Spin Density Wave Fluctuations and p-Wave Pairing in Sr_2RuO_4

Jia-Wei Huo,[1] T. M. Rice,[2,1] and Fu-Chun Zhang[1,3]

[1]Department of Physics and Centre of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong SAR, China
[2]Institut für Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland
[3]Department of Physics, Zhejiang University, Hangzhou 310027, China

(Received 16 January 2013; published 18 April 2013)

Recently, a debate has arisen over which of the two distinct parts of the Fermi surface of Sr_2RuO_4 is the active part for the chiral p-wave superconductivity exhibited. Early theories proposed p-wave pairing on the two-dimensional γ band, whereas a recent proposal focuses on the one-dimensional (α, β) bands whose nesting pockets are the source of the strong incommensurate spin density wave (SDW) fluctuations. We apply a renormalization group theory to study quasi-one-dimensional repulsive Hubbard chains and explain the form of SDW fluctuations, reconciling the absence of long-range order with their nesting Fermi surface. The mutual exclusion of p-wave pairing and SDW fluctuations in repulsive Hubbard chains favors the assignment of the two-dimensional γ band as the source of p-wave pairing.

DOI: 10.1103/PhysRevLett.110.167003 PACS numbers: 74.70.Pq, 74.20.Mn, 75.30.Fv

Sr_2RuO_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 4d bands, a two-dimensional (2D) γ band, mainly a d_{xy} orbital, and a pair of quasi-1D (α, β) 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 γ band. The 2D scenario predicts a chiral p-wave paring 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_2RuO_4 is the strong spin density wave (SDW) fluctuations at an incommensurate nesting wave vector spanning the Fermi surfaces of the 4/3 filled (α, β) 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 $T_{3D} \approx 60$ K [11] when the resistivity starts to show a T^2 behavior [14]. Smaller peaks were observed at the wave vectors (π, $2\pi/3$) and ($2\pi/3$, π). To date, these have been discussed within a random phase approximation (RPA) scheme [15–18]. Because of the highly nesting character of the (α, β) 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 (α, β) 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_2RuO_4. Furthermore, our RG scheme shows mutual exclusion of p-wave pairing and

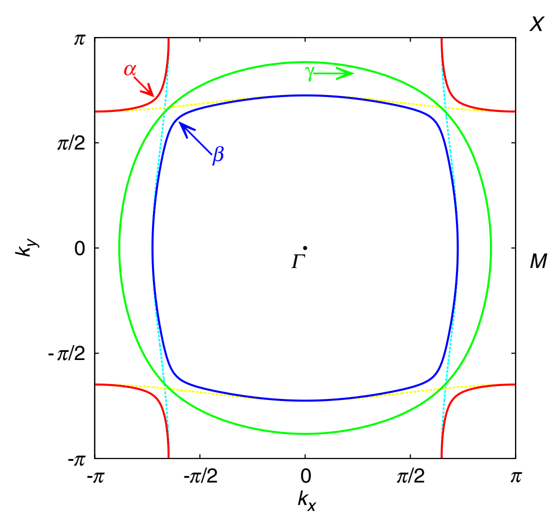

FIG. 1 (color online). Fermi surfaces of Sr_2RuO_4 (solid lines). The quasi-1D (α, β) bands are derived from the d_{xz} and d_{yz} orbitals (dashed lines).

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 experiments, 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 (α, β) bands by neglecting the γ band,

$$\begin{aligned} H_0 &= H^0_{\rm kin} + H_U, \\ H^0_{\rm kin} &= \sum_{m\vec{k}\sigma} \epsilon_{m\vec{k}} c^\dagger_{\vec{k}m\sigma} c_{\vec{k}m\sigma}, \\ H_U &= U \sum_{im} n_{im\uparrow} n_{im\downarrow}. \end{aligned} \tag{1}$$

In the above equations, $\epsilon_{xz(yz),\vec{k}} = v_F(|k_{x(y)}| - k_F)$ with v_F the Fermi velocity and k_F the Fermi wave vector, $c_{\vec{k},m,\sigma}$ is the electron annihilation operator with orbital $m = d_{xz}, d_{yz}$ and momentum $\vec{k}$ and spin σ. H_U is the Hubbard term for the on-site intraorbital interaction and $n_{im\sigma} = c^\dagger_{im\sigma} c_{im\sigma}$. 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 θ changes sign. In the one-loop approximation, $\theta = g_2 - g_1/2$, where g_1 (g_2) is the dimensionless 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

$$\chi^0_{\rm RG}(\vec{q}, T) = \frac{1}{\pi v_F \theta}\left(\frac{E_0}{T}\right)^\theta, \tag{2}$$

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 corresponds to a large temperature (up to 10^3 K) in Sr_2RuO_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 θ is screened to be 0.6θ, which we denote as θ^* from now on.

To have a better modeling for Sr_2RuO_4, we examine the effects on the SDW fluctuations arising from (1) the hybridization and spin-orbit coupling between the two orbitals 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 $H^0_{\rm kin}$ [5]

$$\begin{aligned} \delta H = &\sum_{\vec{k},\sigma}(-2t'' \sin k_x \sin k_y c^\dagger_{\vec{k},xz,\sigma} c_{\vec{k},yz,\sigma} + \text{H.c.}) \\ &+ \eta \sum_{m,n}\sum_{\sigma\sigma'}\sum_{\vec{k}} c^\dagger_{\vec{k},m,\sigma} c_{\vec{k},n,\sigma'} \vec{\ell}_{mn} \cdot \vec{\sigma}_{\sigma\sigma'}. \end{aligned} \tag{3}$$

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

When the above perturbation δH is taken into account, the kinetic energy term becomes $H^\lambda_{\rm kin} = H^0_{\rm kin} + \delta H$, and the quasiparticle spectrum opens a gap 2λ near ($\pm k_F$, $\pm k_F$) with $\lambda = \sqrt{(3t''/2)^2 + \eta^2}$. Therefore, the dispersion for the d_{xz} orbital is modified to

$$\epsilon'_{xz,\vec{k}} \approx v_F(|k_x| - k_F) + \text{sgn}(|k_x| - k_F) L(|k_y|)\lambda, \tag{4}$$

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

$$\begin{aligned} \chi^\lambda_{\rm bare}(\vec{q}, T) = \frac{1}{\pi v_F}\Bigg[&\ln\frac{4T}{E_0 + 2\lambda} \\ &+ \int_0^\infty \ln\left(x + \frac{\lambda}{2T}\right)\text{sech}^2 x dx\Bigg], \end{aligned} \tag{5}$$

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

$$\chi^\lambda_{\rm bare}(\vec{q}, T) \approx \frac{1}{\pi v_F} \ln\frac{T + 2\lambda}{E_0}. \tag{6}$$

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

$$\chi^\lambda_{\rm RG}(\vec{q}, T) = \frac{1}{\pi v_F \theta^*}\left(\frac{E_0}{T + 2\lambda}\right)^{\theta^*}. \tag{7}$$

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

Next, we introduce the interorbital interactions between the two $4d$ orbitals [19]

$$H_I = \sum_{i,m<n,\sigma} \{[U' n_{im\sigma} n_{in\bar{\sigma}} + (U' - J_H) n_{im\sigma} n_{in\sigma} - J_H c^\dagger_{im\sigma} c_{im\bar{\sigma}} c^\dagger_{in\bar{\sigma}} c_{in\sigma}] - J_H [c^\dagger_{im\uparrow} c^\dagger_{im\downarrow} c_{in\uparrow} c_{in\downarrow} + \mathrm{H.c.}]\}, \tag{8}$$

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,

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

where

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

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

$$J_H \frac{T^2}{N^2} \sum_{\vec{k},\vec{k}',i\omega_n,i\omega'_n} G_{xz}(\vec{k} + \vec{Q}, i\omega_n + i\Omega) G_{xz}(\vec{k}, i\omega_n) \times G_{yz}(\vec{k}' + \vec{Q}, i\omega'_n + i\Omega) G_{yz}(\vec{k}', i\omega'_n), \tag{11}$$

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 the ferromagnetic Hund's rule coupling between the two orbitals. Dynamical mean-field theory found that the Hund's rule coupling is important in Sr_2RuO_4 [19]. In our calculations below we use Gutzwiller renormalized values of $\tilde{J}_H \approx 0.13$ 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, $\tilde{J}_H$ can be treated in an RPA-like method, leading to

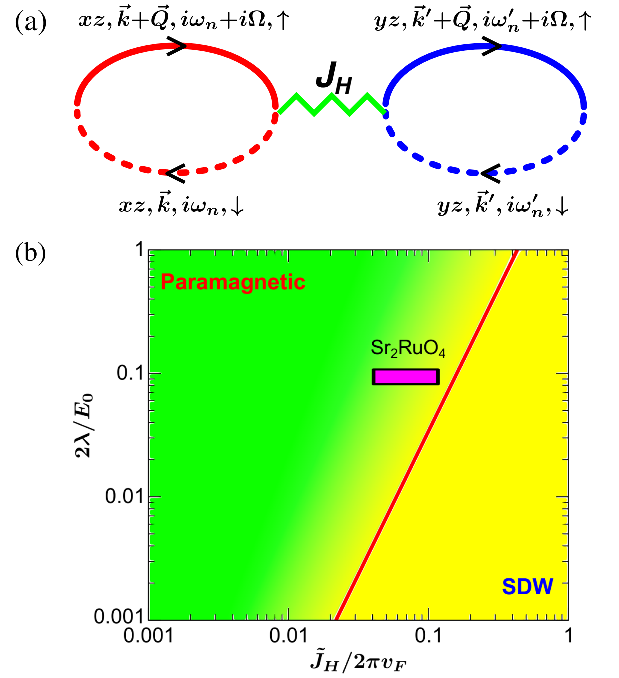

FIG. 2 (color online). (a) The lowest order Feynman diagram for the spin-spin correlation function connecting propagators from different orbitals via the Hund's rule coupling. The red and blue lines stand for electrons in the xz and yz orbitals, respectively. The solid and dashed lines correspond to electrons belonging to the branches containing $+k_F$ and $-k_F$ in the 1D model, respectively. Because of momentum conservation at the vertex, $\vec{Q}$ is locked to be $(2k_F, 2k_F)$. (b) SDW vs paramagnetic phase diagram in the parameter space of λ and $\tilde{J}_H$ at $T = 0$ from Eq. (13). The estimated parameter region for Sr_2RuO_4 is indicated in the paramagnetic phase. In this region, $\tilde{J}_H$ ranges from 0.13 to 0.4 eV, the renormalized and bare values of the Hund's rule coupling.

$$\chi_H(\vec{Q}, T) = \frac{2\chi^\lambda_{\mathrm{RG}}(\vec{Q}, T)}{1 - \frac{\tilde{J}_H}{2}\chi^\lambda_{\mathrm{RG}}(\vec{Q}, T)}. \tag{12}$$

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,

$$T_c^{\mathrm{SDW}} = E_0 \left(\frac{\tilde{J}_H}{2\pi v_F \theta^*}\right)^{1/\theta^*} - 2\lambda. \tag{13}$$

The first term gives an upper limit on T_c^{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 $\tilde{J}_H - \lambda$ parameter space as shown in Fig. 2(b). The parameter set for Sr_2RuO_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 (α, β) bands of Sr_2RuO_4. The interchain hopping $t_\perp$ alone would give rise to a singular SDW response function at the wave vector ($2k_F$, π) since the tight-binding approximation preserves the perfect nesting for quasi-1D systems [21,27]. However, in the case of Sr_2RuO_4, the Fermi surfaces of the (α, β) bands are distorted due to hybridization and spin-orbit coupling between orbitals, as discussed previously. Therefore, the nesting property at ($2k_F$, π) is lost, and a strong enhancement for the SDW fluctuation is not expected.

Another mechanism to affect the SDW response function at ($2k_F$, π) is the superexchange interaction $J_{\rm ex} = 4t_\perp^2/U$ between two neighboring parallel chains. But a rough estimation yields $J_{\rm ex} \ll J_H$, since $t_\perp$ is only about 0.026 eV [2]. Combining the above two effects for the parallel chains, the spin fluctuation response at ($2k_F$, π) 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 Sr_2RuO_4, there is a crossover to 3D Fermi liquid with enhanced SDW fluctuations from (α, β) bands, which we do not treat in detail here. But the transition to the ordered SC state at $T_c^s = 1.5$ K can be treated in mean field, and if the (α, β) 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 $\vec{Q}$ upon cooling through the SC transition at T_c^s [11].

To make our analysis more transparent, we restrict the discussion to one dimension and, thus, consider the following Hamiltonian $H = H_{\rm SC} + H_{\rm int}$, where $H_{\rm int} = U\sum_i n_{i\uparrow}n_{i\downarrow}$ 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 $H_{\rm SC}$ is to incorporate the SC pairing,

$$H_{\rm SC} = \sum_{k,\sigma} v_F(|k| - k_F)c_{k\sigma}^\dagger c_{k\sigma} + \sum_k [\Delta(k)c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \text{H.c.}], \tag{14}$$

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 that spin-orbit coupling locks the $\vec{d}$ vector along the crystal c axis has been made, consistent with the polarized neutron scattering experiment in Sr_2RuO_4 [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]

$$G_{\sigma\sigma'}(k, i\omega_n) = -\delta_{\sigma\sigma'}\frac{i\omega_n + \xi_k}{\omega_n^2 + \xi_k^2 + \Delta_0^2} \tag{15}$$

and

$$F_{\sigma\sigma'}(k, i\omega_n) = \frac{\mathbf{\Delta}_{\sigma\sigma'}(k)}{\omega_n^2 + \xi_k^2 + \Delta_0^2}. \tag{16}$$

Here, $\xi_k = v_F(|k| - k_F)$ and $\mathbf{\Delta}_{\sigma\sigma'}(k) = \Delta(k)\sigma_z i\sigma_y$. Near the Fermi surface, we have, due to the odd parity, $\Delta(k) = \text{sgn}(k)\Delta_0$, with Δ_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

$$\frac{T}{N}\sum_{k,i\omega_n} G_{\uparrow\uparrow}(k, i\omega_n)G_{\downarrow\downarrow}(k + 2k_F, i\omega_n + i\Omega) - F_{\uparrow\downarrow}(k, i\omega_n)F_{\downarrow\uparrow}^\dagger(k + 2k_F, i\omega_n + i\Omega). \tag{17}$$

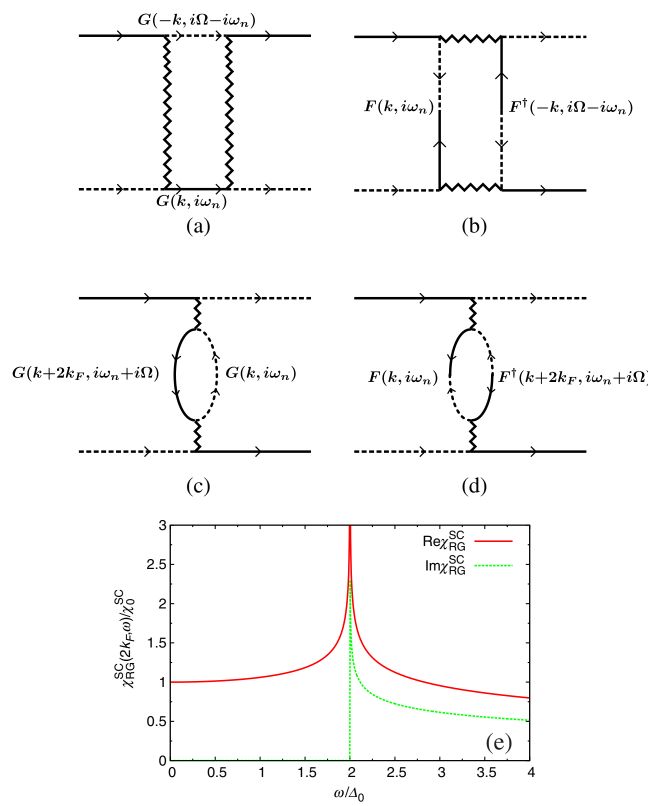

FIG. 3 (color online). (Upper panels) Structure of the vertex diagrams. (a) and (b) are for the particle-particle channel, whereas (c) and (d) are for the particle-hole channel. The solid and dashed lines correspond to electrons belonging to the branches containing $+k_F$ and $-k_F$ in the one-dimensional model, respectively. The wavy lines stand for bare on-site interactions. (Lower panel) Response function as a function of ω at $T = 0$ is shown in (e). Here, $\chi_{\rm RG}^{\rm SC}(2k_F, \omega)$ is scaled by $\chi_0^{\rm SC} \equiv \text{Re}\chi_{\rm RG}^{\rm SC}(2k_F, \omega = 0)$, and θ^* is about 0.41 in the system of interest.

To the leading order in the logarithmic accuracy, this expression is reduced to

$$\frac{1}{2\pi v_F}\left[\ln\frac{\sqrt{|\omega^2-4\Delta_0^2|}}{E_0}-i\frac{\pi}{2}\Theta(\omega-2\Delta_0)\right], \tag{18}$$

with $\Theta(x)$ the Heaviside function, and we have performed an analytic continuation to real frequency ω 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:

$$\begin{aligned}\mathrm{Re}\chi_{\mathrm{RG}}^{\mathrm{SC}}(2k_F,\omega) &= \frac{1}{\pi v_F\theta^*}\left(\frac{E_0}{\sqrt{|\omega^2-4\Delta_0^2|}}\right)^{\theta^*},\\ \mathrm{Im}\chi_{\mathrm{RG}}^{\mathrm{SC}}(2k_F,\omega) &= \frac{\Theta(\omega-2\Delta_0)}{2v_F}\left(\frac{E_0}{\sqrt{|\omega^2-4\Delta_0^2|}}\right)^{\theta^*}.\end{aligned} \tag{19}$$

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 $\vec{Q}$ [16,17]. While early neutron scattering experiments by Braden *et al.* [11] did not show a change in low-energy spectra at $\vec{Q}$, a more complete investigation would be worthwhile to definitively decide if an SC gap opens up in the 1D (α, β) bands at the onset of superconductivity at T_c^s.

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 Sr_2RuO_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 γ band as the source of the superconductivity.

We thank M. Sigrist for useful discussions. J.-W. H. and F.-C. Z. wish to thank S. Raghu for interesting and helpful discussions. This work is partly supported by Hong Kong's RGC Grant No. GRF HKU707211. T. M. R. acknowledges support from the Swiss Nationalfond.

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