Origin of the Non-Fermi Liquid Behavior of $SrRuO_3$

M. S. Laad and E. Müller-Hartmann
Institut für Theoretische Physik, Universität zu Köln, 77 Zülpicher Strasse, 50937 Köln, Germany

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Motivated by the unusual features observed in the transport properties of the ferromagnetic "bad metal" $SrRuO_3$, we construct a model incorporating essential features of the realistic structure of this nearly cubic material. In particular, we show how the t_{2g} orbital *orientation* in the perfectly cubic structure determines the peculiar structure of the hybridization matrix, and demonstrate how the local non-Fermi liquid features arise when interactions are switched on. We discuss the effects of the slight deviation from the cubic structure qualitatively. The model provides a consistent explanation of the features observed recently in the optical response of $SrRuO_3$.

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Strongly correlated electronic systems continue to present new surprises in condensed matter physics. In particular, d-electron systems exhibit fascinating phenomena, from unconventional high-T_c superconductivity to colossal magnetoresistance [1]. These dramatic behaviors are believed to be associated with the fact that the important electronic states are often intermediate between the itinerant and localized limits, necessitating the development of new ideas [2].

Ruthenates constitute a class of d-band oxides occurring in both layered [3,4] as well as nearly cubic forms. The electronic states responsible for both conduction and magnetism (or superconductivity) are associated with bands which involve Ru-4d orbitals hybridized with the O-2p states. The cubic material $SrRuO_3$ exhibits a transition from a high-T paramagnetic metallic to a ferromagnetic metallic state below $T_c^{\mathrm{FM}} = 150$ K [5]. State-of-the-art band structure calculations do produce this basic feature [6]. However, photoemission [7] measurements reveal a much reduced spectral density at the Fermi surface, compared to the results from a band structure calculation. Moreover, the authors of [7] do not observe a clear separation between the "coherent" and incoherent parts of the spectral function, suggesting that the low-energy spectral weight may have a significant incoherent contribution. Actually, the low-energy line shape looks incoherent, in contrast to the inverse photoemission spectra, where a coherent part is clearly visible [7]. The mass enhancement factor deduced from this is in excellent agreement with that extracted from the low-T specific heat, showing the importance of correlation effects. More unusual features are observed in transport studies. At low T, a resistivity minimum is observed even as the resistivity itself is very low [8–10]. At higher $T > T_c^{\mathrm{FM}}$, $\rho_{\mathrm{dc}}(T)$ increases linearly with T, passing through the Ioffe-Regel limit [8] without saturation. It exhibits a kink at T_c^{FM} and continues to increase up to 1000 K. In other words, one is dealing with a situation where $k_F l \simeq 1$ (already for $T \simeq 500$ K), suggesting the inapplicability of Boltzmann equation approaches for transport. In fact, this similarity with other "bad metals," as well as with dilute ferromagnetic alloys [8], suggests that a local picture (as opposed to a band description) for transport is required for $SrRuO_3$. Near T_c^{FM}, anomalous critical behavior in $\rho_{\mathrm{dc}}(T)$ has been found by Klein *et al.* [10]. That this is not related to magnetic critical behavior is shown by the fact that the magnetization data are well fit with conventional universal critical exponents. This line of thinking is further reinforced by a recent study [10] probing the deviations from Matthiessen's rule (DMR) in $SrRuO_3$ and $CaRuO_3$. The latter is not a ferromagnet down to the lowest temperatures. Interestingly, however, the similarity in the radiation-induced change in the resistivity for *both* samples indicates that the observed DMR is not caused by magnetic ordering. More recently, Kostic *et al.* [11] have studied the infrared conductivity of $SrRuO_3$ from 50 cm^{-1} to 40 000 cm^{-1} at temperatures ranging from 40 to 300 K. Quite astonishingly, $\sigma(\omega) \simeq \omega^{-\alpha}$ with $\alpha = 1/2$ deep into the ferromagnetic phase ($T = 40$ K) instead of the ω^{-2} form characteristic of Fermi liquids. This form is close to the phenomenological fit used for doped cuprates [12]. Motivated by the strong correlation features observed experimentally, Ahn *et al.* [13] attempted to model the optical spectrum in terms of the response of a one-band Hubbard model in $d = \infty$. However, the low-T response in the $d = \infty$ Hubbard model is that of a correlated Fermi liquid, and Ahn *et al.* themselves point out the importance of extra scattering mechanisms to understand the non-FL (Fermi liquid) falloff in $\sigma(\omega)$. In particular, they speculate that factors like the p-d hybridization and its interplay with Mott-Hubbard physics might provide some insight into the physics of ruthenates.

Given the similarity in their optical response, one is tempted to look for a possible explanation in terms of theories proposed to understand the non-FL metallic phase of cuprates. In sharp contrast to the cuprates, however, $SrRuO_3$ is not close to any quantum critical point. There are no antiferromagnetic spin fluctuations, and neither does it undergo a Mott transition. Actually, it is not clear whether $SrRuO_3$ is close to a Mott transition. The ferromagnetic spin fluctuations cannot be the cause of the non-FL features, since these features are observed well below T_c^{FM}. The scattering rate extracted from an extended "Drude" fit increases *linearly* with frequency, and remains high above T_c^{FM}. At high $T > T_c^{\mathrm{FM}}$, $\sigma(\omega)$ even appears to increase with frequency in the far infrared, reminiscent of strongly disordered systems. However, the nature of such strong scattering and, in particular, its microscopic origin, is completely unclear, given that this system has negligible extrinsic disorder [8]. One is led, therefore, to search for the origin of the (intrinsic) strong scattering in the peculiarities of the material itself.

A proper understanding of the anomalies should, in the final analysis, be linked to the peculiarities in the local quantum chemistry (or the basic electronic structure) of this material. In this connection, it is interesting to notice that Cox *et al.* [14] have reported *three* flat bands crossing the Fermi surface: one e_g band between Γ and X, and two t_{2g} bands between the X and M points in the Brillouin zone. The microscopic origin of these features are, however, obscured in the numerics.

The appearance of a ferromagnetic metallic state at low T in SrRuO$_3$ is understood as follows. In SrRuO$_3$, the crystal field breaks the first Hund's rule, and the four Ru d electrons then partially fill the t_{2g} states, giving rise to a local spin $S = 1$ at each site, consistent with the measured magnetization ($M \simeq 1\mu_B$) at low T. The t_{2g}^4 configuration implies a threefold orbital degeneracy since the fourth electron can go into any of the three t_{2g} orbitals. If this were the whole story (i.e., if we ignored the O-$2p$ bands), one would expect SrRuO$_3$ to be a $S = 1$, antiferromagnetic Mott insulator (probably with some kind of orbital ordering). We claim that this orbital degeneracy in the perfectly cubic system is the origin of the strong intrinsic scattering observed experimentally (see below). Band structure calculations [14] as well as photoemission measurements, however, point to the important role of self-doping in this material, introducing a small concentration of holes into the O-$2p$ band via charge transfer processes, which put a small concentration of additional electrons into the t_{2g} orbitals. The Ru $4d_{xy,yz,zx}$-O $2p$ hybridization then drives the resulting mixed-valent system metallic and ferromagnetic via the double-exchange mechanism.

The spin-orbit coupling in SrRuO$_3$ is estimated to be of order 0.4 eV. The analysis here requires some care, because the spin-orbit interaction in the $4d$ shell is usually antiferromagnetic: $H_{\mathrm{so}} = \lambda \mathbf{L} \cdot \mathbf{S}$. In the t_{2g} sector relevant for the ruthenates, however, the angular momentum operator $\mathbf{L}$ with magnitude 1 has, except for the reversed sign, the same matrix elements among the eigenfunctions xy, yz, zx as a fictitious angular momentum $\tilde{\mathbf{l}} = 1$, i.e., $\mathbf{L} = g_l \tilde{\mathbf{l}}$ with $g_l = -1$. Hence, $H_{\mathrm{so}} \simeq -\lambda \tilde{\mathbf{l}} \cdot \mathbf{S}$, so $\tilde{\mathbf{l}}$ couples *ferromagnetically* to the local spin $S = 1$. Since the magnetization operator is $\mathbf{M} = 2\mathbf{S} + g_l \tilde{\mathbf{l}}$, with $g_l = -1$, this leads to a twofold reduction in M ($= 2S - \tilde{l}$). However, we believe that the strong hybridization in concert with orbital frustration (see below) quenches the orbital moment in the solid. The situation is very similar to LaTiO$_3$, where strong hybridization in the t_{2g} sector leads to an orbital-liquid state [15]. This connection is made more transparent by observing that the minority-spin electron in the triply degenerate t_{2g}^4 configuration in SrRuO$_3$ is very similar to that of the single electron in a similar environment in LaTiO$_3$.

In what follows, we propose a microscopic model for SrRuO$_3$ which ties together (i) the local quantum chemistry, (ii) the relevant interactions, and (iii) the observed non-Fermi liquid anomalies within one approach. In particular, we show how the t_{2g} orbital orientation determines the peculiar structure of the hybridization matrix (see below), and how the non-FL behavior arises (within a single-impurity picture) when local Coulomb interactions are switched on.

We start by deriving the hybridization (Ru $4d_{xy,yz,zx}$-O $2p$) matrix for the nearly cubic structure of SrRuO$_3$. To begin with, we shall assume a perfect cubic structure, and consider the effects of the slight distortion later in the paper.

Considering the local orbital structure of the Ru-O octahedron, the relevant electronically active states involve the hybridization of the triply degenerate Ru-$4d_{xy,yz,zx}$ and O-$2p_{x,y,z}$ states. In this situation, the hopping part is written as

$$H_{\mathrm{hop}} = -t \sum_{\mathbf{l}\sigma} [d_{xy\mathbf{l}\sigma}^{\dagger} P_{\mathbf{l}\sigma} + \mathrm{c.t.} + \mathrm{H.c.}], \tag{1}$$

where $P_{\mathbf{l}\sigma} = (p_{y,\mathbf{l}+\mathbf{x}/2,\sigma} - p_{y,\mathbf{l}-\mathbf{x}/2,\sigma} + p_{x,\mathbf{l}+\mathbf{y}/2,\sigma} - p_{x,\mathbf{l}-\mathbf{y}/2,\sigma})$ and $p_{\alpha,\mathbf{l}\pm\beta/2}$ means the p_α orbital placed at the center of the bond(s) leaving site i in the $\pm\beta$ direction. In Eq. (1), c.t. (cyclic terms) means terms which arise by a cyclic permutation of x, y, z. Notice that the d_{xy} orbital *does not* hybridize with $p_{z,l\pm\alpha/2}$ and $p_{\alpha,l\pm z/2}$ ($\alpha = x, y$) because of symmetry reasons. It is precisely this peculiarity resulting from the local quantum chemistry of SrRuO$_3$ which, together with the orbital degeneracy mentioned above, is responsible for its anomalous behavior, as we show below.

The hopping part of the Hamiltonian Eq. (1) describes a planar hybridization of each of the t_{2g} $4d$ orbital of Ru with a hybridizing O-$2p$ (Wannier) orbital in close formal analogy to the $3d_{x^2-y^2}$-$2p_\sigma$ hybridization in the CuO$_2$ planes in cuprates.

In order to make the peculiarity mentioned above more transparent, we Fourier transform the hopping part (1), giving

$$H_{\mathrm{hop}}(t_{2g}) = -2it \sum_{\mathbf{k}\sigma} [d_{xy\mathbf{k}\sigma}^{\dagger}(s_x p_{yx\mathbf{k}\sigma} + s_y p_{xy\mathbf{k}\sigma}) + \mathrm{c.t.} + \mathrm{H.c.}], \tag{2}$$

using the short notations, $s_\alpha = \sin(k_\alpha/2)$ ($\alpha = x, y, z$), and defining the hybridizing (Wannier) orbitals, $w_{yz\mathbf{k}} = -i(s_y p_{zy\mathbf{k}} + s_z p_{yz\mathbf{k}})/f_{yz}$, $w_{xz\mathbf{k}} = -i(s_z p_{xz\mathbf{k}} + s_x p_{zx\mathbf{k}})/f_{zx}$, and $w_{xy\mathbf{k}} = -i(s_x p_{yx\mathbf{k}} + s_y p_{xy\mathbf{k}})/f_{xy}$. Writing $f_{\alpha\beta} = (s_\alpha^2 + s_\beta^2)^{1/2}$ and going back to the

Wannier representation we get, finally,

$$H_{\rm hop}(t_{2g}) = -t \sum_{\langle lm\rangle\sigma} [T_{yz}(m) d^{\dagger}_{yzl\sigma} w_{yz,l+m\sigma} + \text{c.t.} + \text{H.c.}], \tag{3}$$

with $T_{\alpha\beta}(m) = \langle 2(s_\alpha^2 + s_\beta^2)^{1/2} e^{i\mathbf{k}\cdot\mathbf{m}}\rangle_{\mathbf{k}}$. Thus, in the perfect cubic symmetry, the band structure is purely two dimensional in each direction solely as a consequence of the orbital *orientation*. This intrinsic frustration in the otherwise perfectly cubic structure leads to large quantum disorder and dynamically quenches the t_{2g} orbital moments in $\mathrm{SrRuO_3}$.

We now consider the interaction part of the Hamiltonian. The local, intraorbital Hubbard interaction is large, as can be seen from the satellite feature in photoemission being situated $\simeq 5$ eV below the Fermi energy. We can thus roughly estimate $U_{dd} \simeq 5$ eV (the results obtained below are insensitive to its actual value). The Hund's rule coupling is of the order of magnitude of the exchange splitting ($\simeq 0.5$ eV). The nearest neighbor Ru-O interaction, U_{pd}, can be estimated to be $U_{pd} \simeq (e^2/a\epsilon) \simeq 1.5$–$2$ eV. Setting $U_{dd} \to \infty$, we write the interaction term as [16]

$$H_{\rm int} = U_{pd} \sum_{\langle lm\rangle\sigma} n_{ld\sigma}(n^x_{l+m,w,\sigma'} + n^y_{l+m,w,\sigma'} + n^z_{l+m,w,\sigma'}). \tag{4}$$

Thus, the total Hamiltonian reads

$$H = H_{\rm hop}(t_{2g}) + H_{\rm int}. \tag{5}$$

The peculiar feature coming from the local quantum chemistry of $\mathrm{SrRuO_3}$ is now clear. The $w_{z\alpha}$ do not hybridize with the d_{xy} orbitals, but interact with a strength U_{pd}; $w_{x\alpha}$ do not hybridize with the d_{yz}, and the $w_{y\alpha}$ do not hybridize with the d_{zx}. Hence, for example, the term $U_{pd}\sum_{\langle lm\rangle\sigma} n_{ldxy\sigma} n^z_{l+m,w,\sigma'}$ provides a nonhybridizing (screening) channel that strongly scatters the w_z-band carriers. Within the impurity approximation, local non-Fermi liquid behavior [17] now arises from the competition of this term, which drives the system to a non-FL state characterized by x-ray edge singularities, and the hybridization, which would drive the system to a FL fixed point if the nonhybridizing channel were absent. The situation is somewhat reminiscent of the picture proposed in the context of marginal Fermi liquids in cuprates [17]. The origin of the local non-FL behavior is quite different, however, in our case. In what follows, we show that the true low-energy response is indeed power law in nature, as seems to be indicated by optical measurements.

Let us first consider the simplified situation when the screening channel (the term $U_{pd}\sum_{\langle lm\rangle\sigma} n_{ldxy\sigma} n^z_{l+m,w,\sigma'}$) is inoperative. In this case, the hybridization term drives the system to a local Fermi liquid fixed point, as is understood from the observation that t_{pd} is a relevant variable [17]. This problem can then be mapped onto the problem of quasiparticles hopping in an effective medium determined by a complex self-energy, $\Sigma(\omega)$, having the correct Fermi liquid form at low energy,

$$\Sigma_{w\alpha\beta}(\omega) = -(U_{pd}\rho_0)^2\left[\frac{4\omega}{\pi} + i\,\frac{\pi\rho_0}{2}(\omega^2 + \pi^2 T^2)\right], \tag{6}$$

so that the effective model *without* the screening channel can be written as

$$H^0_{\rm eff} = \sum_{k\sigma\alpha\beta} [\epsilon_{\alpha\beta}(\mathbf{k}) + \Sigma_{\alpha\beta}(\omega)] w^{\dagger}_{\alpha\beta\mathbf{k}\sigma} w_{\alpha\beta\mathbf{k}\sigma}. \tag{7}$$

Since $\Sigma_{w\alpha\beta}(\omega)$ has the FL form, we ignore it in what follows. The presence of the screening channel modifies the effective Hamiltonian, which now reads

$$H_{\rm eff} = H^0_{\rm eff} + U_{pd} \sum_{l\mathbf{k}\mathbf{k}',\alpha\beta\gamma\sigma\sigma'} n_{ld\alpha\beta\sigma} w^{\dagger}_{\gamma\mathbf{k}\sigma'} w_{\gamma\mathbf{k}'\sigma'},$$

where $\alpha\beta = xy, yz, zx$ in pairs, and $\gamma = z$, when $\alpha\beta = xy$, etc. This is recognizable as a model where the *absence* of the $d_{\alpha\beta} - w_\gamma$ hybridization results in x-ray edgelike singularity right at the Fermi surface, resulting in breakdown of Fermi liquid theory. We again emphasize that this strong scattering off the "localized" w_γ orbital results from the intrinsic feature of the quantum chemistry of $\mathrm{SrRuO_3}$, namely, from the orbital degeneracy in the t_{2g} sector and the peculiar structure of the hybridization matrix derived above, and is not related to extrinsic disorder-induced localization.

To obtain an analytic insight into the origin of the anomalous non-FL features in the optical response, we make some simplifications which will not qualitatively modify the conclusions. The dispersive band just below the Fermi level is approximated by $\epsilon_{\alpha\beta}(k) = A - Bk^2$ for small k. Furthermore, we assume that the lattice form factors are assumed constant, since they are expected to be smooth functions of k. The above approximations remove the dependence of two-particle quantities on k as well as on the orbital indices, and the problem is thereby transformed into that of a band of w electrons scattered locally by a localized d hole potential right at the Fermi surface. As is known [18], this problem is exactly soluble in the impurity limit; we work only in the metallic phase, and so choose a Lorentzian unperturbed density of states (DOS). As long as there is no band splitting, we expect this simplification to hold qualitatively. The w electron DOS is now given by [19]

$$\rho_w(\omega) = \frac{1 - n_d}{\omega^2 + D^2} + \frac{n_d}{(\omega - U_{pd})^2 + D^2}, \tag{8}$$

where D is the w bandwidth. The localized d-hole spectral function is [19]

$$\rho_d(\omega) \simeq (1 - n_w)\frac{\theta(\omega - \mu)}{|\omega - \mu|^{1-\eta}} + n_w \frac{\theta(\omega - U_{pd} - \mu)}{|\omega - U_{pd} - \mu|^{1-\eta}}, \tag{9}$$

where $\pi\eta = \tan^{-1}(\pi\rho_w(0)U_{pd})$ is the s-wave scattering phase shift of the w electrons. Here $\rho_w(0)$ is the density of states of the w fermions at the Fermi surface, and equals $1/D\pi$ for the Lorentzian used here. The optical response has contributions from both of the above. The most singular intraband contribution to $\sigma(\omega)$ results from $\rho_d(\omega)$ above. Indeed, by a simple scaling argument [20],

$$\sigma_{\text{intra}}(\omega) = \frac{\text{const}}{(i\omega)^{1-2\eta}}\,. \tag{10}$$

With a plausible ratio $U_{pd}/D \simeq 1$, we obtain $\eta = 1/4$ and the optical conductivity at small ω, $\sigma_{\text{intra}}(\omega) = C\omega^{-1/2}$ as indeed observed experimentally.

The above relation holds up to an upper energy cutoff of order of D. There is also a nonsingular contribution from the w-DOS at higher energies. It is obvious that this is very different from a FL-like description, where $\sigma(\omega) \simeq \omega^{-2}$.

The above holds for a perfectly cubic lattice. In practice, in $\mathrm{SrRuO_3}$, the lattice is slightly distorted from the perfect cubic structure. Given this, one expects that the threefold orbital degeneracy in the t_{2g} sector will be slightly lifted, and that the hybridization matrix will contain a small term corresponding to $d_{xy} - w_z$ hybridization. Indeed, we expect that the strict orthogonality of the $p_{x,y,z}$ orbitals in the perfect cubic structure is violated in the presence of a slight lattice distortion, resulting in a term $t'_{pd}\sum_{il\sigma}(d^{\dagger}_{ixy\sigma}p_{i+l/2,z\sigma} + \text{H.c.})$ in Eq. (1). This cuts off the infrared singularity by a low-energy quasicoherent scale related to t'_{pd}. At sufficiently low T (within the local approach), t'_{pd} will become relevant [21], making the system scale to a low-T FL fixed point. Given the small distortion observed in $\mathrm{SrRuO_3}$, we expect this scale to be quite small, consistent with the $T_0 < 40$ K [22] below which a T^2 component in the dc resistivity is indeed observed. A quantitative estimate of T_0 is, however, out of the scope of the present work.

Finally, we touch briefly on the difference between $\mathrm{SrRuO_3}$ and other cases where orbital degeneracy effects might be important. For example, in $\mathrm{SrVO_3}$, the deviation from the perfect cubic structure is larger than in the ruthenate [1]. In our modeling, this would lead to a larger recoil in the impurity problem, stabilizing correlated FL behavior over a wider T scale.

In conclusion, we have developed a model incorporating the basic local quantum chemical aspects of the structure of the nearly cubic ferromagnetic bad metal $\mathrm{SrRuO_3}$. We have pointed at the threefold degeneracy of the t_{2g}^4 configuration, as well as at the peculiar features in the hybridization matrix, whose structure is controlled by the orbital *orientation* in the t_{2g} sector, and is effectively two dimensional in the perfectly cubic structure. Finally, we have shown how a non-Fermi liquid metallic state is generated within an impurity picture when interactions are switched on, and argued how a small distortion cuts off the low-energy singularity, generating a low-energy coherence scale. The model explains the non-FL features observed in optical spectra in a consistent way.

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[1] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).

[2] A. Georges *et al.,* Rev. Mod. Phys. **68**, 13 (1996).

[3] Y. Maeno, Physica (Amsterdam) **282-287C**, 206 (1997).

[4] Tamio Oguchi, Phys. Rev. B **51**, 1385 (1995).

[5] C. B. Eom *et al.,* Science **258**, 1766 (1992).

[6] P. B. Allen *et al.,* Phys. Rev. B **53**, 4393 (1996).

[7] K. Fujioka *et al.,* Phys. Rev. B **56**, 6380 (1997).

[8] T. H. Geballe *et al.,* J. Phys. Condens. Matter **8**, 10 111 (1996).

[9] G. Cao *et al.,* Phys. Rev. B **56**, 321 (1997).

[10] L. Klein *et al.,* Phys. Rev. Lett. **77**, 2774 (1996).

[11] P. Kostic *et al.,* Phys. Rev. Lett. **81**, 2498 (1998).

[12] P. W. Anderson, Phys. Rev. B **55**, 11 785 (1997). See also D. van der Marel, Phys. Rev. B **60**, R765 (1999).

[13] J. S. Ahn *et al.,* Phys. Rev. Lett. **82**, 5321 (1999).

[14] P. A. Cox *et al.,* J. Phys. Condens. Matter **16**, 6221 (1983).

[15] G. Khaliullin and S. Maekawa, Phys. Rev. Lett. **85**, 3950 (2000).

[16] Terms like $U_{pd}\sum_{lmm'\sigma\sigma'\alpha\beta\gamma} n_{ld\sigma}w^{\dagger}_{l+m\sigma'}w_{l+m'\sigma'}$ will be generated in general. These have no qualitative effect on the discussion in the text, since they do not modify the main feature coming from competition of the hybridization and the presence of the screening channel in our model.

[17] See Ref. [2], and references therein, relating to the "solution" of the multiband Hubbard model with extra screening channels in $d = \infty$.

[18] G. M. Zhang and L. Yu, Phys. Rev. Lett. **81**, 4192 (1998).

[19] K. D. Schotte *et al.,* Phys. Rev. **182**, 479 (1968).

[20] P. W. Anderson, Phys. Rev. B **55**, 11 785 (1997).

[21] The effect of t'_{pd} is to block the singularity caused by strong scattering of the "light" p carriers by the "infinitely heavy" d hole (caused by $U_{pd}\sum_{\langle ij\rangle\sigma} n^{xy}_{id\sigma}n^{z}_{jp\sigma'}$); the problem then becomes equivalent to allowing the infinitely heavy d hole to acquire a heavy, but finite mass, leading to recoil and destruction of the low-energy singular features below a temperature (energy) scale related to t'_{pd}. See E. Müller-Hartmann *et al.,* Phys. Rev. B **3**, 1102 (1971).

[22] A. P. MacKenzie *et al.,* Phys. Rev. B **58**, R13 318 (1998).