Local *f*-electron superconductivity in an interacting conduction band

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Using a mean-field approach we study the effect of interactions between conduction electrons on the appearance of superconductivity of local *f* electrons within the context of an Anderson lattice. We consider both the effects of local and nearest-neighbor Coulomb repulsions between the conduction electrons. At the mean-field level the addition of these terms renormalizes the parameters of the original Anderson Hamiltonian, as expected. At low densities the effect of the interactions is to increase the superconducting critical temperature T_c, while at high densities ($n \leqslant 2$) the interactions decrease T_c or suppress the superconductivity altogether.

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A consistent description of the overall properties of heavy-fermion systems has been achieved assuming a description in terms of an Anderson lattice.[1] In this model delocalized (conduction) free electrons hybridize with strongly interacting localized states (typically f orbitals). In the Anderson lattice the energy of a single electron in an f orbital (e.g., $4f^1$) is ϵ_0, and the energy of two electrons in the same f orbital ($4f^2$) is $2\epsilon_0+U_f$, where U_f is the on-site Coulomb repulsion. The energy of the $4f^2$ state is much larger than the energy of the $4f^1$ state and it is usual in many theoretical treatments to take the limit $U_f \rightarrow \infty$.

Experimentally it is found that these systems show a rich phase diagram. Their complex phase diagrams arise from an interplay between Kondo screening of local moments, the antiferromagnetic [Ruderman-Kittel-Kasuya-Yosida (RKKY)] interaction between the moments, and superconducting correlations between the heavy quasiparticles. Therefore, these systems display paramagnetic, antiferromagnetic, and superconducting phases at low temperatures.[2] Particularly interesting is the competition between antiferromagnetism and superconductivity, which in certain uranium systems leads to the coexistence[3] of both ordered phases.

The limit $U_f=\infty$ has been studied using the slave boson technique.[4,5] In particular, it has been found that in the disordered phase superconducting instabilities arise in the p and d-wave channels because of the effective (RKKY) interaction between the f electrons.[6] The superconductivity of the Anderson lattice was studied in the context of high-T_c materials[7] using a $1/N$ expansion to leading order in the normal phase and to the first order in the ordered phase where the critical temperature was studied as a function of doping for an s-wave pairing. Mean-field studies of superconductivity in the Anderson lattice both at finite U_f and at $U_f=\infty$ were recently carried out,[8,9] explicitly introducing an attractive interaction between the f electrons to study the ordered phase directly. Also, the competition between magnetic order and superconductivity has recently been studied considering the conditions for the formation of a local moment in the presence of superconducting correlations,[10] taking a RKKY interaction explicitly into account.[11]

On the other hand, it was stressed recently that any realistic description of heavy fermions should also take into account the interactions between conduction electrons. These are usually considered free for reasons of simplicity, but their interactions are certainly not negligible. In particular it was stressed that deviations of the compound $Nd_{2-x}Ce_xCuO_4$ from the standard Kondo picture are probably due to interactions in the conduction band.[12] Using the dynamical field theory[13] it was shown for a half-filled system that the effect of the interactions is to increase the hybridization effectively. Also, recently it was shown that the effect of correlations is to narrow the effective conduction band leading to an enhanced Kondo scale at low temperatures,[14] as observed in $Nd_{1-x}Ce_xCuO_4$. The main effect of the interactions was concluded to be an increased spin polarization of the conduction electrons.

In this work we study the influence of a Hubbard-like interaction between conduction electrons on the superconducting properties of these systems. We consider the interaction between the f electrons to be infinite, and introduce local and nearest-neighbor repulsions between the conduction electrons. We use a mean-field approach as previously done for the free conduction electrons.[9] A mean-field approach yields interesting results, as shown recently.[15]

We consider an extended version of the Anderson lattice model, which includes a density-density attraction between the electrons occupying neighboring f orbitals of the form $H_J=\frac{1}{2}J\Sigma_{\langle i,j\rangle,\sigma,\sigma'}n^f_{i,\sigma}n^f_{j,\sigma'}$. This term explicitly describes an effective attraction between neighboring f sites ($J<0$) which is responsible for superconductivity in the local f electrons. In addition we consider interactions between the conduction electrons. We consider a local interaction of the form $H_{U_{c0}}=U_{c0}\Sigma_i n^c_{i\uparrow}n^c_{i\downarrow}$, where $n^c_{i\sigma}$ is the number of conduction electrons with spin σ at site i. We also consider Coulomb repulsion between nearest neighbors of the form $H_{U_{c1}}=U_{c1}\Sigma_{\langle i,j\rangle}\Sigma_{\sigma,\sigma'}n^c_{i\sigma}n^c_{j\sigma'}$ In general the Coulomb repulsion between the conduction electrons will be screened and will only extend to a few neighbors.

The effective mean-field Hamiltonian can be written as

$$
\begin{aligned}
H_{eff}=&\tilde{H}_{eff}+\sum_{\vec{k}\sigma}(\tilde{\epsilon}_f-\tilde{\mu})f^\dagger_{\vec{k}\sigma}f_{\vec{k}\sigma}\\
&+\sum_{\vec{k}\sigma}\left(-2(t+2U_e\mathcal{G})\sum_{i=x,y,z}\cos k_i-\tilde{\mu}\right)c^\dagger_{\vec{k}\sigma}c_{\vec{k}\sigma}\\
&+\sqrt{z_f}V\sum_{\vec{k}\sigma}(f^\dagger_{\vec{k}\sigma}c_{\vec{k}\sigma}+c^\dagger_{\vec{k}\sigma}f_{\vec{k}\sigma})\\
&+z_f\sum_{\vec{k}\sigma>0}(f^\dagger_{\vec{k}\sigma}f^\dagger_{-\vec{k},-\sigma}\Delta_{\vec{k}\sigma}+f_{-\vec{k},-\sigma}f_{\vec{k},\sigma}\Delta^*_{\vec{k}\sigma}).
\end{aligned}
$$

Here $\tilde{H}_{eff}=(\epsilon_f-\epsilon_0)(z_f-1)N_S-U_d n_c^2 N_S+2U_e\bar{z}\mathcal{G}^2 N_S-(N_S/2J)\Sigma_\sigma\Delta_\sigma^*\Delta_\sigma$, ϵ_f is the renormalized energy of the f orbitals due to the on-site repulsion, $U_d=\frac{1}{4}U_{c0}+\alpha\bar{z}U_{c1}$, $U_e=(1-\alpha)U_{c1}$, $\tilde{\mu}=\mu-2U_d n_c-2U_e\bar{z}$, and $\tilde{\epsilon}_f=\epsilon_f-2U_d n_c-2U_e\bar{z}$. We consider a three-dimensional cubic lattice in which the conduction band is given by $\epsilon_{\vec{k}}=-2t\Sigma_{i=x,y,z}\cos k_i$. The c and f operators are fermionic and obey the usual anticommutation relations. The hybridization potential V is assumed to be momentum independent, N_s is the number of lattice sites, and $\bar{z}$ is the number of nearest neighbors. We implement the condition $U_f=\infty$ within the slave-boson formulation,[5] in which the empty f site is represented by a slave boson b_i and the physical annihilation operator f_i is replaced with $b^\dagger{}_i f_i$. Condensation of the slave bosons can be described by the replacement $b_i\rightarrow\langle b_i\rangle=\langle b^\dagger{}_i\rangle=\sqrt{z_f}$. The mean-field treatment of the interaction term H_J involves the usual decoupling of destruction and annihilation operators, but we associate a boson operator with every f operator in order to prevent double occupancy at the f sites. Also taking the boson condensation into account, we obtain the superconducting part of the mean-field Hamiltonian from the substitution[9,16] $f^\dagger f^\dagger f f\rightarrow z_f f^\dagger f^\dagger\langle z_f f f\rangle$ +H.c. The gap function $\Delta_{\vec{k},\sigma}=\eta_{\vec{k}}\Delta_\sigma$, and the superconducting order parameter Δ_σ is given by $\Delta_\sigma=(z_f J/N_s)\Sigma_{\vec{k}}\eta_{\vec{k}}\langle f_{-\vec{k},-\sigma}f_{\vec{k},\sigma}\rangle$, where $\eta_{\vec{k}}$ denotes any of the possible pairing symmetries[17] $\eta_{\vec{k}}^{(s)}=\sqrt{\frac{2}{3}}[\cos(k_x)+\cos(k_y)+\cos(k_z)]$, $\eta_{\vec{k}}^{(p,i)}=\sqrt{2}\,\sin(k_i)$, and $\eta_{\vec{k}}^{(d_{x^2-y^2})}=\cos(k_x)-\cos(k_y)$ for s, p, and d waves, respectively. Electron pairing in the superconducting phase occurs in a state with a zero total pair momentum. The mean-field decoupling of the interactions between the conduction electrons is done by factorizing the number operators like $n_{i\sigma}^c=\langle n_{i\sigma}^c\rangle+(n_{i\sigma}^c-\langle n_{i\sigma}^c\rangle)$. The nearest-neighbor term can be factorized in two ways. The first way (with a weight α) is by obtained decoupling, as for the local term. On the other hand, the nearest-neighbor term can also be decoupled considering a resonating-valence-bond- (RVB-) like form where we couple the nearest neighbors (with weight $1-\alpha$) and introducing $\mathcal{G}=\langle c_i^\dagger c_j\rangle$ as a variational parameter for the effective Hamiltonian. As we will see below an important quantity is the gap between the band center and the renormalized f level given by $\epsilon_f-2U_d n_c$ (taking $U_e=0$).

The mean-field equations, obtained varying the mean-field Hamiltonian with respect to the variational parameters, are solved self-consistently.[9] Most of our results are obtained considering that the pairing has a d-wave symmetry. At the end we will compare the results for the other two symmetries, the extended s wave and the p wave. The various pairings yield results that are qualitatively similar.

We may also consider the extreme limit where the Coulomb repulsion between the conduction electrons is very large. The case where $U_{c0}\rightarrow\infty$ may be handled by introducing a second set of slave bosons to implement the condition of no-double occupancy in the conduction electrons. The set of slave bosons appears in the hopping term (tight-binding band), as in the t-J model, and in the hybridization. The parameters of the original Anderson Hamiltonian are therefore further renormalized.

We begin by considering the influence of the Coulomb repulsion on the superconducting critical temperature T_c as a function of the electronic density n. We recall that it is convenient to define a parameter $U_d=\frac{1}{4}U_{c0}+\bar{z}U_{c1}$, which is the result of the combined effects of a local repulsion and of a nearest-neighbor repulsion treated in a usual Hartree-Fock decoupling. Since the number of nearest-neighbors is large for three-dimensional systems, $\bar{z}=6$, it is seen that it is necessary to include the effect of the nearest-neighbor interactions since even a small U_{c1} gives a comparable contribution. Also, the contribution of terms like U_e is important due to the $\bar{z}$ factor. However, further neighbors are not considered since it is expected that the screening will be effective at larger distances due to the exponential decay factor.

In Fig. 1 we compare the effects of U_d and U_e on the critical temperature as a function of density, n. The parameters are $\epsilon_0=-1.5$, $J=-3$, and $V=1.2$ (unless otherwise stated, these parameter values are used throughout). For low densities as U_d (or U_e) increases T_c also increases, while at high densities the effect of the interactions is opposite. Figures 1(a) and 1(b) are qualitatively similar (note that U_e is about ten times smaller, to produce similar effects). We recall that when $U_d=0$ and $U_e\neq 0$ we are considering the effect of only nearest-neighbor interactions and a RVB-like decoupling. At low densities the f states have low populations and the superconductivity does not arise. Also, at densities close to 2 the f states are very populated and superconductivity is depressed since the Cooper pairs cannot move (since $U_f=\infty$). Introducing repulsions between the conduction electrons will increase the population of the f states. Therefore at low densities more f electrons are available to pair and, with increasing U_d (or U_e), T_c increases. At high densities the effect is opposite.

To further clarify the results let us first consider a regime of high densities and focus on a value of $n=1.4$. As ϵ_0 or V increase n_f decreases for any value of U_d. For fixed values of ϵ_0 or V, as U_d increases n_f also increases. As stated above the effect of the repulsion is to increase n_f at the expense of n_c (since n is fixed). Clearly if n_f increases with U_d for a fixed pair (ϵ_0,V) then z_f decreases and naturally the pairing order parameter decreases, since it is proportional to $z_f=1-n_f$; therefore T_c also decreases. The dependence of T_c on ϵ_0 for $n=1.4$ is very similar to the behavior as a function of n. The same occurs as a function of the hybridization, as shown in Fig. 2, where we show the influence of U_d. As U_d increases, the peak of T_c, as a function of V, shifts to the right; the same occurs as a function of ϵ_0.

Let us now consider the regime of low densities, and let us focus our attention on a particular value $n=0.4$. As U_d increases n_f also increases for a fixed pair (ϵ_0,V), as expected, but the behavior as a function of V is not monotonic at low values of the interaction in contrast to the case at higher densities. In Fig. 3 we show T_c as a function of V for various values of U_d. As a general trend as U_d increases T_c increases as well (except for some crossovers that occur at either low V or ϵ_0).

As stated above, the f-level energy can be renormalized as $\tilde{\epsilon}_f=\epsilon_f-2U_d n_c$ (taking $U_e=0$). This renormalization is the

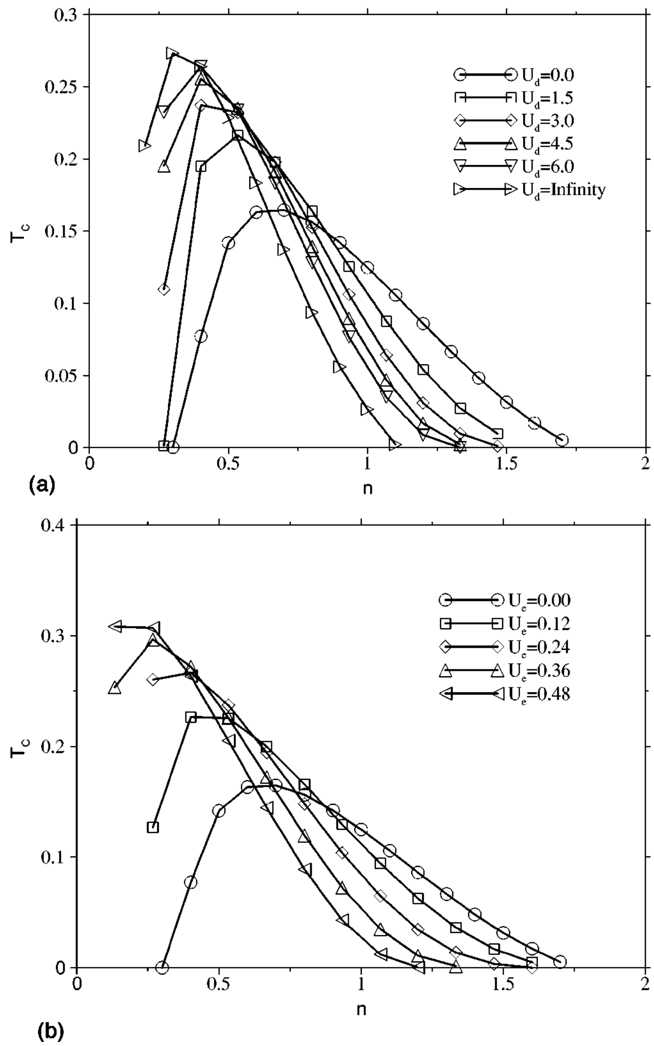

FIG. 1. Superconducting critical temperature T_c as a function of electronic density n for several values of (a) U_d and (b) U_e. The other parameters in this figure and in all others, unless explicitly stated, are $\epsilon_0 = -1.5$, $J = -3$ and $V = 1.2$ in units of t.

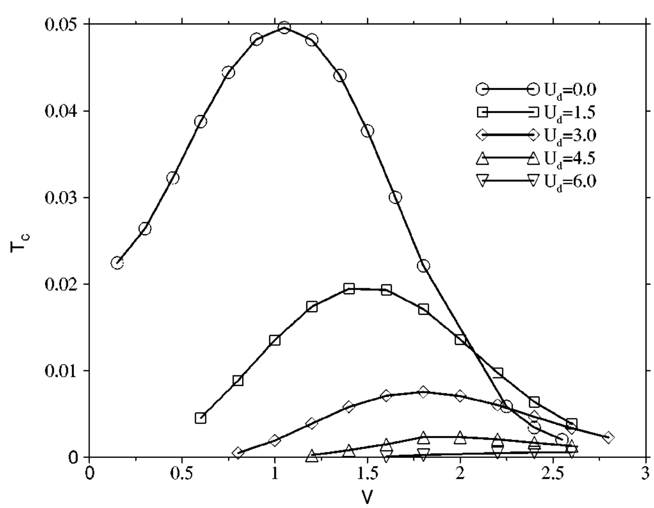

FIG. 2. Critical temperature T_c as a function of the hybridization V for several values of U_d at $n = 1.4$.

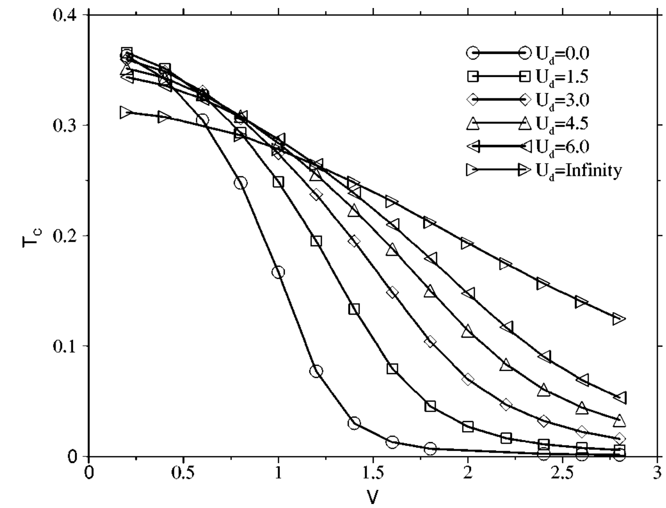

FIG. 3. Critical temperature T_c as a function of the hybridization V for different values of U_d for $n = 0.4$.

energy difference between the center of the conduction band and the *f*-level energy. A study of T_c as a function of ϵ_0 shows that there is a shift in the peak position of T_c as a function of ϵ_0 which is due to this energy difference. In Fig. 4 we plot T_c as a function of $\epsilon_f - 2U_d n_c$ for different values of ϵ_0 and of U_d for both $n = 1.4$ and 0.4, and we find a universal curve in both cases. This shows that the critical temperature is essentially determined by this energy difference. As a side remark we note that if we take $U_d = 0$ and carry out the same study as a function of U_e either for $n = 1.4$ or 0.4 we do not exactly find a universal curve. The reason is that while T_c as a function of ϵ_0 for different values of U_d has peaks that shift to lower values of ϵ_0 as U_d grows but with similar heights, their heights increase slightly as U_e increases.

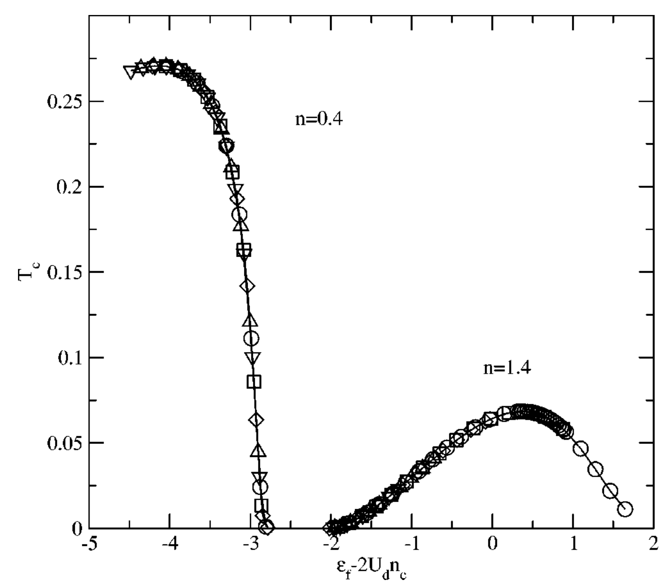

FIG. 4. Critical temperature T_c as a function of the energy difference between the center of the conduction band and the renormalized *f*-level energy $\epsilon_f - 2U_d n_c$ for $n = 1.4$ and $n = 0.4$. An universal curve is obtained for several pairs of the bare *f*-level energy ϵ_0, and of U_d.

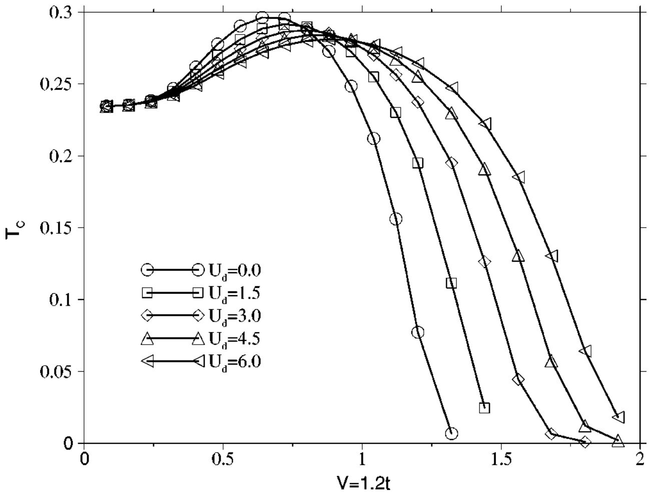

FIG. 5. Critical temperature T_c as a function of pressure for several values of U_d. We take $V/t=1.2$ constant (keeping the other parameters constant and $n=0.4$).

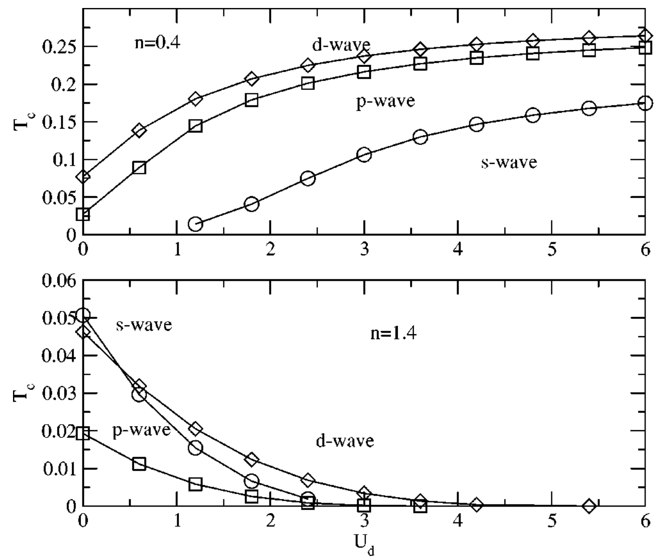

FIG. 6. Critical temperature T_c as a function of U_d for the various pairing symmetries for (a) $n=0.4$ and (b) $n=1.4$.

It is also interesting to see how the critical temperature varies in the presence of an externally applied pressure. Recently there has been a great interest in the effects of pressure, particularly in the context of coexistence of magnetism and superconductivity in these materials.[18] Increasing pressure is expected to increase both the hopping and the hybridization, keeping V/t constant,[19] while probably keeping other parameters approximately constant in a first approximation. It was shown that a d-wave superconducting phase expels the magnetic phase of $CeCu_2Si_2$ when the magnetic critical temperature crosses the superconducting critical temperature as the pressure increases. A similar result was found theoretically within a mean-field treatment considering a finite U_f.[10] In Fig. 5 we consider the effects of U_d (similar results are obtained varying U_e) on the critical temperature as a function of V (with $V/t=1.2$) at $n=0.4$. Consider first $U_d=0$. The effect of the increase of the hybridization is to decrease T_c. However, since we keep V/t fixed, we also increase the hopping. The overall effect is that at small V and small hopping T_c increases. When we approach $t=1$, T_c decreases quickly. The effect of the interactions, as before, is to slow down this decrease; therefore, a peak structure appears that shifts to higher values of V as U_d (or U_e) increase.

Finally in Fig. 6 we compare the three pairing symmetries. At low densities we see that for all U_d the highest T_c is for the d-wave symmetry and the lowest is for the extended s-wave symmetry. For $n=1.4$ and for $U_d=0$ (as previously shown[9]) the highest T_c is for the extended s wave. As U_d increases there is a crossover between the various symmetries. The main conclusion, however, is that the behavior of the various symmetries is qualitatively similar.

To summarize, the consequence of the inclusion of Coulomb repulsions between the conduction electrons is, within a mean-field approximation, to renormalize the parameters of the Anderson Hamiltonian, as expected. Previously it was shown[9] that, considering a free conduction band, superconductivity between the f electrons is suppressed both at low and high densities ($n\leqslant 2$). The addition of Coulomb repulsions between the conduction electrons generally decreases n_c and increases n_f (at a constant n). Therefore, at low densities the effect of the interactions is to favor superconductivity and at high densities is to inhibit it. It was also found in this work that the critical temperature depends in a universal way on the energy difference between the center of the conduction band and the renormalized f-level energy, both at low and high densities, considering different pairs of values of ϵ_0 and U_d.

The construction of a more realistic Hamiltonian for these systems is important, as we stressed at the beginning. While within the mean-field approximation the effect of the extra terms is understood, it also reveals that significant changes in the behavior of the system do occur.

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[1] D.M. Newns and N. Read, Adv. Phys. **36**, 799 (1987).

[2] C.M. Varma, Comments Solid State Phys. **11**, 221 (1985); Z. Fisk, D.W. Hess, C.J. Pelhick, D. Pimes, J.L. Smith, J.D. Thompson, and J.O. Willis, Science **239**, 33 (1988); P. Schlottmann, Phys. Rep. **181**, 1 (1989); Robert H. Heffner and Michael R. Norman, Comments Condens. Matter Phys. **17**, 361 (1996).

[3] N.D. Mathur, F.M. Grosche, S.R. Julian, I.R. Walker, D. Freye, R. Haselwimmer, and G. Lonzarich, Science **394**, 39 (1998); K. Ishida, Y. Kawasaki, K. Tabuchi, K. Kashima, Y. Kitaoka, K. Asayama, C. Geilbel, and F. Steglich, Phys. Rev. Lett. **82**, 5353 (1999); R. Caspary, P. Hellmann, M. Keller, G. Sparn, C. Wassilew, R. Köhler, C. Geibel, C. Schank, F. Steglich, and N. Phillips, *ibid.* **71**, 2146 (1993); R. Feyerherm, A. Amato, F.N. Gygax, A. Schenck, C. Geibel, F. Steglich, N. Sato, and T.

Komatsubara, *ibid.* **73**, 1849 (1994); N. Bernhoeft, N. Sato, B. Roessli, N. Aso, A. Hiess, G.H. Lander, Y. Endoh, and T. Komatsubara, *ibid.* **81**, 4244 (1998); N. Aso, B. Roessli, N. Bernhoeft, R. Calemczac, N.K. Sato, Y. Endoh, T. Komatsubara, A. Hiess, G.H. Lander, and H. Kadowaki, Phys. Rev. B **61**, R11 867 (2000).

[4] A.J. Millis and P.A. Lee, Phys. Rev. B **35**, 3394 (1987).

[5] P. Coleman, Phys. Rev. B **29**, 3035 (1984); **35**, 5072 (1987).

[6] A. Houghton, N. Read, and H. Won, Phys. Rev. B **37**, 3782 (1988); M. Lavagna, A.J. Millis, and P.A. Lee, Phys. Rev. Lett. **58**, 266 (1987).

[7] D.M. Newns, M. Rasolt, and P.C. Pattnaik, Phys. Rev. B **38**, 6513 (1988).

[8] S. Robaszkiewicz, R. Micnas, and J. Ranninger, Phys. Rev. B **36**, 180 (1987); A. Romano, C. Noce, and R. Micnas, *ibid.* **55**, 12 640 (1997); Acta Phys. Pol. A **91**, 381 (1997).

[9] M.A.N. Araújo, N.M.R. Peres, P.D. Sacramento, and V.R. Vieira, Phys. Rev. B **62**, 9800 (2000).

[10] M.A.N. Araújo, N.M.R. Peres, and P.D. Sacramento, Phys. Rev. B **65**, 012503 (2002).

[11] M. A. N. Araújo, N. M. R. Peres, and P. D. Sacramento (unpublished).

[12] T. Brugger, T. Schreimer, G. Roth, P. Adelman, and G. Czjzek, Phys. Rev. Lett. **71**, 2481 (1993); P. Fulde, V. Zevin, and G. Zwicknagl, Z. Phys. B: Condens. Matter **92**, 133 (1993); G. Khauliullin and P. Fulde, Phys. Rev. B **52**, 9514 (1995).

[13] T. Schork and S. Blawid, Phys. Rev. B **56**, 6559 (1997).

[14] W. Hofstetter, R. Bulla, and D. Vollhardt, Phys. Rev. Lett. **84**, 4417 (2000).

[15] C. Hurscroft, A.K. McMahan, and R.T. Scalettar, Phys. Rev. Lett. **82**, 2342 (1999); N.M.R. Peres, P.D. Sacramento, and M.A.N. Araújo, Phys. Rev. B **64**, 113104 (2001).

[16] A.E. Ruckenstein, P.J. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).

[17] C. Bastide and C. Lacroix, J. Phys. C **21**, 3557 (1988).

[18] P. Gegenwart, C. Langhammer, C. Geibel, R. Helfrich, M. Lang, G. Sparn, F. Steglich, R. Horn, L. Donnevert, A. Link, and W. Assmus, Phys. Rev. Lett. **81**, 1501 (1998); G. Bruls, B. Wolf, D. Finsterbusch, P. Thalmeier, I. Kouroudis, W. Sun, W. Assmus, B. Lüthi, M. Lang, K. Gloos, F. Steglich, and R. Modler, *ibid.* **72**, 1754 (1994); G.M. Luke, A. Keren, K. Kojima, L.P. Le, B.J. Sternlieb, W.D. Wu, Y.J. Uemura, Y. Onuki, and T. Komatsubara, *ibid.* **73**, 1853 (1994).

[19] B.H. Bernhard and C. Lacroix, Phys. Rev. B **60**, 12 149 (1999).