) \) for \( d_{xz} \) and \( d_{yz} \) orbitals, respectively.

To first order in the interorbital interactions, the only nonvanishing term is

\[ J_H \frac{T^2}{N^2} \sum_{\vec{k},\vec{k}',\omega_n,i\omega_n} G_{xz}(\vec{k} + \vec{Q}, i\omega_n + i\Omega) G_{xz}(\vec{k}, i\omega_n) \] 
\[ \times G_{xz}(\vec{k}', i\omega_n + i\Omega) G_{xz}(\vec{k}', i\omega_n), \] (11)

with a corresponding diagram shown in Fig. 2(a). Note that the wave vector for the response function \( \vec{Q} = (2k_F, 2k_F) \) is the same for both \( d_{xz} \) and \( d_{yz} \) orbitals due to the conservation of momentum in the scattering process in Fig. 2(a). Another important consequence is that only the Hund’s rule coupling contributes to the SDW response function, while other on-site interaction terms in Eq. (8) are not involved. This result originates from the spin configuration in Fig. 2(a). In this sense, the Hund’s rule coupling assists the spin-flip processes between different orbitals. An intuitive physical picture is that the spin-flip processes are coherent even in different orbitals, due to the ferromagnetic Hund’s rule coupling between the two orbitals. Dynamical mean-field theory found that the Hund’s rule coupling is important in \( \text{Sr}_2\text{RuO}_4 \) [19]. In our calculations below we use Gutzwiller renormalized values of \( J_H = 0.13 \) eV to take into account the strong on-site repulsion between holes [26].

The full dressed joint SDW response function in Eq. (9) is obtained by first including the intraorbital interaction \( U \) in an RG scheme, which means that the bare bubbles in Fig. 2(a) are replaced with the dressed ones in Eq. (7). However, due to the 2D perpendicular scattering nature of the Hund’s rule coupling term, \( J_H \) can be treated in an RPA-like method, leading to

\[ \chi_H(\vec{Q}, T) = \frac{2\chi_{RG}(\vec{Q}, T)}{1 - J_H^2 \chi_{RG}(\vec{Q}, T)}, \] (12)

The divergence of \( \chi_H(\vec{Q}, T) \) in Eq. (12) gives an estimate of the mean-field transition temperature to long-range SDW order,

\[ T_c^{\text{SDW}} = E_0 \left( \frac{J_H}{2\pi v_F} \right)^{1/\theta'} - 2\lambda. \] (13)

The first term gives an upper limit on \( T_c^{\text{SDW}} \) due to the Hund’s rule coupling, which is about 50 K, similar to \( T_{3D} \). The presence of the second term, of order \( 10^3 \) K, guarantees that the ground state is paramagnetic. To illustrate the underlying physics, we construct the phase diagram in the \( J_H - \lambda \) parameter space as shown in Fig. 2(b). The parameter set for \( \text{Sr}_2\text{RuO}_4 \) is in the paramagnetic region, but near the phase boundary to SDW order. Therefore, the strongly enhanced response function generated by Hund’s rule coupling at \( \vec{Q} \) naturally explains the strong enhancement of the SDW signal near \( \vec{Q} \) in the experiments [11].
Next, we briefly comment on how interchain tunneling between parallel chains affects the SDW in the quasi-1D 
(\alpha, \beta) bands of Sr₂RuO₄. The interchain hopping \(t_\perp\) alone would give rise to a singular SDW response function at the
wave vector \((2k_F, \pi)\) since the tight-binding approximation preserves the perfect nesting for quasi-1D systems [21,27]. However, in the case of Sr₂RuO₄, the Fermi surfaces of the \((\alpha, \beta)\) bands are distorted due to hybridization and spin-orbit coupling between orbitals, as discussed previously. Therefore, the nesting property at \((2k_F, \pi)\) is lost, and a strong enhancement for the SDW fluctuation is not expected.

Another mechanism to affect the SDW response function at \((2k_F, \pi)\) is the superexchange interaction \(J_{\text{ex}} = 4t_\perp^2/U\) between two neighboring parallel chains. But a rough estimation yields \(J_{\text{ex}} \ll J_H\) since \(t_\perp\) is only about 0.026 eV [2]. Combining the above two effects for the parallel chains, the spin fluctuation response at \((2k_F, \pi)\) should be much weaker than that at \((2k_F, 2k_F)\), as observed in the experiment [13].

Finally, we consider the effects that follow from SC pairing order in 1D bands on the magnetic response. In Sr₂RuO₄, there is a crossover to 3D Fermi liquid with enhanced SDW fluctuations from \((\alpha, \beta)\) bands, which we do not treat in detail here. But the transition to the ordered SC state at \(T_c = 1.5\) K can be treated in mean field, and if the \((\alpha, \beta)\) bands are the active bands, this should be observable in neutron scattering experiments. Early measurements did not find a change in the magnetic response at \(\tilde{Q}\) upon cooling through the SC transition at \(T_c\) [11].

To make our analysis more transparent, we restrict the discussion to one dimension and, thus, consider the following Hamiltonian \(H = H_{\text{SC}} + H_{\text{int}}\), where \(H_{\text{int}} = U \sum_i n_i \sum_j \) is the Hubbard on-site interaction term, which can be reduced to the standard form describing different scattering processes with \(g_1 = g_2 = U/\pi v_F\) [21,28], and \(H_{\text{SC}}\) is to incorporate the SC pairing,

\[
H_{\text{SC}} = \sum_{k,\sigma} v_F([k] - k_F)c_{k\sigma}^\dagger c_{k\sigma} + \sum_k [\Delta(k)c_{k\uparrow}^\dagger c_{-k\downarrow} + \text{H.c.}],
\]

which models 1D electrons with \(p\)-wave SC pairing \(\Delta(k)\) and can be solved in the mean-field approximation. We assume that the mean-field results are stabilized via the interchain couplings. The assumption spin-orbit coupling locks the \(\tilde{d}\) vector along the crystal \(c\) axis has been made, consistent with the polarized neutron scattering experiment in Sr₂RuO₄ [29]. While there is a crossover to 3D Fermi liquid above the SC transition temperature in experiment, here our aim is to show the effect of SC order on the SDW fluctuations by using a quasi-1D model.

In Nambu’s spinor representation, the normal and anomalous Green’s functions are given by [30]

\[
G_{\sigma'\sigma}(k, i\omega_n) = -\delta_{\sigma'\sigma} - \frac{i\omega_n + \xi_k}{\omega_n^2 + \xi_k^2 + \Delta_0^2}
\]

and

\[
F_{\sigma'\sigma}(k, i\omega_n) = \frac{\Delta_{\sigma'\sigma}(k)}{\omega_n^2 + \xi_k^2 + \Delta_0^2}.
\]

Here, \(\xi_k = v_F([k] - k_F)\) and \(\Delta_{\sigma'\sigma}(k) = \Delta(k)\sigma_2\sigma\). Near the Fermi surface, we have, due to the odd parity, \(\Delta(k) = \text{sgn}(k)\Delta_0\), with \(\Delta_0\) the SC gap near the Fermi surface. The calculation of SDW response function in the SC state is straightforward. It is interesting that the contributions from the particle-particle and particle-hole diagrams cancel each other, similar to the case in the Luttinger liquid case. The particle-hole bubble diagram can be expressed as

\[
\frac{T}{N} \sum_{k,\omega_n} G_{\parallel}(k, i\omega_n)G_{\parallel}(k + 2k_F, i\omega_n + i\Omega) - F_{\parallel}(k, i\omega_n)F_{\parallel}(k + 2k_F, i\omega_n + i\Omega).
\]

FIG. 3 (color online). (Upper panels) Structure of the vertex diagrams. (a) and (b) are for the particle-particle channel, whereas (c) and (d) are for the particle-hole channel. The solid and dashed lines correspond to electrons belonging to the branches containing \(+k_F\) and \(-k_F\) in the one-dimensional model, respectively. The wavy lines stand for bare on-site interactions. (Lower panel) Response function as a function of \(\omega\) at \(T = 0\) is shown in (e). Here, \(\chi_{\parallel\parallel}^{\text{SC}}(2k_F, \omega)\) is scaled by \(\chi_{\parallel\parallel}^{\text{RG}}(2k_F, \omega = 0)\), and \(\theta^*\) is about 0.41 in the system of interest.
To the leading order in the logarithmic accuracy, this expression is reduced to

$$\frac{1}{2\pi v_F} \left[ \ln \sqrt{\omega^2 - 4\Delta_0^2} - i\frac{\pi}{2} \Theta(\omega - 2\Delta_0) \right],$$

(18)

with $\Theta(x)$ the Heaviside function, and we have performed an analytic continuation to real frequency $\omega$ at zero temperature. The structure of this expression is also similar to its counterpart in the normal state. Because of this analogy, the RG flow equations for the interaction constants $g_1$ and $g_2$ should be the same as those for the non-SC case [21,28]. Therefore, in the case of $\theta^* > 0$, the SDW fluctuation is expected as usual.

A standard RG analysis yields the final results for the SDW response function in the SC state as follows:

$$\text{Re}_{\text{RG}}^{\text{SC}}(2k_F, \omega) = \frac{1}{\pi v_F \theta^*} \left( \frac{E_0}{\sqrt{\omega^2 - 4\Delta_0^2}} \right)^{\theta^*},$$

$$\text{Im}_{\text{RG}}^{\text{SC}}(2k_F, \omega) = \frac{\Theta(\omega - 2\Delta_0)}{2v_F} \left( \frac{E_0}{\sqrt{\omega^2 - 4\Delta_0^2}} \right)^{\theta^*},$$

(19)

As shown in Fig. 3(e), if one looks at the low-energy properties $\omega \to 2\Delta_0$, the response function diverge as $\chi \sim |\omega - 2\Delta_0|^{-\theta^*/2}$. This result indicates that the transition to superconductivity in the 1D bands will open a gap in the low-energy spectra at wave vector $Q$. While early neutron scattering experiments by Braden et al. [11] did not show a change in low-energy spectra at $Q$, a more complete investigation would be worthwhile to definitively decide if an SC gap opens up in the 1D ($\alpha$, $\beta$) bands at the onset of superconductivity at $T_c^\ast$.

In summary, we have applied an RG scheme starting from the 1D analysis for single chains to explain the strong SDW fluctuations and the absence of SDW order at temperatures above the crossover to 3D Fermi liquid behavior with the strong on-site Hubbard repulsion estimated for $\text{Sr}_2 \text{RuO}_4$. The mutual exclusion in the 1D RG theory of enhancement in the SDW and simultaneously in the $p$-wave pairing channel is in favor of the 2D $\gamma$ band as the source of the superconductivity.

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[12] This wave vector is equivalent to $(4\pi/3, 4\pi/3)$ in the electron notion.
[26] The effect of strong on-site repulsion suppresses the probability of having two electrons from distinct orbitals at the same site to be 1/3. Thus, $J_H$ is reduced by a Gutzwiller factor of 1/3, compared with the bare value $J_H = 0.4$ eV in Ref. [19].