Superconductivity in the SU(N) Anderson lattice at $U=\infty$

M. A. N. Araújo
Departamento de Física, Universidade de Évora, Rua Romão Ramalho, 59, P-7001 Évora Codex, Portugal

N. M. R. Peres
Departamento de Física, Universidade de Évora, Rua Romão Ramalho, 59, P-7001 Évora Codex, Portugal

P. D. Sacramento
Departamento de Física and CFIF, Instituto Superior Técnico, Avenida Rovisco Pais, 1049-001 Lisboa, Portugal

V. R. Vieira
Departamento de Física and CFIF, Instituto Superior Técnico, Avenida Rovisco Pais, 1049-001 Lisboa, Portugal
(Received 3 February 2000)

We present a mean-field study of superconductivity in a generalized N-channel cubic Anderson lattice at $U=\infty$ taking into account the effect of a nearest-neighbor attraction J. The condition $U=\infty$ is implemented within the slave-boson formalism considering the slave bosons to be condensed. We consider the f-level occupancy ranging from the mixed valence regime to the Kondo limit and study the dependence of the critical temperature on the various model parameters for each of three possible Cooper pairing symmetries (extended s-, d-, and p-wave pairing) and find interesting crossovers. It is found that the d- and p-wave order parameters have, in general, very similar critical temperatures. The extended s-wave pairing seems to be relatively more stable for electronic densities per channel close to one and for large values of the superconducting interaction J.

I. INTRODUCTION

The superconducting behavior of heavy-fermion materials has attracted much attention due to its nonconventional properties.[1] Despite the large amount of work trying to understand heavy-fermion superconductivity, the normal state properties, the symmetry of the order parameter, the origin of superconductivity and the interplay between superconductivity and magnetism are still interesting and open questions.

Some of these materials, such as $UAgCu_4$, UCu_7, U_2Zn_{17}, order antiferromagnetically at low temperatures while others (such as UBe_{13}, $CeCu_2Si_2$, UPt_3) order in a superconducting state and others show no ordering (such as $CeAl_3$, $UAuPt_4$, $CeCu_6$, UAl_2).[1] There are materials which order both antiferromagnetically and become superconducting as the temperature drops (e.g., URu_2Si_2, $U_{0.97}Th_{0.03}Be_{13}$) and it has recently been found that UPd_2Al_3 shows coexistence of superconductivity and local moment antiferromagnetism.[2] All these materials have very large specific heat coefficients γ, indicating very large effective masses, hence the designation heavy fermions.

The superconducting properties of a system depend on the type of ground state that the system exhibits in the normal phase. The large specific heat γ coefficient can have two very different origins: a Kondo-impurity behavior,[3] in which case γ behaves as the inverse of the Kondo temperature T_K, or a Kondo-lattice behavior, in which case γ is controlled by a large density of states at the Fermi energy. The large density of states arises from a hybridization mechanism between the conduction band and localized electronic states (f states, say).[4]

Even though the large effective masses indicate strong correlations between the electrons, these behave in many cases as essentially ''free,'' with renormalized parameters, as explained by the Fermi-liquid theory. However, there has recently been growing evidence that other materials have properties that do not fit the Fermi-liquid picture.[5] The reason could be either disorder,[6] vicinity to a quantum phase transition,[7] or unusual impuritylike behavior such as the one described by generalized models, as the n-channel Kondo model.[8] The n-channel Kondo lattice shows interesting behavior and it has been shown to be an incoherent metal at low temperatures with a residual entropy that is usually lifted via ordering at very low temperatures.[9]

A consistent description of the overall properties of the heavy-fermion behavior has been achieved assuming that a generalization of the impurity Anderson model to the lattice case is valid.[4,10] 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. Moreover, these systems are often characterized by large angular momentum, due to the spin-orbit coupling.[3,4] In general, both the large values of U and the large total angular momentum must be included in any model used to describe the properties of heavy-fermion materials.

The SU(N) Anderson lattice Hamiltonian is believed to give a good description of the normal state of Kondo-lattice systems.[4] The limit $U=\infty$ is considered in many calculations since the experimental U values are large. The Anderson lattice model predicts Fermi-liquid-like properties in the normal nonmagnetic state. The theoretical results give a good description of many materials and explain the main features

at low temperatures such as universality, large effective masses, the Kondo resonance at the Fermi level. At the single-impurity level the picture is clear. In the Kondo limit the f level has an occupation close to one leading to a localized spin that is shielded by a conduction electron spin cloud. This compensation of the spin explains why some of these compounds do not order magnetically. The main point to be explained in the lattice case is the competition between the Kondo compensation of the localized spins and the magnetic interactions between them. In these materials this interaction is mediated by the conduction electrons Ruderman-Kittel-Kasuya-Yosida (RKKY) type. Actually, since the Kondo temperature is very small it is difficult to explain why the RKKY does not always prevail. Related to this competition is the effectiveness of the compensating cloud around each f level. The size of this cloud has been subject of controversy. Arguments show that it should be a large scale of the order of v_F/T_K (Ref. 11) but other arguments claim to be $\sim a$ (a is the lattice constant).[12] This is a relevant issue in the lattice case related to Nozières exhaustion problem which states that there are not enough conduction electrons to screen the f levels.

To increase the complexity the system may also order into a superconducting state. Many questions have been raised starting from the result that the discontinuity of the specific heat at T_c is large, of the order of the specific heat itself in the normal phase (which originates in the heavy fermions). This indicates that pairing occurs between the heavy f-level electrons, which will then form the condensate. Within the Anderson lattice model the strong correlations and the hybridization are responsible for the high effective masses and 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[13] slave boson formalism together with a large-N approach, various attempts have been made to search for the existence of superconducting instabilities in the infinite-U Anderson-lattice model. It was proposed[14] that slave bosons 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.[15]

Assuming that the normal state is a Fermi liquid, several other studies of superconductivity have been carried out on the Anderson lattice model and generalizations of it.[16–19] By adding an attractive nearest-neighbor interaction between the f electrons, so as to explicitly provide an attractive channel leading to superconductivity, a mean-field study has been carried out as a function of the local repulsion U. Romano, Noce, and Micnas[19] have found a superconducting ground state for finite values of U, but no superconductivity was found for large values of onsite Coulomb repulsion, in the Anderson lattice. This is so because the authors consider the Kondo regime (this is, $\epsilon_0 \ll \mu$ where μ is the chemical potential), where the occupation number of an f orbital n_f is close to two for small U. Therefore, upon increasing the interaction U, this number is reduced to one, blocking charge transport in the f band.

In this paper we carry out a mean field study of superconductivity in the $U=\infty$ Anderson lattice where an attractive interaction between neighboring f orbitals is explicitly introduced in order to simulate an effective interaction (which might have various causes) leading to superconductivity. Since $U=\infty$, we are restricted to f-level occupancies in the range $0<n_f<1$. In the mixed valent regime, where n_f is between zero and one, charge movement is allowed among the f orbitals, even when $U=\infty$. We study the dependence of the critical temperature and f-level ocupancy on the various model parameters for different Cooper pairing symmetries. The paper is organized as follows. In Sec. II we present the model Hamiltonian we use in our study and derive the mean field equations. Particular attention is paid on the form of the superconducting pairing term. In Sec. III we present our calculations of the critical temperature as function of the several parameters of the model and we summarize our findings in Sec. IV.

II. THE MODEL HAMILTONIAN

We consider an extended version of the Anderson lattice model, which includes a density-density attraction between the electrons occupying neighboring f orbitals. This form of interaction enables us to consider three possible symmetries for electron pairing: s, d, and p wave. The Hamiltonian is given by

$$H=H_c^0+H_f^0+H_{cf}+H_U+H_J, \tag{1}$$

where

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

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

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

$$H_U=U\sum_{i,m\neq m'}n_{i,m}n_{i,m'}, \tag{5}$$

and

$$H_J=\frac{1}{2}J\sum_{\langle i,j\rangle,m,m'}n_{i,m}n_{j,m'}, \tag{6}$$

where i and j are nearest neighbor sites and $n_{i,m}=f_{i,m}^{\dagger}f_{i,m}$. The c and f operators are fermionic and obey the usual anticommutation relations. The hybridization potential V is assumed to be momentum independent. The term H_U represents the strong onsite repulsion between the f orbitals and in the rest of this work we shall consider $U=\infty$. The term H_J explicitly describes an effective attraction between neighboring f sites ($J<0$) which is responsible for superconductivity. The total angular momentum projection m takes on N values.[10,13] We shall assume that the local angular momentum of the f sites is half-integer and, therefore, that N is even.

The term H_J may be rewritten in momentum space as

$$H_J=\sum_{\vec{Q},\vec{k},\vec{k}'}\sum_{m,m'}\frac{J_{\vec{k},\vec{k}'}}{2}f^{\dagger}_{\vec{Q}/2+\vec{k}',m}f^{\dagger}_{\vec{Q}/2-\vec{k}',m'}\times f_{\vec{Q}/2-\vec{k},m'}f_{\vec{Q}/2+\vec{k},m}, \tag{7}$$

where the interaction $J_{\vec{k},\vec{k}'}=J\Sigma_{\vec{\delta}}\exp i(\vec{k}-\vec{k}')\cdot\vec{\delta}$ and the summation over $\vec{\delta}$ runs over the nearest neighbors. Considering the case of a cubic lattice, the interaction $J_{\vec{k},\vec{k}'}$ may be separated into terms with *s*-, *p*-, and *d*-wave symmetries as[20]

$$J_{\vec{k},\vec{k}'}=J\left(\eta^{(s)}_{\vec{k}}\eta^{(s)}_{\vec{k}'}+\sum_{i=x,y,z}\eta^{(p,i)}_{\vec{k}}\eta^{(p,i)}_{\vec{k}'}\right)+J(\eta^{(d_{x^2-y^2})}_{\vec{k}}\eta^{(d_{x^2-y^2})}_{\vec{k}'}+\eta^{(d_{r^2-3z^2})}_{\vec{k}}\eta^{(d_{r^2-3z^2})}_{\vec{k}'}),$$

where

$$\eta^{(s)}_{\vec{k}}=\sqrt{\frac{2}{3}}[\cos(k_x)+\cos(k_y)+\cos(k_z)],$$

$$\eta^{(p,i)}_{\vec{k}}=\sqrt{2}\sin(k_i),$$

$$\eta^{(d_{x^2-y^2})}_{\vec{k}}=\cos(k_x)-\cos(k_y),$$

$$\eta^{(d_{r^2-3z^2})}_{\vec{k}}=\frac{1}{\sqrt{3}}[\cos(k_x)+\cos(k_y)-2\cos(k_z)]. \tag{8}$$

Electron pairing in the superconducting phase will occur in the state with total pair momentum $\vec{Q}=0$.

We implement the condition $U=\infty$ within the slave-boson formulation due to Coleman,[13] in which the empty *f* site is represented by a slave boson b_i and the physical operator f_i in Eq. (4) is replaced with $b^{\dagger}{}_i f_i$. Condensation of the slave-bosons can be described by the replacement $b_i\rightarrow\langle b_i\rangle=\langle b^{\dagger}{}_i\rangle=\sqrt{z}$. The mean-field treatment of the interaction term H_J involves the usual decoupling of destruction and annihilation operators but, in keeping with the spirit of Coleman's slave boson formalism, we associate a boson operator with every *f* operator in Eq. (7) in order to prevent double occupancy at the *f* sites. Taking also into account the boson condensation, we obtain the superconducting part of the mean-field Hamiltonian from the substitution $f^{\dagger}f^{\dagger}ff\rightarrow zf^{\dagger}f^{\dagger}\langle zff\rangle+\text{H.c.}$ Following these ideas we write down the effective Hamiltonian as[21]

$$H_{eff}=\sum_{\vec{k},m}[(\epsilon_{\vec{k}}-\mu)c^{\dagger}_{\vec{k},m}c_{\vec{k},m}+(\epsilon_f-\mu)f^{\dagger}_{\vec{k},m}f_{\vec{k},m}]+\sqrt{z}V\sum_{\vec{k},m}(f^{\dagger}_{\vec{k},m}c_{\vec{k},m}+c^{\dagger}_{\vec{k},m}f_{\vec{k},m})+\frac{1}{2}\sum_{\vec{k},m}(zf^{\dagger}_{\vec{k},m}f^{\dagger}_{-\vec{k},m},\Delta_{\vec{k},m}+zf_{-\vec{k},m'}f_{\vec{k},m}\Delta^{*}{}_{\vec{k},m})-\frac{N_s}{2J}\sum_m\Delta^{*}{}_m\Delta_m+(\epsilon_f-\epsilon_0)(z-1)N_s, \tag{9}$$

where N_s denotes the number of lattice sites and ϵ_f is the renormalized energy of the *f* orbitals due to the on-site repulsion. The angular momentum projection $m'=-m$ if electron pairing in a singlet state (*s* or *d* wave) is considered and $m'=m$ in the case of *p* wave pairing. The gap function $\Delta_{\vec{k},m}=\eta_{\vec{k}}\Delta_m$ and the superconducting order parameter Δ_m is given by

$$\Delta_m=\frac{zJ}{N_s}\sum_{\vec{k}}\eta_{\vec{k}}\langle f_{-\vec{k},m}f_{\vec{k},m}\rangle, \tag{10}$$

where $\eta_{\vec{k}}$ denotes any of the possible pairing symmetries considered in Eq. (8).

The density of the boson condensate *z* minimizes the free energy of the system and ϵ_f is obtained after imposing local particle (boson+fermion) conservation at the *f* sites:

$$z=1-\frac{1}{N_s}\sum_{\vec{k},m}\langle f^{\dagger}_{\vec{k},m}f_{\vec{k},m}\rangle, \tag{11}$$

$$\epsilon_f-\epsilon_0=-\frac{V}{2\sqrt{z}N_s}\sum_{\vec{k},m}(\langle f^{\dagger}_{\vec{k},m}c_{\vec{k},m}\rangle+\langle c^{\dagger}_{\vec{k},m}f_{\vec{k},m}\rangle)-\frac{N_s}{zJ}\sum_m\Delta^{*}_m\Delta_m. \tag{12}$$

Equation (11) states that the mean number of electrons at an *f* site is $1-z$.

In order to derive the gap equation and the spectrum of elementary excitations we use the Gorkov Green's function approach. The anomalous Green's functions that we need to consider are

$$\mathcal{F}^{\dagger}_{f,m}(\vec{k},\tau-\tau')=\langle T_\tau f^{\dagger}_{\vec{k},m}(\tau)f^{\dagger}_{-\vec{k},-m}(\tau')\rangle, \tag{13}$$

$$\mathcal{F}^{\dagger}_{cf,m}(\vec{k},\tau-\tau')=\langle T_\tau c^{\dagger}_{\vec{k},m}(\tau)f^{\dagger}_{-\vec{k},-m}(\tau')\rangle, \tag{14}$$

and we must also define three other Matsubara Green's functions: one that is associated with the conduction electrons, another one for the *f* electrons and the third one is related to the hybridization of the *f* and *c* bands:

$$\mathcal{G}_{c,m}(\vec{k},\tau-\tau')=-\langle T_\tau c_{\vec{k},m}(\tau)c^{\dagger}_{\vec{k},m}(\tau')\rangle, \tag{15}$$

$$\mathcal{G}_{f,m}(\vec{k},\tau-\tau')=-\langle T_\tau f_{\vec{k},m}(\tau)f^{\dagger}_{\vec{k},m}(\tau')\rangle, \tag{16}$$

$$\mathcal{G}_{cf,m}(\vec{k},\tau-\tau')=-\langle T_\tau c_{\vec{k},m}(\tau)f^{\dagger}_{\vec{k},m}(\tau')\rangle. \tag{17}$$

After Fourier transforming these functions into frequency space, we may write down their equations of motion (Gorkov's equations) according to the Hamiltonian (9):

$$(-i\omega_n+\epsilon_f-\mu)\mathcal{G}_{f,m}(\vec{k},i\omega_n)+V\sqrt{z}\mathcal{G}_{cf,m}(\vec{k},i\omega_n)+Jz^2\Delta_m(\vec{k})\mathcal{F}^{\dagger}_{f,m}(\vec{k},-i\omega_n)=-1, \tag{18}$$

$$(-i\omega_n+\epsilon_{\vec{k}}-\mu)\mathcal{G}_{cf,m}(\vec{k},i\omega_n)+V\sqrt{z}\mathcal{G}_{f,m}(\vec{k},i\omega_n)=0, \tag{19}$$

$$(-i\omega_n-\epsilon_{\vec{k}}+\mu)\mathcal{F}^{\dagger}_{cf,m}(\vec{k},i\omega_n)-V\sqrt{z}\mathcal{F}^{\dagger}_{f,m}(\vec{k},i\omega_n)=0, \tag{20}$$

$$(-i\omega_n-\epsilon_f+\mu)\mathcal{F}^{\dagger}_{f,m}(\vec{k},i\omega_n)-V\sqrt{z}\mathcal{F}^{\dagger}_{cf,m}(\vec{k},i\omega_n)$$
$$+Jz^2\Delta^{\dagger}_m(\vec{k})\mathcal{G}_{f,m}(-\vec{k},i\omega_n)=0. \quad (21)$$

Diagonalization of the above equations yields the energies of the poles of the Green's functions (excitation energies) and the corresponding residues (coherence factors). The solutions are of the form

$$\mathcal{G}(\vec{k},i\omega)=-\sum_{i=1,2}\sum_{\alpha=\pm}\frac{u_i^{\alpha}}{i\omega_n+\alpha E_i}. \quad (22)$$

The coherence factors, u_i^{α} and the excitation energies, E_i are given in the Appendix.

The Green's functions have to be determined self-consistently using the mean field equations (10)–(12). These equations can be rewritten in terms of Green's functions as

$$z=1-\frac{T}{N_s}\sum_{\vec{k},m}\sum_{i\omega_n}\mathcal{G}_{f,m}(\vec{k},i\omega_n), \quad (23)$$

$$\epsilon_f-\epsilon_0=-\frac{VT}{\sqrt{z}N_s}\sum_{\vec{k},m}\sum_{i\omega_n}\mathcal{G}_{cf,m}(\vec{k},i\omega_n)-\frac{N_s}{zJ}\sum_m\Delta_m^*\Delta_m, \quad (24)$$

$$\Delta_m=\frac{zJT}{N_s}\sum_{\vec{k}}\sum_{i\omega_n}\eta_{\vec{k}}\mathcal{F}_{f,m}(\vec{k},i\omega_n). \quad (25)$$

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:

$$n=1-z+\frac{T}{N_s}\sum_{\vec{k},m}\sum_{i\omega_n}\mathcal{G}_{c,m}(\vec{k},i\omega_n). \quad (26)$$

III. RESULTS

In what follows we consider a cubic lattice in which the conduction band dispersion has the simple tight-binding form

$$\epsilon_{\vec{k}}=-2t\sum_{i=x,y,z}\cos(k_i),$$

so that $D=6t$ is half the bandwidth. We have used the subroutine HYBRD.F from MINPACK in order to solve the four coupled equations (23)–(26).

The possible pairing symmetries expressed in Eq. (8) have been studied separately. The two $\eta_{\vec{k}}$ functions corresponding to the d-wave symmetry in Eq. (8) describe different spatial orientations of the angular momentum of the Cooper pairs and give degenerate solutions. This same remark also applies to the three p-wave $\eta_{\vec{k}}$ functions in Eq. (8).

The critical temperatures T_c are obtained solving the mean-field equations using the normal state Green's functions. On the other hand, the study of $\Delta(T)$, $z(T)$, $\epsilon_f(T)$, and the specific heat requires solving the mean-field equations with the full Green's functions. In the normal phase, the slave boson condensation temperature, T_z, above which $z=0$, is given by $T_z=(\epsilon_f-\mu)/\ln(N-1)$. If $N=2$, z is always finite. For larger values of N, and in particular in the limit $N\to\infty$, $z\to 0$ as the temperature increases. Correspondingly, $n_f\to 1$ and the f-electron superconductivity is inhibited. Therefore, for large values of N it is expected that the mean-field theory will not yield superconductivity. One then has to take into account the boson fluctuations. We will focus our attention in the case $N=2$, relevant for instance for Ce and Yb materials, but we will return to this point later.

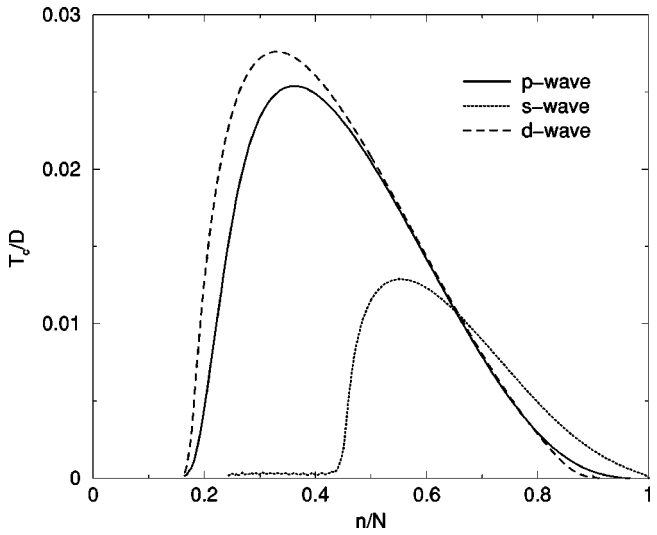

FIG. 1. The critical temperature as function of the total density of electrons per channel, for the $U=\infty$ Anderson lattice. The parameters are $N=2$, $\epsilon_f=-0.25D$, $V=0.2D$, and $J=-0.5D$. The hopping integral $t=1$ and $D=6t$.

Figure 1 shows the behavior of the superconducting critical temperatures T_c as function of the particle density per channel n/N, for each of the three pairing symmetries. It is readily seen that the critical temperatures associated with d- and p-wave pairing follow similar trends and that the d-wave symmetry exhibits the highest T_c up to densities of about $n/N\approx 0.6$. At higher densities, a crossover occurs into a regime where the extended s-wave pairing becomes the most stable, for the parameters considered.

The value of T_c vanishes at low densities because the f-level occupancy also becomes small in that limit ($z\to 1$) and Cooper pairing occurs only between the f electrons in the model under consideration. In the high density limit, T_c vanishes because each f level is almost fully occupied with one electron ($z\to 0$), and freezing of the charge fluctuations [arising from the term $f^{\dagger}f^{\dagger}$ in Eq. (9)] occurs because of the infinite on-site repulsion.

Heavy-fermion behavior in the normal phase occurs when the chemical potential μ lies close to the peak of the density of states (hence the strong effective mass). This peak is the equivalent of the Kondo resonance peak which appears in the single-impurity problem. For the lattice problem, two strong peaks appear due to hybridization between the conduction electron band and the dispersionless band of localized f states, leading to the large electron's effective mass. For densities above $n/N\approx 0.7$ the chemical potential becomes close to the density of states peak in the lower band.

In the superconducting phase the full solution of Eqs. (23)–(26) yields a renormalized excitation energy spectrum. In Fig. 2 we show the band structure for $n/N=0.7$ in the

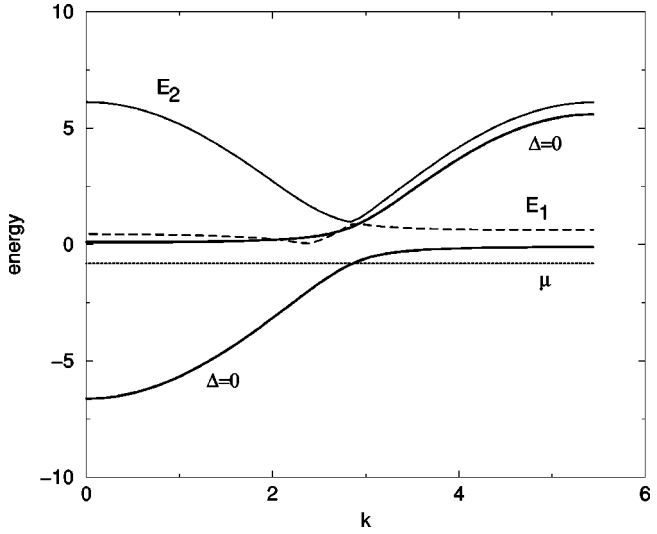

FIG. 2. Band structure of the normal and superconducting states, along the direction $k_x=k_y=k_z$ in momentum space ($k=\sqrt{3}k_x$), at zero temperature. The total electronic density per channel is $n/N=0.7$ and the other parameters are the same as in Fig. 1. The symmetry of the superconducting order parameter is extended *s* wave. The excitation energies E_1 and E_2 are given by Eqs. (A2) and (A3).

normal and superconducting phases. It is clear that for this density μ is in the flat region of the band in the normal state.

It is seen from Fig. 1 that as the density per channel n/N approaches 1, the value of T_c is strongly reduced until it eventually vanishes. From the same figure one can also see that the critical temperature of the *s*-wave state at $n/N\approx 0.7$, for instance, is higher than that of the *d*- or *p*-wave states. For the model parameters considered in Fig. 1 this means that as the temperature of a normal system is lowered, the system would first enter a superconducting state with extended *s*-wave symmetry. On lowering further the temperature, the nature of the superconducting state becomes a mixture of different symmetries. This sequence of phase transitions would be different had we chosen different parameters: our calculations show that if J/D is less than about 0.4, then the critical superconducting temperature of a system with $n/N\approx 0.7$ would correspond to a *d*-wave order parameter (see left panel of Fig. 3).

The dependence of T_c on the parameters V, ϵ_0 and J shows interesting crossovers. If ϵ_0 is well below the chemical potential μ then the *f* level is highly populated and the system cannot become superconducting unless the hybridization parameter V is large enough. On the other hand, if ϵ_0 is not too low a superconducting ground-state is obtained even for small values of V. As can be seen from the right panel of Fig. 3, T_c first increases with V up to a maximum value, but as V is further increased, large charge quantum fluctuations at the *f* orbitals are induced and superconductivity is destroyed. Moreover, the *d*- and *p*-wave superconductivity seem to be more stable than the *s* wave for large values of V. That this result is consistent with Fig. 1 can be easily understood as follows: upon increasing the hybridization between the *f* orbitals and the conduction band, the electron occupation in the *f* sites is reduced and Fig. 1 already showed that depletion of the *f* band has the effect of reducing T_c and increasing the stability of *d*-wave pairing relative to *p*- and *s*-wave pairing.

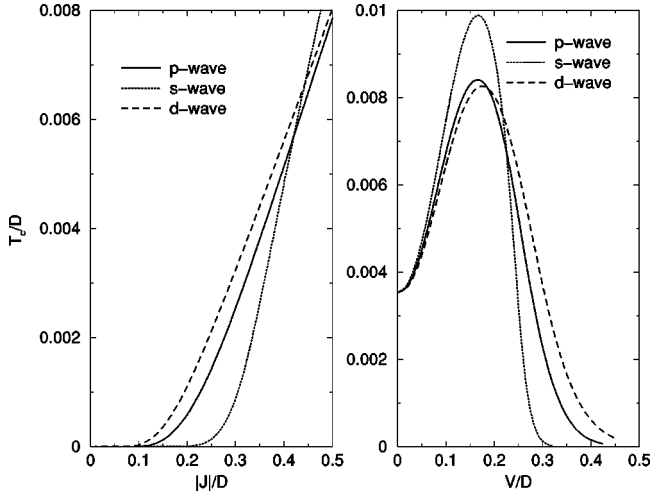

FIG. 3. Left panel: The critical temperature T_c as function of the coupling J. Right panel: The critical temperature T_c as function of the hybridization parameter V. The total electronic density per channel is $n/N=0.7$ and the other parameters are the same as in Fig. 1.

The temperature dependence of the gap function in the superconducting phase is the standard one. In Fig. 4 we show a typical case. The crossing of the *d*- and *p*-order parameters close to T_c is related with the same crossing observed in $z(T)$. Since close to T_c, $z(T)$ for the superconducting *d* phase becomes slightly higher than for the superconducting *p* phase, the *d*-wave phase has an effective superconducting coupling that is slightly higher than the *p*-wave coupling, leading to an higher T_c.

In Fig. 5 we show the dependence of T_c on the *f*-level position. It is seen that the *d*-wave state has always a higher T_c than the *p* wave over the range of ϵ_0 values considered. But the *s*-wave critical temperature exhibits a much stronger dependence on ϵ_0. In particular, *s*-wave pairing seems to be more strongly depressed for low ϵ_0.

In a normal system at zero temperature the renormalized *f*-level energy ϵ_f is located above the chemical potential and

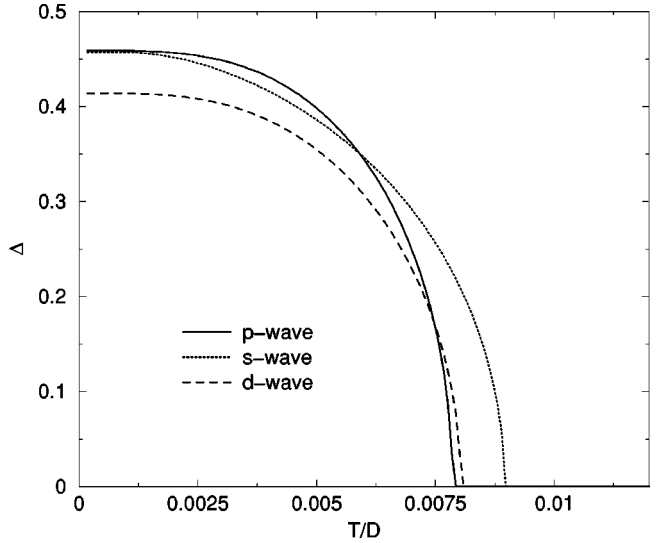

FIG. 4. Superconducting gap $\Delta(T)$ as functions of the temperature for the three symmetries considered. The parameters are the same as in Fig. 1.

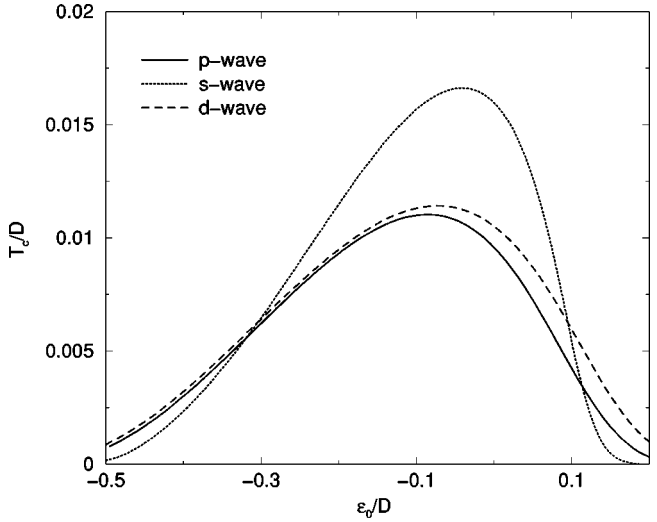

FIG. 5. The critical temperature T_c as function of the f-level bare energy ϵ_0. The total electronic density per channel is $n/N=0.7$ and the other parameters are the same as in Fig. 1.

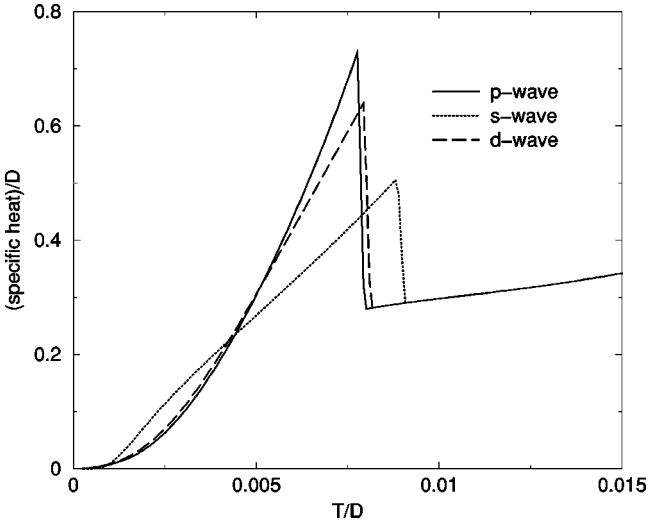

FIG. 7. Specific heat $C(T)$ as function of the temperature for the three symmetries considered. The parameters are the same as in Fig. 1.

$\epsilon_f-\mu$ is of the order of the Kondo temperature for the equivalent single-imputity problem. Keeping the particle density fixed, both ϵ_f and μ increase with temperature but the difference $\epsilon_f-\mu$ decreases. Our calculations show that T_c is smaller than $\epsilon_f-\mu$ by a factor of about 10 (see Fig. 6) over almost the entire range of densities considered in Fig. 1. In Fig. 6 we present T_c, ϵ_f, and μ for the extended s-wave order parameter (the curves for the other symmetries are qualitatively the same). The susceptibility $dn_f/d\epsilon_f$, in the region of densities characterized by $n/N\simeq 0.7$ or larger, is very small since the f-level density of states is much larger than the c-level one, leading to a negative feedback changing the chemical potential in such a way as to keep ϵ_f close to μ. This is very clear from Fig. 6, where ϵ_f is indeed close to μ, for electronic densities where the density of states is large.

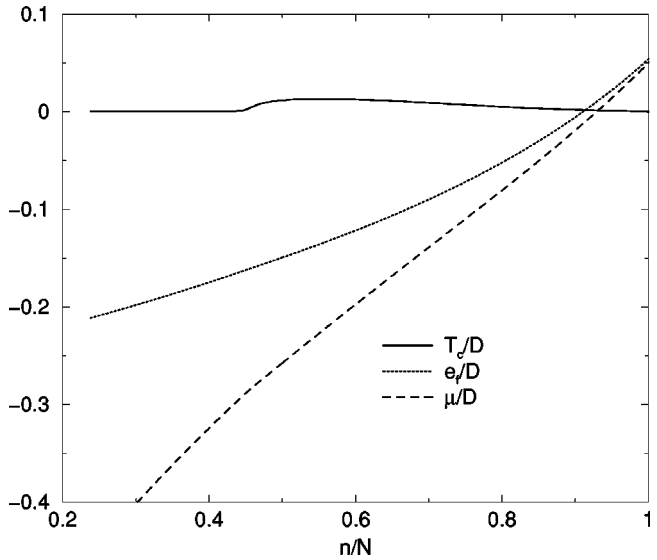

FIG. 6. Critical temperature T_c, renormalized energy level ϵ_f, and chemical potencial μ as function of n/N. The value of $\epsilon_f-\mu$ is much larger than T_c. The symmetry of the superconducting order parameter is extended s wave, and the other symmetries follow the same trends. The parameters are the same as in Fig. 1.

This is consistent with the picture that the pairing is developed by the excitations of the system resulting from the Kondo compensated lattice.

Finally we calculate the specific heat for the various symmetries. The nonconventional pairing symmetry leads to a power law behavior at low T in the superconducting phase. In Fig. 7 we show the specific heat for the various symmetries as a function of temperature. The specific heat jump at the transition is $\Delta C/C\sim 1.6,1.3,0.8$ for the p, d, s symmetries, respectively. We have found that the specific heat at low T has a T^2 dependence for the p, d symmetries, and has an exponential behavior for the s-wave case.

Considering now the effect of increasing the number of channels N, we find that T_c decreases by one order of magnitude or more, as N changes from $N=2$ to $N=4$. For the parameters considered in the figures, the effect is most dramatic for s, p-wave symmetries, where superconductivity is absent for $N\geqslant 4$. Furthermore, we found that the critical temperature of a system with a d-wave order parameter is less sensitive to the number of channels N, as compared to the other symmetries.

IV. SUMMARY

Heavy-fermions show a rich and complex behavior at low temperatures. In particular, the interplay between magnetic correlations, the Kondo effect, and superconducting correlations is a difficult problem to solve. This is further complicated since neither the mechanism nor the pairing symmetry are fully established. In this paper we have focused on the superconducting order assuming that the superconducting correlations are the dominant ones. Using a generalized Anderson lattice model with nearest-neighbor attraction between the f electrons and with infinite-U local Coulomb repulsion, we studied the various pairing symmetries using a mean-field approach. In this way it is possible to compare the various solutions in contrast to an approach where, starting from the normal phase, the leading instabilities are identified.

The results show that there are several crossovers between the s-, d-, and p-wave pairing symmetries as the parameters

of the model are varied. In contrast to a previous mean-field approach we find superconducting order, even though $U=\infty$. The reason is that we focus on a regime where $0<n_f<1$, while the previous work concentrated on a regime where $1<n_f<2$ (for finite U). Since we consider only the case $U=\infty$, n_f has to be smaller than one due to the Coulomb repulsion. In the previous work as U grows the density $n_f\rightarrow 1$ the f electrons become more localized inhibiting superconductivity. We find the same qualitative behavior as we approach the Kondo regime from the mixed valent regime. For small values of ϵ_0 we tend to a regime where $n_f\rightarrow 1$ and superconductivity is suppressed.

In the mean-field approach if $z\rightarrow 0 (n_f\rightarrow 1)$ the gap function $\Delta_m\rightarrow 0$. This happens for large densities $n/N\rightarrow 1$. For $n_f\rightarrow 0$ superconductivy is supressed, since the superconducting coupling is among the f electrons. Also, if N is large $z\rightarrow 0$ at lower temperatures. In particular, p-wave and extended s-wave symmetries are strongly suppressed. For $N=2$ z is always finite. For larger values of N in general it will be necessary to consider the boson fluctuations and a treatment beyond mean-field will be required. For systems where the spin degeneracy is low we expect the results to be qualitatively correct.

We have found that the d-wave and p-wave symmetries yield similar transition temperatures. For large nearest-neighbor attraction the extended s-wave pairing is preferred. Otherwise, the d-wave symmetry seems to be more robust, in particular as N grows. Clearly, we are not considering magnetic correlations in our mean-field study and therefore the description applies to systems where there are no local moments (and therefore $T_c<T_K$) and where $T_c>T_{\mathrm{RKKY}}$.

We found that superconductivity is preferred in a mixed valent regime (due to the infinite Coulomb repulsion). There are materials that are mixed valent and superconductors.[22–27] In the framework of weak coupling BCS theory one would expect that the local magnetic character of the f states should be pair breaking. However, the heavy fermion superconductivity in the Kondo limit (integer valent case) reveals that the pairing is of another nature that compensates the pair breaking effects of the local magnetic character. For materials such as $CeRu_3Si_2$ there is a considerable mixed valent character and accordingly the effective masses are not high. Also, the Wilson ratio is close to one indicating a conventional weak-coupling BCS superconductor. Other mixed valent superconductors are not conventional superconductors. It would be interesting to identify systems that by changing the mixed-valent character could change the superconducting temperature, T_c. In the framework of our model this would require f states with large U values. The nearest-neighbor attraction could be due to several mechanisms like spin fluctuations or slave boson fluctuations (Coulombic nature).

ACKNOWLEDGMENTS

We would like to thank P. Estrela for bringing Refs. 23–27 to our attention. This research was supported by PRAXIS under Grant No. 2/2.1/FIS/302/94.

APPENDIX: POLES AND COHERENCE FUNCTIONS FOR THE GREEN'S FUNCTIONS

The algebraic solutions of Eqs. (18)–(21) for the Green's functions $\mathcal{G}_{f,m}(\vec{k},i\omega_n)$, $\mathcal{G}_{cf,m}(\vec{k},i\omega_n)$, $\mathcal{F}^{\dagger}_{f,m}(\vec{k},i\omega_n)$, and $\mathcal{G}_{c,m}(\vec{k},i\omega_n)$ have the form

$$\mathcal{G}(\vec{k},i\omega_n)=-\sum_{i=1,2}\sum_{\alpha=\pm}\frac{u_i^{\alpha}}{i\omega_n+\alpha E_i}, \tag{A1}$$

and the coherence factors u_i^{α} and the excitations energies E_i are given below.

The energies E_i have the form

$$E_1=\sqrt{\gamma/2-\sqrt{\gamma^2/4-\beta}}, \tag{A2}$$

$$E_2=\sqrt{\gamma/2+\sqrt{\gamma^2/4-\beta}}, \tag{A3}$$

with γ and β given by

$$\gamma=(\epsilon_f-\mu)^2+(\epsilon_{\vec{k}}-\mu)^2+2V^2z+|Jz^2\Delta(\vec{k})|^2, \tag{A4}$$

$$\beta=[(\epsilon_{\vec{k}}-\mu)(\epsilon_f-\mu)-V^2z]^2+|Jz^2\Delta(\vec{k})|^2(\epsilon_{\vec{k}}-\mu)^2. \tag{A5}$$

The u_i^{α} factors for $\mathcal{G}_{f,m}(\vec{k},i\omega_n)$ are given by

$$u_1^{+}=F(E_1+\epsilon_{\vec{k}}-\mu)X_1, \tag{A6}$$

$$u_1^{-}=F(E_1-\epsilon_{\vec{k}}+\mu)Y_1, \tag{A7}$$

$$u_2^{+}=-G(E_2+\epsilon_{\vec{k}}-\mu)X_2, \tag{A8}$$

$$u_2^{-}=-G(E_2-\epsilon_{\vec{k}}+\mu)Y_2, \tag{A9}$$

where the functions X_i and $Y_i (i=1,2)$ are given by

$$X_i=(\epsilon_{\vec{k}}-\mu)(\epsilon_f-\mu)-(\epsilon_{\vec{k}}-\epsilon_f-2\mu)E_i+E_i^2-zV^2, \tag{A10}$$

$$Y_i=(\epsilon_{\vec{k}}-\mu)(\epsilon_f-\mu)+(\epsilon_{\vec{k}}-\epsilon_f-2\mu)E_i+E_i^2-zV^2, \tag{A11}$$

and the functions F and G are given by

$$F=\frac{1}{2E_1(E_2^2-E_1^2)},\quad G=\frac{1}{2E_2(E_2^2-E_1^2)}. \tag{A12}$$

The u_i^{α} factors for $\mathcal{F}^{\dagger}_{f,m}(\vec{k},i\omega_n)$ are given by

$$u_1^{+}=-Jz^2\Delta(\vec{k})F[E_1^2-(\epsilon_{\vec{k}}-\mu)^2],\quad u_1^{+}=-u_1^{-}, \tag{A13}$$

$$u_2^{+}=-Jz^2\Delta(\vec{k})G[E_2^2-(\epsilon_{\vec{k}}-\mu)^2],\quad u_2^{+}=-u_2^{-}. \tag{A14}$$

The u_i^{α} factors for $\mathcal{G}^{\dagger}_{cf,m}(\vec{k},i\omega_n)$ are given by

$$u_1^{+}=-V\sqrt{z}FX_1,\quad u_1^{-}=FY_1, \tag{A15}$$

$$u_2^{+}=V\sqrt{z}GX_2,\quad u_2^{-}=-GY_2. \tag{A16}$$

The u_i^{α} factors for $\mathcal{G}_{c,m}(\vec{k},i\omega_n)$ are given by

$$u_1^{+}=FQ_1,\quad u_1^{-}=-FR_1, \tag{A17}$$

$$u_2^{+}=-GQ_2,\quad u_2^{-}=GR_2, \tag{A18}$$

where

$$Q_i=(\epsilon_{\vec{k}}-\mu-E_i)|Jz^2\Delta(\vec{k})|^2+(\epsilon_f+E_i)X_i, \tag{A19}$$

$$R_i=(\epsilon_{\vec{k}}-\mu+E_i)|Jz^2\Delta(\vec{k})|^2-(-\epsilon_f+E_i)Y_i. \tag{A20}$$

[1] C.M. Varma, Comments Solid State Phys. **11**, 221 (1985); Z. Fisk *et al.*, 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).
[2] N. Bernhoeft, N. Sato, B. Roessli, N. Aso, A. Hiess, G.H. Lander, Y. Endoh, and T. Komatsubara, Phys. Rev. Lett. **81**, 4244 (1998).
[3] A. C. Hewson, *The Kondo Problem to Heavy-fermions* (Cambridge University Press, Cambridge, 1997).
[4] D.M. Newns and N. Read, Adv. Phys. **36**, 799 (1987).
[5] See, for instance, J. Phys.: Condens. Matter **8**, 1 (1986).
[6] V. Dobrosavljevic, T.R. Kirkpatrick, and G. Kotliar, Phys. Rev. Lett. **69**, 1113 (1992); O.O. Bernal *et al.*, *ibid.* **75**, 2023 (1995).
[7] B. Andraka and A.M. Tsvelik, Phys. Rev. Lett. **67**, 2886 (1991); A.M. Tsvelik and M. Reizer, Phys. Rev. B **48**, 9887 (1993).
[8] P. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980); P. Schlottmann and P.D. Sacramento, Adv. Phys. **42**, 641 (1993); D.L. Cox and A. Zawadowski, *ibid.* **47**, 599 (1998).
[9] M. Jarrell, H. Pang, D.L. Cox, and K.H. Luk, Phys. Rev. Lett. **77**, 1612 (1996); F.B. Anders, M. Jarrell, and D.L. Cox, *ibid.* **78**, 2000 (1997); M. Jarrell, H. Pang, and D.L. Cox, *ibid.* **78**, 1996 (1997); P.D. Sacramento and V.R. Vieira, Phys. Rev. B **58**, 11 119 (1998).
[10] A.J. Millis and P.A. Lee, Phys. Rev. B **35**, 3394 (1987).
[11] P. Nozières, Ann. Phys. (Paris) **10**, 19 (1985); V. Barzykin and I. Affleck, Phys. Rev. B **57**, 432 (1998).
[12] J. Gan, J. Phys.: Condens. Matter **6**, 4547 (1994); V. Barzykin and I. Affleck, Phys. Rev. Lett. **76**, 4959 (1996).
[13] P. Coleman, Phys. Rev. B **29**, 3035 (1984); **35**, 5072 (1987).
[14] M. Lavagna, A.J. Millis, and P.A. Lee, Phys. Rev. Lett. **58**, 266 (1987).
[15] A. Houghton, N. Read, and H. Won, Phys. Rev. B **37**, 3782 (1988).
[16] S. Robaszkiewicz, R. Micnas, and J. Ranninger, Phys. Rev. B **36**, 180 (1987).
[17] B. Nathanson and O. Entin-Wohlman, Phys. Rev. B **49**, 15 377 (1994).
[18] Gayatri Pal and P. Rudra, Phys. Rev. B **49**, 14 139 (1994).
[19] A. Romano, C. Noce, and R. Micnas, Phys. Rev. B **55**, 12 640 (1997); Acta Phys. Pol. A **91**, 381 (1997).
[20] C. Bastide and C. Lacroix, J. Phys. C **21**, 3557 (1988).
[21] Note that $f_i^\dagger f_i = f_i^\dagger b_i f_i b_i^\dagger = f_i^\dagger f_i - f_i^\dagger f_i b_i^\dagger b_i$. The second term will give zero when it acts on any state of the basis. The anomalous term $f^\dagger f^\dagger$ however, violates the constraint of no double occupancy and therefore we take the order parameter as in Eq. (10). This same procedure has been used in the context of the *t-J* model in A.E. Ruckenstein, P.J. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).
[22] J.M. Lawrence, P.S. Riseborough, and R.D. Parks, Rep. Prog. Phys. **44**, 1 (1981).
[23] D. Wohlleben and J. Röhler, J. Appl. Phys. **55**, 1904 (1984).
[24] U. Rauchschwalbe, W. Lieke, F. Steglich, C. Godart, L.C. Gupta, and R.D. Parks, Phys. Rev. B **30**, 444 (1984).
[25] K.S. Athreya, L.S. Hausermann-Berg, R.N. Shelton, S.K. Malik, A.M. Umarji, and G.K. Shenoy, Phys. Lett. **113A**, 330 (1985).
[26] W. Schmitt and G. Güntherodt, J. Magn. Magn. Mater. **47**, 583 (1985).
[27] S.K. Malik, A.M. Umarji, G.K. Shenoy, and M.E. Reeves, J. Magn. Magn. Mater. **54**, 439 (1986).