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Hund's rule coupling as the microscopic origin of the spin-triplet pairing in a correlated and degenerate band system

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Abstract. We propose that the spin-triplet pairing can originate from the intraatomic Hund's rule exchange in a degenerate d-band system. The role of this interaction in the pairing is decisive when accounted for in conjunction with rather strong correlations induced by the direct Coulomb interactions. The superconducting-gap value is obtained in the saddle-point approximation for the Coulomb correlations, treated in the auxiliary Bose field approach, which is combined with the mean-field approximation of the BCS type for the pairing part.

The existence of an electronic counterpart of the spin-triplet superfluid ^{3}He has not been demonstrated as yet. The discovery of superconductivity in a strongly anisotropic system Sr_2RuO_4 [1] was followed by a conjecture [2] that this compound may provide an example such a system. This conjecture is supported by the fact that the three-dimensional analogue $SrRuO_3$ is an unusual metallic ferromagnet [2]. However, two specific features of those system should be emphasized. First, both the Ca_2RuO_4 and $Sr_2Ru_{1-x}Ir_xO_4$ are Mott insulators with the spin $S = 1$ [4]. On the other hand in the Sr_2RuO_4 system we encounter a large T^2 term in resistivity, the Korringa-type relaxation in the nmR and a relatively large linear specific heat coefficient γ. So, this system can be regarded as an almost localized Fermi liquid [5]. Second, from an electronic point of view the Ru^{4+} ion contains two holes in a triply degenerate t_{2g} state, which hybridizes with the $2p\pi^*$ states due to oxygen in the nominal $2p^6$ configuration. Hence, the orbital effects in conjunction with the intraatomic Hund's rule coupling determine the system properties. Therefore, a natural question arises and concerns the connection between the Hund's rule (ferromagnetic) coupling and the triplet pairing. This question bears a direct analogy to that relating the antiferromagnetic kinetic exchange interaction and the singlet pairing in high-T_c and heavy-fermion systems [6].

In this paper we propose a mechanism of spin-triplet pairing as originating from the intraatomic ferromagnetic (Hund's rule) coupling, which is furnished by the circumstance that the paired electrons can occupy locally different orbitals with quenched or zero orbital moment, so we can neglect the spin–orbit interaction. To make our argument transparent we consider here the simplest situation of a doubly degenerate band. It is easy to generalize the present results to an arbitrary degeneracy $D > 1$; the main restrictions are caused by the band filling and the magnitude of the correlations. Our model thus differs from the spin-fluctuation mechanism [7], as well as from that induced by the intersite Coulomb interaction [8], as it includes pairing by the local exchange interaction in real space, which takes place between rather strongly

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correlated electrons. We demonstrate that the paired state appears already on the saddle-point-approximation level; thus, the fluctuation-induced contribution can also be included as a higher order processes. We also show that the solution mediated by the intraatomic exchange leads in a straightforward manner to a nonstandard gap and, in particular, to the relation between the linear specific heat coefficients $\gamma_S \sim \gamma_N/2$ [9] for superconducting (S) and normal (N) phases. More importantly, the sizable value of critical temperature $T_S \approx 1$ K appears only when the band filling n is substantially greater than unity and less than half filling. Hence, the triplet pairing emerges when both the ferromagnetism with orbital ordering ($n \approx 1$) [10] or antiferromagnetism ($n \approx 2$) [11] become unstable. The results match roughly the band filling encountered in Sr_2RuO_4, where we have on average $(2/3)$ d holes per band per Ru atom.

We start from the simplest Hamiltonian for electrons in a $D = 2$-fold degenerate and correlated narrow band, which has the form

$$\mathcal{H} = \sum_{ijl\sigma} t_{ij} a^{\dagger}_{il\sigma} a_{jl\sigma} + U \sum_{il} n_{il\uparrow} n_{il\downarrow} + (U - J) \sum_{i} n_{i1} n_{i2} - 2J \sum_{i} (\boldsymbol{S}_{i1} \cdot \boldsymbol{S}_{i2} + \tfrac{3}{4} n_{i1} n_{i2}). \quad (1)$$

We have assumed that the hopping integrals t_{ij} are the same for both orbitals $l = 1, 2$. Also, the intraorbital Coulomb interaction is U, and the interorbital interaction has been taken as $U - J$, where $J > 0$ is the magnitude of the Hund's rule coupling. Both of these assumptions should not be crucial as we consider the physical quantities involving integration over the single-particle energies. To emphasize the physics of the problem we consider the equivalent (canonical) orbital model, since the generalization to the case of anisotropic band of e_g or t_{2g} symmetry does not pose any conceptual difficulty and will be dealt with separately.

The properties of the system characterized by (1) depend crucially on the magnitude of U and $J > 0$ (both parameters are taken relative to the bare bandwidth $W = 2z|t|$, where z is the number of nearest neighbours). The condition for the onset of ferromagnetism in the Hartree–Fock approximation has the form of the form of the Stoner criterion $U_{eff}\rho(\epsilon_F) = 1$, where $U_{eff} \equiv U + (D - 1)J$, with $D = 2$ and $\rho(\epsilon_F) \sim 1/W$ being the density of states at the Fermi energy, per atom per spin. However, in the correlated state the contribution to the system energy $\sim U$ is multiplied by the probability $d^2 \equiv \langle n_{il\uparrow} n_{il\downarrow} \rangle$ of encountering a double occupancy on the same orbital, whereas the negative contribution $\sim J$ is proportional to the local moment $m_0 \equiv \langle (\sum_l \boldsymbol{S}_{il})^2 \rangle$. With the growing ratios U/W and J/W the direct Coulomb correlations are suppressed ($d^2 \to 0$), whereas the local moment grows ($m_0 \to S(S + 1)$), (where $S = n/2$ is the total spin of aligned $n \leqslant D$ electrons). In effect, the local spin-triplet correlations induced by the Hund's rule become essential close to (but below) the Stoner threshold, since the exchange energy overcomes the direct Coulomb contribution. Thus, the Stoner criterion for the correlated state should be also modified, as discussed below.

The Hund's rule pairing is be expressed formally by the spin-triplet-pair-creation operators (acting on the vacuum state) defined as follows

$$A^{\dagger}_{i1} = a^{\dagger}_{i1\uparrow} a^{\dagger}_{i2\uparrow} \qquad A^{\dagger}_{i-1} = a^{\dagger}_{i1\downarrow} a^{\dagger}_{i2\downarrow} \qquad A^{\dagger}_{i0} = \frac{1}{\sqrt{2}} (a^{\dagger}_{i1\uparrow} a^{\dagger}_{i2\downarrow} + a^{\dagger}_{i1\downarrow} a^{\dagger}_{i2\uparrow}) \quad (2)$$

through which one can express the Hund's rule exchange part

$$\boldsymbol{S}_{i1} \cdot \boldsymbol{S}_{i2} + \tfrac{3}{4} n_{i1} n_{i2} = \sum_{m=-1}^{1} A^{\dagger}_{im} A_{im} \quad (3)$$

In this representation the interorbital correlations are included explicitly in the pairing.

The correlations are accounted for in the auxiliary- (slave-) boson scheme through the following characterization of the atomic states [12]:

$$|0\rangle = e^{\dagger}_i |v\rangle \qquad |l\sigma\rangle = p^{\dagger}_{il\sigma} f^{\dagger}_{il\sigma} |v\rangle \qquad |2l\rangle = d^{\dagger}_{il} f^{\dagger}_{il\uparrow} f^{\dagger}_{il\downarrow} |v\rangle$$

$$|2\sigma\bar{\sigma}\rangle = d^\dagger_{i\sigma} f^\dagger_{i1\sigma} f^\dagger_{i2\bar{\sigma}}|v\rangle \qquad |2\sigma\rangle = t^\dagger_{i\sigma} f^\dagger_{i1\sigma} f^\dagger_{i2\sigma}|v\rangle$$
$$|3l\sigma\rangle = s^\dagger_{il\sigma} f^\dagger_{il\sigma} f^\dagger_{i\bar{l}\uparrow} f^\dagger_{i\bar{l}\downarrow}|v\rangle \qquad |4\rangle = g^\dagger_i f^\dagger_{i1\uparrow} f^\dagger_{i1\downarrow} f^\dagger_{i2\uparrow} f^\dagger_{i2\downarrow}|v\rangle. \tag{4}$$

The notation is self-explanatory: the Bose fields label respectively empty (e), singly occupied ($p_{l\sigma}$), doubly occupied configurations on the same orbital (d_l), on different orbitals (d_σ) and equal-spin (t_σ) triplet states, as well as the triple (s_σ) and the quadruple (g) occupancies. Such formulation allows for a treatment of the dominant terms $\sim U$ beyond the Hartree–Fock (H–F) approximation, as the result reduces to those obtained in H–F scheme with both U and J substantially smaller than W. The Hund's rule pairing is associated with two electrons on different orbitals, therefore we must project out triple and quadruple occupancies from interaction (3) and leave the fermionic part for double occupancies. After some algebra we obtain explicitly:

$$A^\dagger_{im}A_{im} = t^\dagger_{i\sigma}t_{i\sigma}B^\dagger_{im}B_{im} + s^\dagger_{i1\sigma}s_{i1\sigma} + s^\dagger_{i2\sigma}s_{i2\sigma} + g^\dagger_i g_i$$
$$\text{for } (m,\sigma) = (1,\uparrow) \text{ or } (-1,\downarrow)$$
$$A^\dagger_{i0}A_{i0} = \tfrac{1}{2}(d^\dagger_{i\uparrow}d_{i\uparrow}n_{i1\uparrow}n_{i2\downarrow} + d^\dagger_{i\uparrow}d_{i\downarrow}S^+_{i1}S^-_{i2} + s^\dagger_{i1\uparrow}s_{i1\uparrow} + s^\dagger_{i2\downarrow}s_{i2\downarrow} + g^\dagger_i g_i)$$
$$+\tfrac{1}{2}(d^\dagger_{i\downarrow}d_{i\downarrow}n_{i1\downarrow}n_{i2\uparrow} + d^\dagger_{i\downarrow}d_{i\uparrow}S^-_{i1}S^+_{i2} + s^\dagger_{i1\downarrow}s_{i1\downarrow} + s^\dagger_{i2\uparrow}s_{i2\uparrow} + g^\dagger_i g_i) \tag{5}$$

where $n_{il\sigma} = f^\dagger_{il\sigma}f_{il\sigma}$, $S^\sigma_{il} = f^\dagger_{il\sigma}f_{il\bar{\sigma}}$, $B^\dagger_{i1} = f^\dagger_{i1\uparrow}f^\dagger_{i2\uparrow}$ etc. In addition to the above relations we have the constraints [12], which in the present notation have the form:

$$Q_{il\sigma} = p^\dagger_{il\sigma}p_{il\sigma} + d^\dagger_{il}d_{il} + t^\dagger_{i\sigma}t_{i\sigma} + d^\dagger_{i\sigma}d_{i\sigma} + \sum_\sigma s^\dagger_{i\bar{l}\sigma}s_{i\bar{l}\sigma} + s^\dagger_{il\sigma}s_{il\sigma} + g^\dagger_i g_i - f^\dagger_{il\sigma}f_{il\sigma} = 0 \tag{6}$$

$$R_i = e^\dagger_i e_i + \sum_{l\sigma} p^\dagger_{il\sigma}p_{il\sigma} + \sum_l d^\dagger_{il}d_{il} + \sum_\sigma (t^\dagger_{i\sigma}t_{i\sigma} + d^\dagger_{i\sigma}d_{i\sigma}) + \sum_{l\sigma} s^\dagger_{il\sigma}s_{il\sigma} + g^\dagger_i g_i - 1 = 0 \tag{7}$$

As a result, the effective starting Hamiltonian with inclusion of constraints (6) and (7) is defined as: $\mathcal{H} \to \mathcal{H} - \sum_{il\sigma}\lambda^{(1)}_{il\sigma}Q_{il\sigma} - \sum_i \lambda^{(0)}_i R_i - \mu\hat{N}_e$, where μ is the chemical potential for N_e fermions, $\hat{N}_e = \sum_{il\sigma}\hat{n}_{il\sigma}$ and $\lambda^{(0)}_i$ and $\lambda^{(1)}_{il\sigma}$ are the Lagrange multipliers.

A brief physical characterization of the formalism just introduced is in place. As is well known, the slave-boson approach in the case of the Hubbard model reproduces on one hand the main features of the Gutzwiller approach (see e.g. [20]), and on the other provides an interpolation between the Hartree–Fock and kinetic exchange limit, where it gives correctly the t^2/U contribution to the ground state energy in the mean-field approximation (see e.g. [19]). It also provides agreement with the principal results concerning the thermodynamics of the almost localized systems in the dynamic field approach (cf [16]). Therefore, the approach can be regarded as a good single-particle interpolative approach between the regimes of weakly and strongly correlated electrons. However to include the spin-fluctuation contribution [17, 18] we have to consider the Gaussian fluctuation around the saddle-point solution. The aim of this paper is to show that there is a nontrivial saddle-point contribution to the pairing, and to draw attention to its nontrivial consequences. The full analysis requires the inclusion of the quantum fluctuations and will be quite cumbersome in view of the large number of auxiliary fields introduced above.

In what follows we will make the saddle-point approximation and thus replace Bose operators with their expectation values and also put $t_{i1} = t_{i-1} = d_{i\sigma} \equiv t$, $\lambda^{(0)}_i = \lambda^{(0)}$, $\lambda^{(1)}_{il\sigma} = \lambda^{(1)}$ and, subsequently, make the BCS-type decomposition of the pairing part, as for the 3d orbitals we have that $J \approx (0.2\text{–}0.1)U$ (see also below). By carrying out this procedure, we obtain the effective Fermi liquid with renormalized characteristics such as the hopping integral and the magnitude of the pairing potential. However, this effective picture is not a free-particle picture, as we have to determine the renormalized parameters from the self-consistency

conditions. Explicitly, the effective Hamiltonian in the saddle-point approximation and with the local pairing included takes the following form

$$\mathcal{H} = \sum_{kl\sigma}(\Phi\epsilon_k - \bar{\mu})n_{kl\sigma} + 2NUd^2 + 4N(U-J)t^2 + 2N(3U-5J)(2s^2+g^2) + \lambda^{(0)}N(e^2+4p^2+2d^2+4t^2+4s^2+g^2-1) + 4\lambda^{(1)}N(p^2+d^2+2t^2+3s^2+g^2) - 2Jt^2\sum_{i,m=-1,0,1} B^\dagger_{im}B_{im} \tag{8}$$

where $\bar{\mu} = \mu + \lambda^{(0)}$ and the band narrowing factor due to the correlations is

$$\Phi = \frac{16}{n(4-n)}[p(e+t) + (t+d)(p+s) + s(t+g)]^2. \tag{9}$$

The local pairing part is now expressed by the condensed Bose amplitude t combined with the BCS-type triplet-pairing amplitudes $\langle f^\dagger_{i1\sigma} f^\dagger_{i2\sigma'}\rangle$. The Bose amplitudes renormalize a rather large bare coupling constant J of a few tenths of an eV by at least an order of magnitude (see the figures below) and reduce the drastically the critical temperature. This renormalization is caused by the circumstance that we have to project out all local configurations except triplets.

Hamiltonian (3) contains *local real-space pairing* $\sim B^\dagger_{im}B_{im}$. Decomposing the pairing operators in the mean-field manner of Bardeen–Cooper–Schrieffer type: $B^\dagger_{im}B_{im} \to \langle B^\dagger_{im}\rangle B_{im} + \mathrm{HC} - |\langle B_{im}\rangle|^2 + \frac{3}{4}(\langle n_{i1}\rangle n_{i2} + n_{i1}\langle n_{i2}\rangle - \langle n_{i1}\rangle\langle n_{i2}\rangle)$, and taking the Fourier transform to the momentum space we obtain the Hamiltonian in the weak coupling (BCS approximation)

$$\mathcal{H} \approx \mathcal{H}_{BCS} = \sum_{kl\sigma} E_k n_{kl\sigma} + \sum_k [\Delta_1 f^\dagger_{k1\uparrow} f^\dagger_{-k2\uparrow} + \Delta_{-1} f^\dagger_{k1\downarrow} f^\dagger_{-k2\downarrow} + \Delta_0(f^\dagger_{k1\uparrow} f^\dagger_{-k2\downarrow} + f^\dagger_{k1\downarrow} f^\dagger_{-k2\uparrow}) + \mathrm{HC}] + E_0 \tag{10}$$

with $E_k \equiv \Phi\epsilon_k - \tilde{\mu}$, $\tilde{\mu} \equiv \mu + \lambda^{(0)} - \frac{3}{4}Jt^2n$, and $\Delta_m = \Delta_{\sigma\sigma'} = (-2Jt^2/N)\sum_k \langle f^\dagger_{k1\sigma} f^\dagger_{-k2\sigma'}\rangle$, and E_0 expressing the remaining (operator-free) terms. Note that the weak-coupling approximation is applicable when $Jt^2 \ll W\Phi$. This condition is fulfilled and is checked *a posteriori*. Also, to obtain a good Hartree–Fock approximation for the energy in the normal state we must divide the term $\frac{3}{4}(\langle n_{i1}\rangle n_{i2} + n_{i1}\langle n_{i2}\rangle - \langle n_{i1}\rangle\langle n_{i2}\rangle)$ by $(\frac{n}{4})^2$ in E_k and E_0. Then in the Nambu convention, we can rewrite (10) in the form

$$\mathcal{H}_{BCS} = \sum_k \boldsymbol{f}_k \mathbf{H}_k \boldsymbol{f}_k + E_0 + \sum_k E_k \tag{11}$$

with $\boldsymbol{f}^\dagger_k \equiv (f^\dagger_{k1\uparrow}, f^\dagger_{k1\downarrow}, f_{-k2\uparrow}, f_{-k2\downarrow})$, and

$$\mathbf{H}_k = \begin{pmatrix} E_k & 0 & \Delta_1 & \Delta_0 \\ 0 & E_k & \Delta_0 & \Delta_{-1} \\ \Delta_1^* & \Delta_0^* & -E_k & 0 \\ \Delta_0^* & \Delta_{-1}^* & 0 & -E_k \end{pmatrix} \equiv \begin{pmatrix} E_k\hat{\sigma}_0 & \hat{\Delta} \\ \hat{\Delta}^\dagger & -E_k\hat{\sigma}_0 \end{pmatrix} \tag{12}$$

where $\hat{\sigma}_0$ is the unit 2×2 matrix. This effective Hamiltonian expresses a two-band spin-triplet paired state with an interorbital pairing. Therefore, the pairing will become important in the correlated state, since the number of local triplet pairs grows with U and eventually becomes $\sim(n-1)^2$. Note also that the gap is $\boldsymbol{k}$ independent, since it involves intraatomic pairing. This circumstance provides one of the principal differences with the case of liquid ^{3}He. Here we have a two-orbital ($l = 1, 2$) situation with the quenched d-orbit moment.

Parametrizing the gap in the standard form [13]

$$\Delta \equiv \mathrm{i}(\boldsymbol{d}\cdot\hat{\sigma})\hat{\sigma}_y = \begin{pmatrix} -d_x + \mathrm{i}d_y & d_z \\ d_z & d_x + \mathrm{i}d_y \end{pmatrix} \tag{13}$$

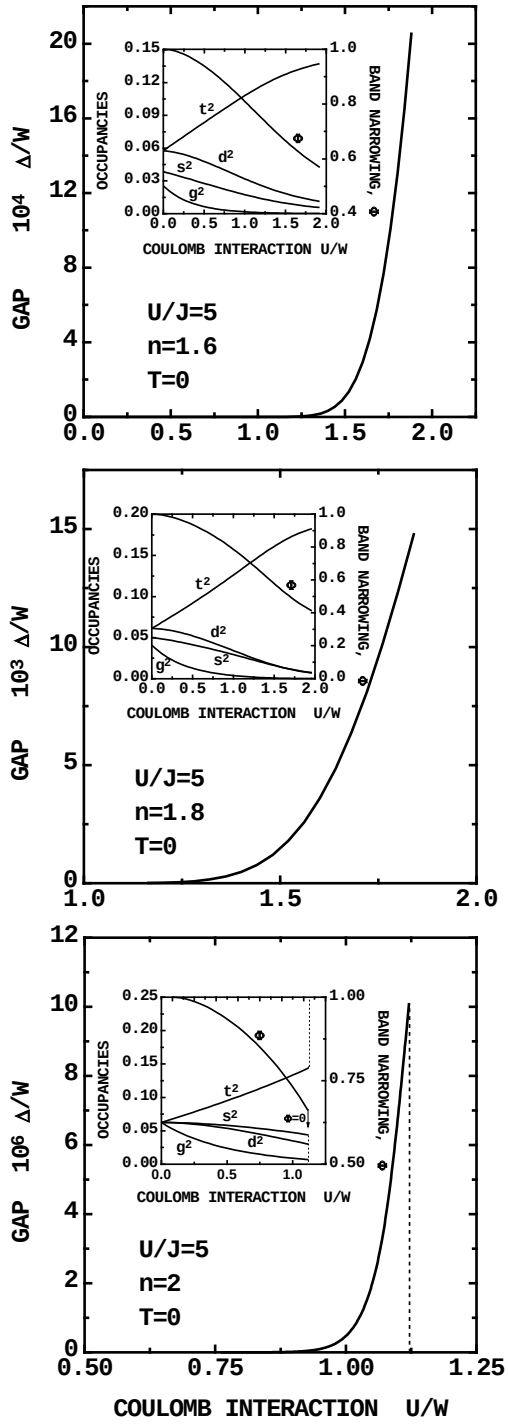

Figure 1. The superconducting gap as a function of the amplitude of direct Coulomb interaction U/W for $n = 1.6$, 1.8 and 2.0 (from top to bottom, respectively). The vertical dashed line in the bottom panel marks the Mott localization threshold. The insets provide the magnitude of the Bose fields and the band narrowing Φ, all against U/W.

we obtain the eigenvalues $\pm\lambda_{ks} \equiv [E_k^2 + |\boldsymbol{d}|^2 + s|\boldsymbol{q}|^2]^{1/2}$, with $s = \pm 1$, and $\boldsymbol{q} = \mathrm{i}(\boldsymbol{d} \times \boldsymbol{d}^*)$. Hence, the free energy functional has the form

$$F = -2k_B T \sum_{\boldsymbol{k},s=\pm 1} \ln[1 + \exp(-\beta\lambda_{ks})] + 2\sum_{\boldsymbol{k}}[E_{\boldsymbol{k}} - (\lambda_{\boldsymbol{k}+} + \lambda_{\boldsymbol{k}-})/2] + E_0 + \mu N_e. \tag{14}$$

Minimization with respect to d_i^* yields the gap equation

$$\hat{\Delta} = \frac{Jt^2}{N}\sum_{ks}\frac{\tanh(\beta\lambda_{ks}/2)}{2\lambda_{ks}}\mathrm{i}(\boldsymbol{Q}_s \cdot \hat{\sigma})\hat{\sigma}_y \tag{15}$$

where $\boldsymbol{Q}_s = \boldsymbol{d} + s\frac{\boldsymbol{q}\times\boldsymbol{d}}{|\boldsymbol{q}|}$. In the situation with the local (on-site) pairing one can expect that $\Delta_{-1} = \Delta_1 = \Delta_0$, so that $|\boldsymbol{d}^2| = |\boldsymbol{q}|$ and $\Delta^2 = 2|\boldsymbol{d}|^2$. In that situation

$$\begin{cases} \lambda_{\boldsymbol{k}+} = \sqrt{E_k^2 + \Delta^2} \\ \lambda_{\boldsymbol{k}-} = E_{\boldsymbol{k}} \end{cases} \tag{16}$$

i.e. roughly half of the quasiparticle spectrum is gapped, and the gap is obtained by the BCS equation. In other words, the linear specific heat term γ_S appears also in the superconducting state and is about half of the value γ_N in the normal state.

To illustrate our results we computed the magnitude of the zero-temperature gap as a function of the Coulomb interaction U/W, for different values of band filling $n \geqslant 1$ and $U/J = 5$. The amplitudes d, t, s and g of the Bose fields have been obtained from the minimization of F in the normal state, as the pairing is treated in the weak-coupling limit. The calculated results for $n = 1.6$, 1.8 and 2.0 are displayed on the panel composing figure 1 (for the bare density of states $\rho^0 = 1/W$). The optimized values of the Bose amplitudes, as well as the band narrowing Φ, are displayed in the insets. Note that in each case t^2 grows substantially with U/W and so does the gap. For the $n = 1.4$ case, displayed in figure 2, the gap is an order of magnitude smaller compared to that for $n = 1.6$. For $W \approx 1$ eV the gap is of the order of 1 K for reasonable value of parameters in the almost localized Fermi-liquid regime. For $n = 1$, the effective gap Δ/W is negligible ($\sim 10^{-12}$). For $n \to 2$ the gap never becomes substantial (cf the bottom of figure 1), as the Mott-insulator boundary (cf the dashed line) is reached first via the first-order transition. Furthermore, for $n = 2$, $g^2 = e^2$ and $s^2 = p^2$ because of the electron–hole symmetry. From these figures one can draw the conclusion that the isotropic triplet superconductivity state with the gap parameter

$$\Delta \approx W\Phi\sqrt{\frac{n}{2}\left(2 - \frac{n}{2}\right)}\exp\left(-\frac{W\Phi}{2Jt^2}\right)$$

should be possible to observe for the intermediate band filling $1 < n < 2$. This gap expression is multiplied by the additional factor $D(D-1)/2$ for $D > 2$, if we think in terms of the equivalent-orbital model. One should also note that the paired state appears in the regime, where the *Stoner condition* is not yet fulfilled (see below for details). Also, for $U/W = 1.5$, we have displayed the results for $J/W = 0.3$ and therefore, the Hund's rule coupling is only a small fraction of the band energy as $\Phi \sim 1/2$, and $t^2 \sim 1/5$. The value of the superconducting gap is thus strongly reduced by the presence of the factor t^2, making the BCS-type approximation applicable, if not realistic. More precisely, in the weak-coupling limit we should have $W\Phi \gg Jt^2$. The value of the gap will not grow indefinitely with increasing U (and J), as the *Stoner criterion is crossed*, and the energy of the ferromagnetic state may become quickly lower than that of the superconducting state. This is because the magnetic moment grows linearly with J, not exponentially, as does Δ in the paired state. The exponential factor $\exp(-W\Phi/2t^2J)$ is contained also in the expression for the superconducting

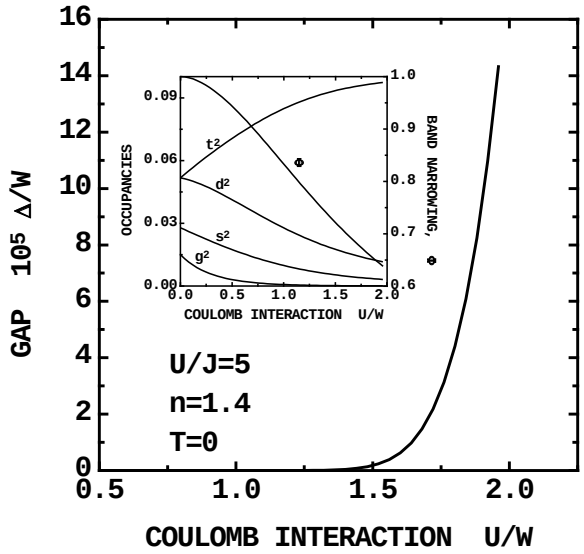

Figure 2. The gap versus U/W for $n = 1.4$, corresponding to 0.7 particles per band per atom. This roughly represents the situation for Sr_2RuO_4.

transition temperature T_S; it contains the ratio of the quasiparticle band energy ($\sim -W\Phi/4$) in the normal state to the effective coupling (Jt^2).

The above weak-coupling approach will be modified in the strong-correlation regime: $U \gg W$, and for $J \gtrsim W$, where J will be replaced by the effective ferromagnetic intersite kinetic exchange $\sim zt^2/(U-3J)$ [15]. However, in this limit the Fermi liquid may not be stable.

As stated above, with increasing Coulomb interactions the triplet paired state stabilizes at the expense of nonmagnetic or antiferromagnetic states. This stabilization does not appear in the Hartree–Fock limit, since then $t = d$, and the gain in Hund's rule exchange energy for any triplet state (for $n > 1$) is not sufficient to overcome the corresponding loss in the band energy. On the other hand, the renormalized Stoner criterion for the onset of the ferromagnetic state in the correlated state has the form [14]

$$\left[1-\left(\frac{U}{U_c}\right)^2\right]\left[1-\frac{U}{W}\frac{1+U/2U_c}{1+(U/U_c)^2}\right]-\frac{J}{W}=0. \tag{17}$$

Taking the critical value for the Mott localization $U_c \approx 2W$, and the actual value $U \approx W$ when the system is close to the first-order localization transition (cf figure 1, bottom), we obtain the critical value $J = J_c$ for the onset of ferromagnetism as $J_c/U = 1/3$. Thus the paired state can be formed when the system is still paramagnetic. *Once the Stoner threshold is crossed over, the Hund's rule starts playing its usual role of the principal factor in magnetic-moment formation*. However, even then the coexistence of the spin-triplet superconductivity and itinerant ferromagnetism is possible. This subject will not be discussed in detail here, as it requires a separate analysis (it will introduce one additional self-consistent equation for the magnetic moment)

From the above discussion, one can draw a general conclusion concerning the pairing in a correlated electronic system. The exclusion of double occupancies on the same orbital favours local interorbital configurations. In this respect, the present pairing is an analogue of

the exchange-induced singlet pairing in the high-T_c systems [15]. However, in our situation, the system is *below* the Mott–Hubbard localization threshold, so it can be described in the Fermi-liquid (albeit almost-localized) category. Actually, the Mott localization is of the first order [14] and takes place *before* the quantum critical point ($\Phi = d = 0$) is reached.

Concluding, our model of pairing, based on the Hund's rule coupling, provides two new important features: (i) it introduces paired states into the standard discussion of the magnetic phase diagram of correlated and degenerate systems, (ii) supplies an opportunity of studying real space pairing in the correlated system with rather well known (Fermi-liquid) nature of the ground state and (iii) it opens up the possibility of studying the coexistence of ferromagnetism and spin-triplet superconductivity. Therefore, it can be regarded as a tractable model situation comprising both the correlated nature of electrons and the exchange-induced local pairing among them.

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