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Magnetic and superconducting instabilities in the periodic Anderson model: a random-phase-approximation study

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Abstract

We study the magnetic and superconducting instabilities of the periodic Anderson model with infinite Coulomb repulsion U in the random-phase approximation. The Néel temperature and the superconducting critical temperature are obtained as functions of electronic density (*chemical pressure*) and hybridization V (*pressure*). It is found that close to the region where the system exhibits magnetic order the critical temperature T_c is much smaller than the Néel temperature, in qualitative agreement with some T_N/T_c ratios found for some heavy-fermion materials. In our study, the magnetic and superconducting physical behaviour of the system has its origin in the fluctuating boson fields effecting the infinite on-site Coulomb repulsion among the f electrons.

1. Introduction

The superconducting and magnetic properties of heavy-fermion materials have recently attracted much attention because of their non-conventional character [1, 2]. These materials have very large specific heat coefficients γ , indicating very large effective quasi-particle masses, hence the designation *heavy fermions*. Some of these materials order antiferromagnetically at low temperatures (examples include UAgCu₄, UCu₇, U₂Zn₁₇) while others (such as UBe₁₃, CeCu₂Si₂, UPt₃) order in a superconducting state and others show no ordering (such as CeAl₃, UAuPt₄, CeCu₆, UAl₂) [1]. Some compounds exhibit phases where antiferromagnetic order coexists with unconventional superconductivity. Examples include: UPd₂Al₃ ($T_N = 14.3$ K and $T_c = 2$ K), UNi₂Al₃ ($T_N = 4.5$ K and $T_c = 1.2$ K), CePd₂Si₂ ($T_N \sim 10$ K and $T_c \sim 0.5$ K) and CeIn₃ ($T_N \sim 10$ K and $T_c \sim 0.15$ K). In the prototype heavy-fermion system Ce_xCu₂Si₂ the coexistence of d-wave superconductivity and magnetic order was clearly identified in a small range of x -values around $x \simeq 0.99$ [3].

Systems that exhibit both superconductivity and antiferromagnetism at low temperature have ratios between the Néel temperature T_N and the superconducting critical temperature T_c of the order of $T_N/T_c \sim 1\text{--}100$. The coexistence of the two types of order can be tuned by external parameters such as external pressure or changes in the stoichiometry [3,4].

A description of the normal-state properties of the heavy-fermion systems has been attempted assuming a generalization of the impurity Anderson model to the lattice [5,6]. 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 $2\epsilon_0 + U$, where U is the on-site Coulomb repulsion. The energy of the $4f^2$ state is much larger than the energy of the $4f^1$ state. Thus, if the charge fluctuations at the f orbital are small, the $4f^1$ electron may behave as a local moment.

The complexity of heavy-fermion systems arises from the interplay between Kondo screening of local moments, the antiferromagnetic Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction between the moments and the superconducting correlations between the heavy quasi-particles. The local moments form in partially filled f shells of Ce and U ions. The absence of magnetic order in some cases could perhaps be due to complete Kondo screening (below the Kondo temperature T_K) or to a spin liquid arrangement of the local moments. In the normal non-magnetic state the Anderson-lattice model predicts Fermi-liquid-like behaviour and explains the main features at low temperatures, such as the large effective masses and the Kondo resonance near the Fermi level. But the main technical difficulty is the competition between the Kondo compensation of the localized spins and the magnetic interaction between them. This interaction is mediated by the conduction electrons (RKKY type). Related to this competition is the effectiveness of the compensating cloud around each f site. The size of this cloud has been a subject of controversy. While some arguments show that it should be of large scale, of the order of v_F/T_K [7], other arguments claim it to be $\sim a$ (a is the lattice constant) [8]. This is a significant issue and is related to Nozières exhaustion problem which states that there are not enough conduction electrons to screen the f moments.

It has been proposed that the mechanism for superconductivity lies in the strong Coulomb interaction between the f electrons, not in a phonon-mediated attraction. Using Coleman's [9] slave-boson formalism together with a large- N approach, various attempts have been made to search for the existence of an effective interaction which might be responsible for superconductivity in the infinite- U Anderson-lattice model. It was proposed [10] that slave-boson fluctuations can provide an effective attraction between the electrons to leading order in $1/N$. Later, a calculation of the electron–electron scattering amplitude to order $1/N^2$ revealed an effective attractive interaction in the p and d channels, which was interpreted as a manifestation of the RKKY interaction, showing that spin fluctuations are an important mechanism [11]. The inclusion of f^0 , f^1 and f^2 states, using two sets of slave bosons, was also considered in the context of the Anderson lattice as a possible description of high- T_c superconductors [12].

The magnetic order in the ground state of Kondo insulators has been studied by Dorin and Schlottmann [13] in the framework of the Anderson-lattice model. The same authors later studied the effect of orbital degeneracy and finite U on a ferromagnetic ground state (their approach did not generate RKKY interactions, thus preventing the study of antiferromagnetic order) [14].

In this work we consider the slave-boson approach to the infinite- U Anderson-lattice model. We treat the boson fields at the mean-field level, thereby enforcing the constraint of one f electron (at most) per site only on average. By splitting the boson operator into a condensate part and an above-the-condensate term, which describes fluctuations, we compute the magnetic and pairing susceptibilities at the random-phase-approximation (RPA) level. For spin-1/2 particles the condensate density at moderate temperatures does not change much

relative to its ground-state value. Therefore we do not expect our results to be of lower quality than those characterizing the ground-state properties. We search for the critical temperatures (T_N and T_c) at which antiferromagnetic order or superconducting (s- or d-wave) pairing occurs in a normal non-magnetic system. We find that the value of T_c is much smaller than the magnetic temperature T_N . Unlike T_N , the superconducting temperature monotonically increases with externally applied pressure.

2. The model and the RPA solution

The PAM Hamiltonian is given by

$$H = H_c^0 + H_f^0 + H_{cf} + H_U, \quad (1)$$

where

$$H_f^0 = \sum_{i,\sigma} (\epsilon_0 - \mu) f_{i,\sigma}^\dagger f_{i,\sigma}, \quad (2)$$

$$H_c^0 = \sum_{\vec{k},\sigma} (\epsilon_{\vec{k}} - \mu) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma}, \quad (3)$$

$$H_{cf} = V \sum_{i,\sigma} (c_{i,\sigma}^\dagger f_{i,\sigma} + f_{i,\sigma}^\dagger c_{i,\sigma}), \quad (4)$$

$$H_U = U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \quad (5)$$

The operators c and f are fermionic and obey the usual anti-commutation relations. The hybridization potential V is assumed to be momentum independent. The term H_U represents the strong on-site repulsion between the f orbitals. We consider $U = \infty$. We implement the condition $U = \infty$ within the slave-boson formulation due to Coleman [9], in which the empty f site is represented by a slave boson b_i and the physical operator f_i in equation (4) is replaced with $b_i^\dagger f_i$ together with the constraints of only one f electron per site. The implementation of this constraint amounts to introducing a Lagrange multiplier λ which will renormalize the bare f-level energy from ϵ_0 to $\epsilon_f = \epsilon_0 + \lambda$. We split the boson operators into two terms:

$$b_q^\dagger = \sqrt{N} \sqrt{z} \delta_{0,\vec{q}} + B_q^\dagger, \quad (6)$$

where z represents the boson condensate and B_q^\dagger represents the fluctuations above the condensate. This procedure leads in leading order to a mean-field Hamiltonian [15, 16]. The corresponding mean-field equations can be written in terms of the Fourier transform of the Green functions:

$$G_{ff,\sigma}(\vec{k}, \tau - \tau') = -\langle T_\tau f_{\vec{k},\sigma}(\tau) f_{\vec{k},\sigma}^\dagger(\tau') \rangle, \quad (7)$$

$$G_{cc,\sigma}(\vec{k}, \tau - \tau') = -\langle T_\tau c_{\vec{k},\sigma}(\tau) c_{\vec{k},\sigma}^\dagger(\tau') \rangle, \quad (8)$$

$$G_{cf,\sigma}(\vec{k}, \tau - \tau') = -\langle T_\tau c_{\vec{k},\sigma}(\tau) f_{\vec{k},\sigma}^\dagger(\tau') \rangle, \quad (9)$$

as

$$z = 1 - \frac{T}{N_s} \sum_{\vec{k},\sigma} \sum_{i\omega_n} \mathcal{G}_{ff,\sigma}(\vec{k}, i\omega_n), \quad (10)$$

and

$$\epsilon_f = \epsilon_0 - \frac{VT}{\sqrt{z}N_s} \sum_{\vec{k},\sigma} \sum_{i\omega_n} G_{cf,\sigma}(\vec{k}, i\omega_n), \quad (11)$$

where N_s denotes the number of lattice sites. Equation (10) states that the mean number of electrons at an f site is $n_f = 1 - z$. For a given number of particles per site, n , these equations must be supplemented with the particle conservation condition which yields the chemical potential μ for any temperature:

$$n = 1 - z + \frac{T}{N_s} \sum_{\vec{k}, \sigma} \sum_{i\omega_n} G_{cc, \sigma}(\vec{k}, i\omega_n). \quad (12)$$

The fluctuations beyond the mean-field approach are described by the Hamiltonian

$$H_{fluct} = \frac{V}{\sqrt{N}} \sum_{\vec{k}, \vec{q}, \sigma} (c_{\vec{k}, \sigma}^\dagger f_{\vec{q}, \sigma} B_{\vec{k}-\vec{q}}^\dagger + B_{\vec{k}-\vec{q}} f_{\vec{q}, \sigma}^\dagger c_{\vec{k}, \sigma}), \quad (13)$$

and will be considered in the calculation of the magnetic susceptibility and superconducting correlation functions below. The calculation, even at the RPA level, of the correlation functions requires knowledge of the boson propagator. The full calculation of the latter is a technically difficult problem in itself, and is still unsolved. There are, however, $1/N$ calculations of $D(\vec{k}, \tau - \tau')$ [6, 10, 11]. Here we follow the work of Evans and Coqblin [17] and use an asymptotic form for the boson propagator given by

$$D(\vec{k}, \tau - \tau') = \langle T_\tau B_{\vec{k}, \sigma}(\tau) B_{\vec{k}, \sigma}^\dagger(\tau') \rangle \sim \frac{1}{\lambda}. \quad (14)$$

We also adopt the same approximation for the propagator $\bar{D}(\vec{k}, \tau - \tau') = \langle T_\tau B_{\vec{k}, \sigma}^\dagger(\tau) B_{\vec{k}, \sigma}(\tau') \rangle$. In the calculation below we shall use mean-field fermionic propagators.

The transverse spin susceptibility for the f electrons is defined as

$$\chi_{-+}(\vec{q}, i\omega_n) = \mu_B^2 \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau S^-(\vec{q}, \tau) S^+(\vec{q}, 0) \rangle, \quad (15)$$

where $\beta = 1/T$ is the inverse temperature, T_τ is the chronological order operator (in imaginary time), $S^-(\vec{q}) = \sum_{\vec{p}} f_{\vec{p}, \downarrow}^\dagger f_{\vec{p}+\vec{q}, \uparrow}$ and $S^+(\vec{q}) = [S^-(\vec{q})]^\dagger$. The calculation at the RPA level yields

$$\chi_{+,-}^f(\vec{q}, i\omega_n) = \frac{\bar{\Gamma}_{ff}^{ff}(\vec{q}, i\omega_n)[1 - J\bar{\Gamma}_{fc}^{cf}(\vec{q}, i\omega_n)]}{[1 - J\bar{\Gamma}_{fc}^{cf}(\vec{q}, i\omega)]^2 - J^2\bar{\Gamma}_{ff}^{ff}(\vec{q}, i\omega_n)\bar{\Gamma}_{cc}^{cc}(\vec{q}, i\omega_n)}, \quad (16)$$

where $J = V^2/(N\lambda)$. The result (16) holds for all values of n_f and is a generalization of that obtained by Evans and Coqblin [17, 18] for the case $n_f = 1$. The functions $\bar{\Gamma}(\vec{q}, i\omega_n)$ above are given by

$$\begin{aligned} \bar{\Gamma}_{ff}^{ff}(\vec{q}, i\omega_n) &= -\frac{1}{\beta} \sum_{\vec{p}, i\omega_m} G_{ff}(\vec{p}, i\omega_m) G_{ff}(\vec{p} + \vec{q}, i\omega_m + i\omega_n), \\ \bar{\Gamma}_{cc}^{cc}(\vec{q}, i\omega_n) &= -\frac{1}{\beta} \sum_{\vec{p}, i\omega_m} G_{cc}(\vec{p}, i\omega_m) G_{cc}(\vec{p} + \vec{q}, i\omega_m + i\omega_n), \\ \bar{\Gamma}_{fc}^{cf}(\vec{q}, i\omega_n) &= -\frac{1}{\beta} \sum_{\vec{p}, i\omega_m} G_{cf}(\vec{p}, i\omega_m) G_{fc}(\vec{p} + \vec{q}, i\omega_m + i\omega_n). \end{aligned}$$

There are three possible superconducting pairing susceptibilities that one can define. These refer to Cooper pairs of either conduction or f electrons, and a hybrid Cooper pair with a conduction and an f electron. We consider the correlation function

$$\Delta_{dd}(\vec{q}, i\omega_n) = \int_0^\beta e^{i\omega_n \tau} \sum_{\vec{k}_1, \vec{k}_2} \eta(\vec{k}_1) \eta(\vec{k}_2) \langle T_\tau d_{\vec{k}_1, \downarrow}(\tau) d_{-\vec{k}_1+\vec{q}, \uparrow}(\tau) d_{\vec{k}_2, \downarrow}^\dagger d_{-\vec{k}_2+\vec{q}, \uparrow}^\dagger \rangle, \quad (17)$$

where $d = c, f$ and $\eta(\vec{k})$ is the Cooper pair structure factor, assumed to be either extended s or d wave. The hybrid pairing correlation function is defined as

$$\Delta_{cf}(\vec{q}, i\omega_n) = \int_0^\beta e^{i\omega_n\tau} \sum_{\vec{k}_1, \vec{k}_2} \langle T_\tau f_{\vec{k}_1, \downarrow}(\tau) c_{-\vec{k}_1 + \vec{q}, \uparrow}(\tau) c_{\vec{k}_2, \downarrow}^\dagger f_{-\vec{k}_2 + \vec{q}, \uparrow}^\dagger \rangle. \quad (18)$$

This definition has been used previously in a mean-field study of the Kondo lattice [19]. At the RPA level the Cooper pair correlation function (17) is given by

$$\Delta_{dd}(\vec{q}, i\omega_n) = \Gamma_{dd}^{dd}(\vec{q}, i\omega_n) + \frac{J\Gamma_{cc}^{fc}(\vec{q}, i\omega_n)\Gamma_{fc}^{cc}(\vec{q}, i\omega_n)}{1 - J[\Gamma_{cf}^{fc}(\vec{q}, i\omega_n) + \Gamma_{cc}^{ff}(\vec{q}, i\omega_n)]}, \quad (19)$$

and the function (18) is given by

$$\Delta_{cf}(\vec{q}, i\omega_n) = \Gamma_{cc}^{ff}(\vec{q}, i\omega_n) + \frac{J\Gamma_{fc}^{fc}(\vec{q}, i\omega_n)\Gamma_{cc}^{ff}(\vec{q}, i\omega_n)}{[1 - J\Gamma_{fc}^{fc}(\vec{q}, i\omega_n)]^2 + J^2[\Gamma_{cc}^{ff}(\vec{q}, i\omega_n)]^2}. \quad (20)$$

The $\Gamma(\vec{q}, i\omega_n)$ functions appearing in the previous expressions are given by

$$\Gamma_{cc}^{cc}(\vec{q}, i\omega_n) = \frac{1}{\beta} \sum_{\vec{p}, i\omega_m} \eta^2(\vec{p}) G_{cc}(\vec{p}, i\omega_m) G_{cc}(-\vec{p} + \vec{q}, -i\omega_m + i\omega_n),$$

$$\Gamma_{fc}^{cc}(\vec{q}, i\omega_n) = \frac{1}{\beta} \sum_{\vec{p}, i\omega_m} \eta(\vec{p}) G_{cc}(\vec{p}, i\omega_m) G_{fc}(-\vec{p} + \vec{q}, -i\omega_m + i\omega_n),$$

$$\Gamma_{cc}^{ff}(\vec{q}, i\omega_n) = \frac{1}{\beta} \sum_{\vec{p}, i\omega_m} G_{ff}(\vec{p}, i\omega_m) G_{cc}(-\vec{p} + \vec{q}, -i\omega_m + i\omega_n),$$

$$\Gamma_{cf}^{fc}(\vec{q}, i\omega_n) = \frac{1}{\beta} \sum_{\vec{p}, i\omega_m} G_{fc}(\vec{p}, i\omega_m) G_{cf}(-\vec{p} + \vec{q}, -i\omega_m + i\omega_n).$$

3. Superconducting and magnetic instabilities

The magnetic and superconducting instabilities of the system are signalled by the poles of the corresponding susceptibilities. Therefore, we search for the temperature T at which the denominators in the RPA expressions for the susceptibilities vanish:

$$K_m(\vec{Q}, 0) = [1 - J\bar{\Gamma}_{fc}^{cf}(\vec{Q}, 0)]^2 - J^2\bar{\Gamma}_{ff}^{ff}(\vec{Q}, 0)\bar{\Gamma}_{cc}^{cc}(\vec{Q}, 0), \quad (21)$$

$$K_{dd}(0, 0) = 1 - J[\Gamma_{cf}^{fc}(0, 0) + \Gamma_{cc}^{ff}(0, 0)], \quad (22)$$

$$K_{cf}(0, 0) = [1 - J\Gamma_{fc}^{fc}(0, 0)]^2 + J^2[\Gamma_{cc}^{ff}(0, 0)]^2, \quad (23)$$

where $\vec{Q} = (\pi, \pi, \pi)$ and where $K_m(\vec{Q}, 0)$, $K_{dd}(0, 0)$ and $K_{cf}(0, 0)$ are the Stoner factors of the correlation functions (16), (19) and (20), respectively. Since heavy-fermion materials are antiferromagnetic materials we seek for poles of $K_m(\vec{Q}, 0)$ at the antiferromagnetic wavevector \vec{Q} . From the definitions of the $\Gamma(\vec{q}, i\omega_n)$ functions we see that the Cooper pair structure factor $\eta(\vec{p})$ does not appear in the Stoner factors $K_{dd}(0, 0)$ and $K_{cf}(0, 0)$. Moreover, we shall see below that the solutions to $K_{dd}(0, 0) = 0$ and $K_{cf}(0, 0) = 0$ lead to the same critical temperature. Therefore, the system's tendency for a certain Cooper pair symmetry only shows up in the intensity of $\Delta_{dd}(0, 0)$ or $\Delta_{cf}(0, 0)$, which is controlled by the numerator of these functions. We also see that both antiferromagnetism and superconductivity are controlled by the same interaction parameter J , which, in turn, depends on hybridization only.

In figure 1 we show a plot of the Néel and superconducting temperatures as functions of the total electronic density n . It is seen that antiferromagnetism can only occur in a very small

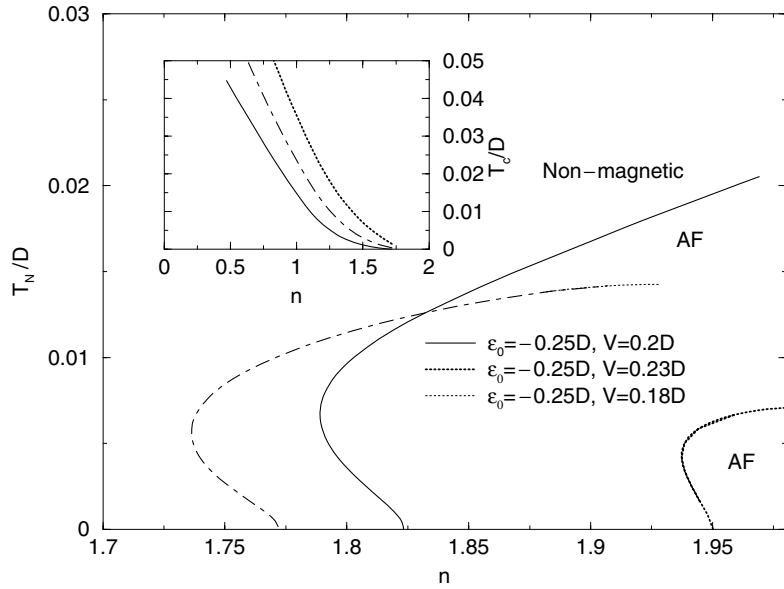


Figure 1. Néel temperatures as functions of the electronic density n . The inset shows the superconducting critical temperature as a function of n . The temperatures are normalized by half the bandwidth, $D = 6t$ and $t = 1$.

region of electronic density. Furthermore, the increase of T_N when $n \rightarrow 2$ corresponds to an increase of the density of n_f electrons towards the Kondo limit ($n_f = 1$). It is also clear that T_N is not a monotonically increasing function of J . Upon reducing V , a larger range of electronic densities can be reached where antiferromagnetic order can be found. From the inset of figure 1 we see that the superconducting temperature T_c is very small ($T_c \sim T_N/50$) close to the density region where the system exhibits antiferromagnetic order.

The dependence of the Néel and superconducting temperatures on pressure has been measured in some heavy-fermion systems [4, 20, 21]. In those studies the Néel temperature is found to decrease as the applied pressure increases and superconducting order is found to develop in a limited range of applied pressures, when the Néel temperature is reduced below ~ 1 K. Let us now see how the critical temperatures in our model vary with the model parameters which, in principle, should depend on externally applied pressure. Increasing pressure should, presumably, make both the hybridization V and the conduction band hopping t increase [22, 23]. In figure 2 we present T_N and T_c versus V , taking the ratio V/t constant. We see that above a certain value of V the magnetic order disappears but the superconducting order remains. We also find that close to the region where the magnetic order vanishes, T_c is much smaller than the maximum value attained by T_N . This is in qualitative agreement with experimental data on some cerium compounds (e.g. CeIn_3), where the ratio $T_N/T_c \sim 100$. Other examples are: $\text{CeCu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$, where T_c as function of pressure displays a positive curvature; and CeRhIn_5 , where the T_c -curve is almost parallel to the pressure axis [26]. For CeCu_2Ge_2 and CeCu_2Si_2 the T_c -curve initially stays almost parallel to the pressure axis, but it shoots up above a certain pressure [27]. Although T_c keeps increasing as V increases, it never reaches values comparable with the maximum value of T_N , even for unreasonable values of V as we can see in the right panel of figure 2. We believe that a better treatment of the boson propagator will lead to a decrease of T_c in agreement with the experiments. We remark that the

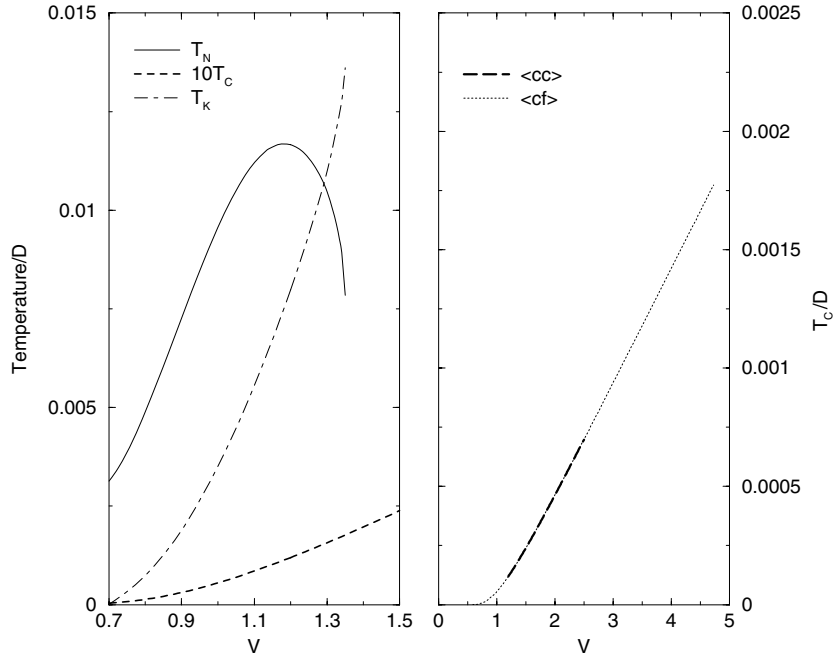


Figure 2. Left: Néel temperature T_N and superconducting critical temperature T_c as functions of V , for a constant ratio of $V/t = 1.2$, electronic density $n = 1.8$ and $\epsilon_0 = -0.25D$. Right: T_c over a very large (unphysical) range of values of V . Note that $T_c \ll T_N$ always. $\langle cc \rangle$ and $\langle cf \rangle$ indicate that T_c has been computed using equations (22) and (23), respectively. The two methods give the same results.

above calculation of T_c is only valid in the situation where the system is non-magnetic because we have not calculated $K_{dd}(0, 0)$ or $K_{cf}(0, 0)$ in the magnetically ordered phase. Furthermore, when T_c is small, the approximation employed for the boson propagator should be improved by including its low-energy part.

For comparison we also plot the temperature T_K defined as the difference between the renormalized f-level energy ϵ_f and the chemical potential [9–11]. This can be very different from the lattice Kondo temperature [24] in the non-magnetic system. Nevertheless, the combined behaviour of T_N and T_K presents the well-known Doniach form showing the interplay between the RKKY and Kondo screening effects. For small values of V , T_K is exponentially small and the system shows antiferromagnetic order. On the other hand, as V increases the Kondo temperature grows, leading to Kondo compensation of the f moments and to a decreasing Néel temperature. For even larger values of V , complete disappearance of the magnetic order takes place and the system shows paramagnetic behaviour (assuming there are enough conduction electrons to compensate all the f local moments). We have also computed the superconducting critical temperature from both equations (22) and (23) and obtained the same T_c , as can be seen in the right panel of figure 2. Along the T_N -curve, n_f decreases from 1 to 0.8, as V increases, and $n_f \approx 0.85$ when T_N is maximum.

Figures 1 and 2 show similar behaviours near the point where $T_N \rightarrow 0$. In both cases T_c starts to increase with a positive curvature. Although in many heavy-fermion systems T_c presents a negative curvature, there are examples where a positive curvature has been observed, such as CePd_2Si_2 under chemical pressure ($T_N = 10$ K, $T_c = 0.2$ K; therefore $T_N/T_c = 50$) [25].

Since our treatment does not take competition between magnetism and superconductivity into account, we cannot tell whether finite values of T_c and T_N imply that both types of order will be present at low temperature. Nevertheless, we found in previous work [23], at the simplest mean-field level, that magnetism and superconductivity may coexist in the system. It follows from the above remarks that the calculation of T_c when T_N is finite requires both the introduction of a better approximation for the boson propagator and extra electronic propagators describing the antiferromagnetic order in the system, as was done in the description of spin waves in the magnetically ordered Mott insulator [28].

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