Ferromagnetism of the Kondo lattice in the low-carrier-concentration limit

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Exact diagonalization of a one-dimensional finite-size system with two conduction electrons is used to demonstrate the existence of an incompletely saturated ferromagnetic ground state in the low-carrier-concentration limit of the Kondo-lattice model. Interactions between the spin-polarization clouds around the electrons play an important part in the stabilization of the ferromagnetic ground state. In a spin-wave analysis of this ground state, two regimes are identified: The very-low-concentration limit is well described by the mean-field approach, whereas with increasing concentration spin fluctuations become important and suppress ferromagnetic order gradually.

I. INTRODUCTION

During the last decade the Kondo-lattice model has attracted much attention for the reason that it might reproduce various physical properties of the heavy-fermion materials.[1] It also represents an example of a strongly correlated electron system, which is of basic theoretical interest. The structure of this model is given by a lattice of localized spins that interact with the conduction electrons via an exchange coupling. The Hamiltonian has the form

$$\mathcal{H}=-\sum_{i,j,s}(t_{ij}c_{is}^{\dagger}c_{js}+\text{H.c.})-J\sum_{i}\mathbf{S}_i\cdot\mathbf{s}_i\ , \tag{1}$$

where c_{is} ($c_{is}^{\dagger}$) denotes the annihilation (creation) operator of a conduction electron at site i with spin s. The vector $\mathbf{S}_i$ is the localized spin operator and

$$\mathbf{s}_i^{\alpha}=(\hbar/2)\sum_{s,s'}c_{is}^{\dagger}\sigma_{ss'}^{\alpha}c_{is'}$$

defines the conduction electron spin operator at the site i. Further, t_{ij} stands for the hopping matrix element between the sites i and j, and J for the exchange-coupling constant. We will restrict this paper to the case of negative J, i.e., antiferromagnetic coupling between localized and electron spin.

The Kondo-lattice model can be derived as an effective model from the more fundamental periodic Anderson model in the strong-coupling limit.[2] Both models have been studied by various approaches like the Gutzwiller or the slave-boson method.[3,4] In this way it could be demonstrated how the quasiparticles in this model form a coherent band with a very heavy effective mass. However, these treatments turned out to be insufficient for the description of magnetic properties or mechanisms of superconductivity found in some heavy-fermion materials. Even the ground-state properties of the model are still a matter of question.

Recently, various numerical studies of the one-dimensional (1D) finite-size Kondo-lattice system considered the ground-state properties by exact-diagonalization or quantum Monte Carlo methods.[5–7] For the case of a half-filled conduction band (one conduction electron per site) these calculations suggest a ground state forming a total spin singlet. On the other hand, in the low-concentration limit an incompletely saturated ferromagnetic state seems to be energetically most favorable.[6,7] This latter result was very recently supported by the rigorous analysis of the case of one conduction electron.[8] This problem is very close to that considered by the Nagaoka theorem, which states that the presence of one hole leads to a ferromagnetic ground state in the infinite-U limit of the half-filled Hubbard model.[9] Actually, the one-electron Kondo-lattice model is identical to the Nagaoka problem in the limit of $J\rightarrow-\infty$. However, in Ref. 8 it was proved that for finite J the ground state is ferromagnetic for considerably less restrictive conditions than necessary in the Nagaoka theorem. Especially, it is valid for all dimensions, despite the fact that the Nagaoka theorem does not apply for 1D systems.[9]

In going beyond the one-particle problem, the interaction between the electrons has to be taken into account. It was shown in Ref. 8 that the conduction electron moves as a quasiparticle dressed by a polarization cloud of the localized spins, i.e., as a spin polaron. In this spin polaron the localized spins tend to align antiparallel to the electron spin. The extension of the cloud is determined by the correlation length of the localized spins. This correlation length ξ is also the length scale of the interaction among spin polarons. Note the J dependence of ξ: ξ is large for J close to zero ($\xi\sim\sqrt{2t/|J|}$) and approaches zero as $J\rightarrow-\infty$. In the latter case the interaction among the spin polarons is reduced to hard-core repulsion only. As we will show below, there are good reasons to believe that due to the interaction among spin polarons for finite J the ferromagnetism proved for the one-particle case can be extended to a (small) finite elec-

tron concentration in the thermodynamic limit. Because in the $U=\infty$ Hubbard model, which is equivalent to the $J=-\infty$ Kondo-lattice model, the holes have only hard-core repulsion, there are discussions whether for the Nagaoka problem a similar extension is possible.[10–14]

The first part of this paper is devoted to the problem of two particles in the Kondo lattice in order to show that the interaction between the two spin polarons favors a ferromagnetic ground state. For that purpose we perform exact diagonalization in 1D finite-size systems. Although it turns out that the ground state depends qualitatively on the form of the boundary conditions, our results strongly support the existence of a ferromagnetic order for the two-electron system.

In a second part we consider the effect of spin fluctuations under the assumption that the ground state is ferromagnetic. By means of a spin-wave analysis of a 3D Kondo lattice we will show that the very-low-carrier-concentration limit may be well described by a mean-field approach. However, a critical concentration exists beyond which spin fluctuations are dominating the behavior of the system.

II. THE KONDO-LATTICE WITH TWO ELECTRONS

In this section we study the ground state of the 1D Kondo lattice with a finite (even) number of sites containing two conduction electrons. Our purpose in treating this model is the confirmation that a Kondo-lattice system with more than one conduction electron prefers also a ferromagnetic ground state, analogous to that in the one-electron case.[8] This system was investigated numerically to some extent already by Hatsugai, Imada, and Nagaosa for other reasons.[6]

It is convenient to consider this system as a ring where the boundary conditions can be defined simply by a phase α attached to an electron traveling once the whole way around the ring. Setting $\alpha=0$ corresponds to periodic boundary conditions (PBC's) in this system and $\alpha=\pi$ to antiperiodic boundary conditions (APBC's). Intermediate α values (twisted boundary conditions) produce states with finite currents. We will concentrate in our numerical study on the ground state for the two extreme boundary conditions, PBC's and APBC's, for reasons that will be explained later.

We use a simplified version of the Hamiltonian in Eq. (1) by setting $t_{ij}=t$ for j nearest neighbor of i, and 0 otherwise. To calculate the ground-state energy the Lanczos method is applied for the exact diagonalization. Subsequently, we obtain the wave function of the state by an inverse iteration method using the conjugate-gradient method (see, for example, Ref. 6 or 7). For this type of numerical calculation the available computer memory limits the size of the system treatable. Therefore the spin and translational symmetry have been used to reduce the needed memory and to increase the treatable system size (number of lattice sites $N\leq 14$ on a nonvectorized computer).

The fact that the conduction band is discretized in our finite-size system leads to problems related with the choice of the boundary conditions. For even N, the PBC's yield to a conduction-electron band with one level at the bottom, $k=0$, whereas for the APBC's there are two degenerate lowest band levels, $k=\pm\pi/N$. Therefore neglecting the interaction part of the Hamiltonian the ground state for two electrons is nondegenerate in the PBC case (spin singlet), but for the APBC's it is fourfold degenerate (any spin configuration of the electrons is degenerate). In both cases a finite energy gap must be overcome to generate excited states in the conduction band. For that reason the ground-state electron-spin configuration tends to be singlet for PBC's even if the interaction part of the Hamiltonian is turned on.

The numerical results for the PBC's suggest that the ground state always forms a total spin singlet (including the localized spins). This is the case for any finite-size system and any value of J ($-3\leq J\leq 0$). The correlation function of the localized spins $K_{ff}(a)=\langle \sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+a}\rangle/N$ is clearly dominated by the Fourier component $\tilde{K}_{ff}(q=2\pi/N)$. Plotting $\tilde{K}_{ff}(q=2\pi/N)$ versus $1/N$ the points lie on a straight line, which extrapolates to a finite value for $N\rightarrow\infty$ [Fig. 1(a)].[15] We take this as the indication that no qualitative change occurs for any parameter J (<0) and N, except for $J\rightarrow-\infty$ where the ground state is highly degenerate in one dimension. On the other hand, the ground state for the APBC breaks the symmetry of the system by having a finite total spin quantum number [$S_{\text{tot}}=(N-2)/2$, incompletely saturated ferromagnet], for any value of J (<0) and N. Consequently, the dominating component of $\tilde{K}_{ff}(q)$ is the one with $q=0$, which gradually approaches the value $\frac{1}{4}$ for increasing N [Fig. 1(b)].

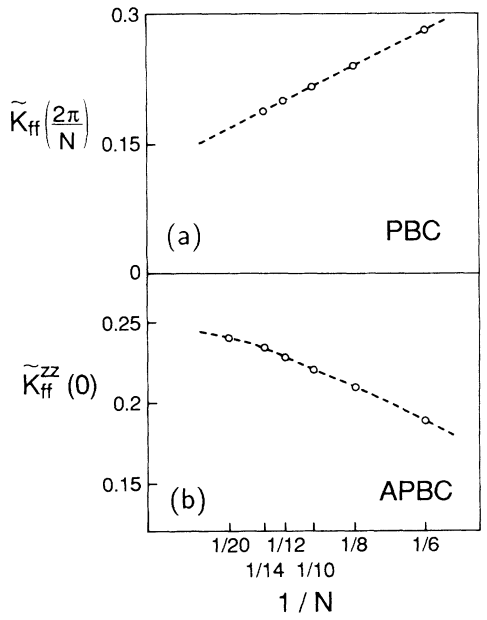

FIG. 1. Correlation of the localized spins: (a) For the total spin singlet state (PBC). The empty circles give the amplitude of the correlation peak in q space at $q=2\pi/N$ for different system sizes N. (b) For the ferromagnetic state (APBC). The empty circles mark the amplitude of the uniform correlation. ($J=-0.2t$; lines are drawn as a guide for the eye.)

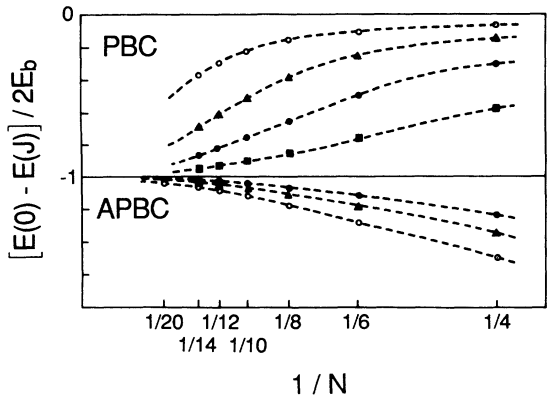

FIG. 2. Energy gain of the ground states in the two-particle system for both boundary conditions, PBC and APBC, for different J and N (see text): empty circle, $J=-0.2t$; filled triangle, $J=-0.5t$; filled circle, $J=-1.0t$; filled square, $J=-2.0t$. (Lines are drawn as a guide for the eye.)

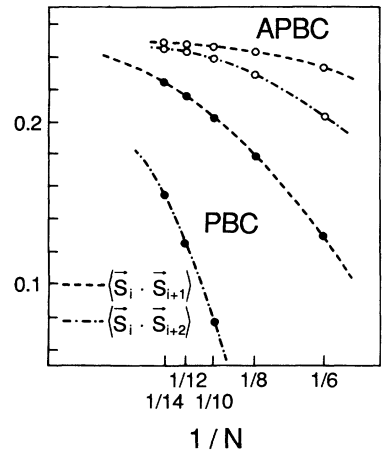

FIG. 3. Nearest- and next-nearest neighbor correlation of the localized spins. Empty circles stand for the ferromagnetic ground state (APBC) and filled circles for the total spin singlet state (PBC). ($J=-0.2t$; lines are drawn as a guide for the eye.)

At first sight it seems discouraging to find such a discrepancy in the qualitative properties of the ground state depending on the chosen boundary conditions. However, this fact provides a good instrument to compare the interaction of two spin polarons if they have preferentially parallel (APBC) or antiparallel (PBC) spin alignment.

As a first point let us consider the energy gain of the two states relative to the free-electron ground-state energy. In Fig. 2 we plot the quantity $[E(0)-E(J)]/2E_b(J)$ for different N and J, where we use for the normalization $E_b(J)$, the energy gain of one electron with a coupling constant J in an infinitely large 1D system (see Ref. 8). The energy gain for the singlet state (PBC) is clearly smaller than for the ferromagnetic one (APBC). For the singlet state even the ground state loses energy compared with the infinitely dilute system ($N\rightarrow\infty$). On the other hand, the interaction between the spin polarons works to lower the energy for the ferromagnetic state. This indicates that parallelly aligned spin polarons (ferromagnet) are energetically favored rather than the antiparallel ones (total spin singlet).

The short-range correlation of the localized spins hints at the tendency of the system toward a ferromagnetic ground state, too. We consider the nearest- and next-nearest-neighbor correlations. For both types of boundary conditions these correlations approach $\frac{1}{4}$ for increasing N, indicating that, at least in the short range, ferromagnetic ordering is developing with increasing N (Fig. 3). It has to be noticed that for large $|J|$ the ferromagnetic correlation of the PBC ground state is suppressed due to the shortening of the correlation length $\xi\ (=\sqrt{2t/|J|}$ for small $|J|)$. Furthermore, the electrons each tend to form an on-site singlet with the localized spins diminishing the correlation, too, as $|J|$ increases. This behavior also affects the relative energy gain of the ferromagnetic ground state compared to that of the singlet ground state as can be easily observed in Fig. 2. The larger the $|J|$, the smaller the relative energy gain is. This is due to the fact that the extension of the interacting spin-polarization clouds is shrinking and that the

TABLE I. Lowest-energy eigenvalues for different coupling constants J and system sizes N for the 1D Kondo-lattice model with two conduction electrons. For PBC the ground state is a total spin singlet, and for the APBC ground state it is an incomplete ferromagnet with spin quantum number $S_{\text{tot}}=(N-2)/2$. The energies and the coupling constant are given in units of the hopping matrix element t.

PBC	$N=6$	$N=8$	$N=10$	$N=12$	$N=14$
$J=-0.2$	−4.013 79	−4.020 99	−4.029 55	−4.039 11	−4.049 07
$J=-0.5$	−4.099 41	−4.149 26	−4.196 82	−4.236 07	−4.266 33
$J=-1.0$	−4.441 88	−4.578 41	−4.667 66	−4.725 13	−4.763 26
$J=-2.0$	−5.557 57	−5.746 70	−5.847 62	−5.906 45	−5.943 36
APBC	$N=6$	$N=8$	$N=10$	$N=12$	$N=14$
$J=-0.2$	−3.635 37	−3.853 18	−3.954 28	−4.009 11	−4.042 11
$J=-0.5$	−3.918 23	−4.121 60	−4.215 96	−4.267 35	−4.298 46
$J=-1.0$	−4.446 52	−4.635 28	−4.723 70	−4.772 20	−4.801 65
$J=-2.0$	−5.648 10	−5.821 37	−5.903 13	−5.947 99	−5.975 18

more the electron spins are locked into singlet states with the localized spin, the less effective their relative polarization is (screening effect).

Now we compare the absolute values of the ground-state energy for the case of PBC and APBC (Table I). With varying phase α these energies change continuously. However, because these two ground states have different quantum numbers, they cannot be connected continuously by turning α from 0 to π. Rather they belong to different branches of the eigenenergy spectrum in the α space. Therefore, they represent local minima if we vary the ground-state energy with respect to α, since for α values away from $n\pi$ (n: integer) the existence of a finite current leads to an increase of the energy. Somewhere in the region $0<\alpha<\pi$ the two levels cross.

Thus, our system considered as a ring may have two different global ground states depending on the system parameters J and N. In Fig. 4 the corresponding phase diagram, J versus N, shows for which parameter pair (J,N) the ground state is in total spin singlet (PBC) or a ferromagnet (APBC). The former state is favored for small J and N, whereas increasing one of the two parameters supports the latter one. The critical line between the two regions is related to the finite-size gap in the conduction-electron band as the approximation $J/4=2t[\cos(\pi/N)-1]$ (dashed line) clearly shows; i.e., the exchange-coupling energy $J\langle \mathbf{S}_i\cdot\mathbf{s}_i\rangle$ is of the same magnitude as the separation of the lowest states in the electron band for the two types of boundary conditions. Therefore, the system would choose the boundary conditions, i.e., α, to minimize its energy for a particular parameter set J and N. Consequently, the system would always turn to a ferromagnet with $S_{\rm tot}=(N-2)/2$ if its size N is large enough (or the electron concentration is small enough).

For better understanding of the properties of the two electrons in this system we also briefly discuss here their correlation functions. The charge-charge correlation function for the PBC ground state shows a very clear change varying the value of J [in Fig. 5(a) plotted for the case of $N=14$]. For $|J|\ll t$ the correlation has a comparatively weak structure very close to the structureless correlation function of the free-electron ground state. However, turning J to more negative values leads to a separation of the two electrons. The electrons tend to form on-site singlets with the localized spins. Thus these singlet objects are strongly repulsive to each other, since two electrons on the same site yield an energy loss of $-3J/2$. This means that the electrons form hard-core polarons with the localized spins as $J\to-\infty$. For the ferromagnetic ground state (APBC) no qualitative and almost no quantitative change is seen in the charge-charge correlation function varying J. For all finite $J<0$ the electrons avoid each other. For $|J|\ll t$ the exchange hole is responsible for this feature, because the ground state breaks the system symmetry, lifting the spin degeneracy of the electrons so that the electrons prefer to have parallel spins. For strong exchange-coupling the electrons behave like hard-core polarons described just above.

The electron spin-spin correlation function shows for both types of ground states the following common

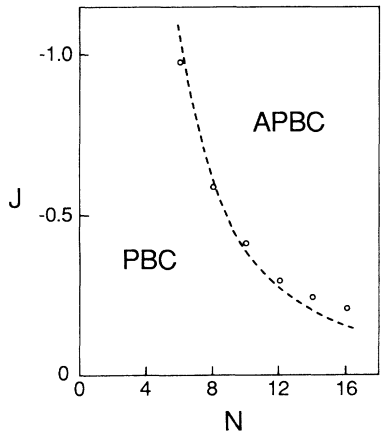

FIG. 4. Phase diagram, J vs N, for the (absolute) ground state. PBC stands for the spin singlet ground state and APBC for the ferromagnetic one (see text).

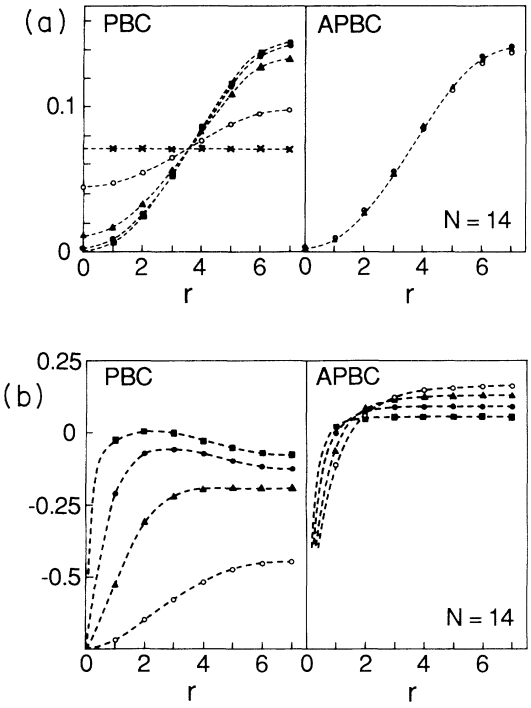

FIG. 5. (a) Charge-charge correlation function of the two electrons in the spin singlet (PBC) and ferromagnetic ground state (APBC) in a system with $N=14$. $\times$, $J=0$; empty circle, $J=-0.2t$; filled triangle, $J=-0.5t$, filled circle, $J=-1.0t$; filled square, $J=-2.0t$. (b) Spin-spin correlation function of the two electrons in the spin singlet (PBC) and ferromagnetic ground state (APBC) in a system with $N=14$. The values given here are the spin-spin correlations normalized by the charge-charge correlation $\langle \mathbf{S}_i\cdot\mathbf{S}_{i+r}\rangle/\langle n_i n_{i+r}\rangle$. For the symbols, see (a). (Lines are drawn as a guide for the eye.)

features [Fig. 5(b)]. The short- as well as the long-range correlation is decreasing with increasing $|J|$ as we expect from the fact that ξ is decreasing as $|J|$ is increasing. For the singlet ground state (PBC) an additional structure is occurring. For large $|J|$ the tendency toward parallel alignment of the electron spins is enhanced. For this effect the cloud of aligned localized spins around each electron is responsible. The two electrons close to each other tend to generate one common parallelly aligned cloud. For $|J| \ll t$ close to zero this effect is covered mainly due to the small size of the system, since the extension of the spin-polarization clouds is about the system size.

Concluding this section, we emphasize that these numerical results strongly support the idea that the ground state of a Kondo-lattice system is ferromagnetic for low carrier concentrations. Therefore, we believe that the rigorous result given for the one-electron case can be extended to the thermodynamic limit with a finite electron concentration. This could not be stated for the $U=\infty$ Hubbard model to date.[10-14,16] There is a qualitative difference between the finite J and the infinite J systems (equivalent to the $U=\infty$ Hubbard model). In the latter system the "spin polarons" have no extension (on-site singlets) and behave like hard-core particles. As pointed out above the relative energy gain due to the spin-polaron interaction is shrinking with $J \to -\infty$, since no information about spin polarization can be exchanged directly between the two spin polarons. Thus, in this situation the spin configuration in the ground state is decided only through the gain of kinetic energy. However, if the spin-polaron clouds overlap, as is the case for finite J, their relative polarization plays a role in the interaction between them, supporting the formation of ferromagnetic long-range order. This fact may give the reason why the infinite J Kondo-lattice model for two electrons need not necessarily yield a ferromagnetic ground state.

III. SPIN-WAVE ANALYSIS

The results of the previous section strongly suggest that the ground state of a Kondo lattice is ferromagnetic even for a small finite number of electrons larger than two. Unfortunately, it is very difficult to give a reliable extrapolation from finite-size calculations to the thermodynamic limit to analyze how the stability of the ferromagnetic ground state depends on the electron concentration. It is generally not possible to fix the electron concentration (number of electrons per lattice sites) for different system sizes except for very special ratios. In order to gain insight into the qualitative behavior of the low-carrier-concentration limit of this model in the thermodynamic limit, we will study here the stability of the ferromagnetic ground state against spin fluctuations by an approximate analytic treatment (Tyablikov-decoupling scheme). The following analysis has the advantage of giving results in a continuous range of concentrations. To make the calculations simple we will study here the ferromagnetic critical temperature in a three-dimensional system.

It is more convenient for the following calculations to write the Hamiltonian H of Eq. (1) in the Fourier space

$$H=\sum_{\mathbf{k},s}\varepsilon(\mathbf{k})c^{\dagger}_{\mathbf{k}s}c_{\mathbf{k}s}-\frac{J}{2N}\sum_{\mathbf{q}}[S_f^{+}(\mathbf{q})S_c^{-}(-\mathbf{q})+S_f^{-}(\mathbf{q})S_c^{+}(-\mathbf{q})+2S_f^{z}(\mathbf{q})S_c^{z}(-\mathbf{q})]\ , \tag{2}$$

where

$$\mathbf{S}_f(\mathbf{q})=\sum_i \mathbf{S}_i e^{i\mathbf{q}\cdot\mathbf{r}_i} \quad \text{and} \quad s_c^{\alpha}(\mathbf{q})=\sum_{\mathbf{k},s,s'} c^{\dagger}_{\mathbf{k}+\mathbf{q},s}\frac{\sigma^{\alpha}_{ss'}}{2}c_{\mathbf{k}s}=\sum_{\mathbf{k}}S_c^{\alpha}(\mathbf{k},\mathbf{q})\ ,$$

and $\varepsilon(\mathbf{k})$ is the electron band spectrum ($\hbar=1$). The magnetic properties of this system can be described by the following susceptibilities (causal Green functions of the spin operators) for the localized (S_f) and the electron spins (S_c):

$$G_{\mu\nu}(\mathbf{q},t)=\langle\langle S_{\mu}^{+}(\mathbf{q},t);S_{\nu}^{-}(-\mathbf{q})\rangle\rangle\ , \tag{3}$$

where $\mu,\nu=f,c$ and $\langle\langle A(t);B\rangle\rangle=-i\Theta(t)\langle[A(t),B]\rangle$ ($\langle\cdots\rangle$ is the thermal expectation value). These susceptibilities can be obtained from their equation of motion. For $G_{ff}(\mathbf{q},t)$ and $G_{cf}(\mathbf{q},t)$ this leads to the following coupled equations:

$$i\frac{d}{dt}G_{ff}(\mathbf{q},t)=\delta(t)\langle 2S_f^{z}(0)\rangle-\frac{J}{2N}\sum_{\mathbf{q}'}\langle\langle 2S_f^{z}(\mathbf{q}+\mathbf{q}',t)S_c^{+}(-\mathbf{q}',t);S_f^{-}(-\mathbf{q})\rangle\rangle$$
$$+\frac{J}{2N}\sum_{\mathbf{q}'}\langle\langle 2S_f^{+}(\mathbf{q}+\mathbf{q}',t)S_c^{z}(-\mathbf{q}',t);S_f^{-}(-\mathbf{q})\rangle\rangle \tag{4}$$

and

$$i\frac{d}{dt}F_{\mathbf{k}}(\mathbf{q},t)=[\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{q})]F_{\mathbf{k}}(\mathbf{q},t)-\frac{J}{2N}\sum_{\mathbf{q}'}\langle\langle S_f^{+}(\mathbf{q}',t)(c^{\dagger}_{\mathbf{k}+\mathbf{q}\uparrow}c_{\mathbf{k}+\mathbf{q}'\uparrow}-c^{\dagger}_{\mathbf{k}+\mathbf{q}-\mathbf{q}'\downarrow}c_{\mathbf{k}\downarrow})(t);S_f^{-}(-\mathbf{q})\rangle\rangle$$
$$+\frac{J}{2N}\sum_{\mathbf{q}'}\langle\langle S_f^{z}(\mathbf{q}',t)(c^{\dagger}_{\mathbf{k}+\mathbf{q}-\mathbf{q}'\uparrow}c_{\mathbf{k}\downarrow}+c_{\mathbf{k}+\mathbf{q}\uparrow}c_{\mathbf{k}+\mathbf{q}'\downarrow})(t);S_f^{-}(-\mathbf{q})\rangle\rangle\ , \tag{5}$$

with $G_{cf}(\mathbf{q},t)=\sum_{\mathbf{k}}F_{\mathbf{k}}(\mathbf{q},t)=\sum_{\mathbf{k}}\langle\langle S_c^{+}(\mathbf{k},\mathbf{q},t);S_f^{-}(-\mathbf{q})\rangle\rangle$. These equations contain fourth-order Green functions,

which in turn lead to equations of motion with again higher-order Green functions. It is, in general, impossible to solve such a hierarchy of coupled equations rigorously. One way to obtain an approximate solution is to decouple these equations at a certain level. The simplest treatment is obtained with a decoupling in lowest order by replacing some of the operators by expectation values (mean fields) in Eqs. (4) and (5), assuming ferromagnetic order in the ground state (Tyablikov decoupling):[17]

$$\begin{aligned} &S_f^z(\mathbf{q}+\mathbf{q}')S_c^+(\mathbf{q}')\approx\langle S_f^z(0)\rangle S_c^+(\mathbf{q})\delta_{\mathbf{q}',-\mathbf{q}}\ , \\ &S_f^+(\mathbf{q}+\mathbf{q}')S_c^z(-\mathbf{q}')\approx\langle S_c^z(0)\rangle S_f^+(\mathbf{q})\delta_{\mathbf{q}',0}\ , \\ &S_f^+(\mathbf{q}')(c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}'\uparrow}-c_{\mathbf{k}+\mathbf{q}-\mathbf{q}'\downarrow}^\dagger c_{\mathbf{k}\downarrow})\approx S_f^+(\mathbf{q})(\langle n_{\mathbf{k}+\mathbf{q}\uparrow}\rangle-\langle n_{\mathbf{k}\downarrow}\rangle)\delta_{\mathbf{q},\mathbf{q}'}\ . \end{aligned} \tag{6}$$

In a strict sense there is no justification for this type of decoupling. Qualitatively this procedure leads to a treatment of independent spin-wave modes. However, we will see below that the self-consistency equations for the mean field, based on a sum rule, takes the missed coupling of the spin-wave modes in an effective way into account again. This method has been applied to various magnetic systems, such as the Heisenberg model, giving very reliable results for the critical temperature.[17]

Using Eq. (6), the equation of motion transformed from the t to the ω space can be written as

$$\begin{aligned} &-\omega G_{ff}(\mathbf{q},\omega)=\frac{1}{2\pi}2\langle S_f^z(0)\rangle-\frac{J}{N}\langle S_f^z(0)\rangle G_{cf}(\mathbf{q},\omega)+\frac{J}{N}\langle S_c^z(0)\rangle G_{ff}(\mathbf{q},\omega)\ , \\ &-\omega F_k(q,\omega)=[\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{q})]F_{\mathbf{k}}(\mathbf{q},\omega)+\frac{J}{N}\langle S_f^z(0)\rangle F_{\mathbf{k}}(\mathbf{q},\omega)+\frac{J}{2N}(\langle n_{\mathbf{k}\downarrow}\rangle-\langle n_{\mathbf{k}+\mathbf{q}\uparrow}\rangle)G_{ff}(\mathbf{q},\omega)\ . \end{aligned} \tag{7}$$

From the second equation we obtain

$$G_{cf}(\mathbf{q},\omega)=\sum_{\mathbf{k}}F_{\mathbf{k}}(\mathbf{q},\omega)=J\chi_c(\mathbf{q},\omega)G_{ff}(\mathbf{q},\omega) \tag{8}$$

with

$$\chi_c(\mathbf{q},\omega)=\frac{1}{2N}\sum_{\mathbf{k}}\frac{\langle n_{\mathbf{k}+\mathbf{q}\uparrow}\rangle-\langle n_{\mathbf{k}\downarrow}\rangle}{\omega+\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{q})+(J/N)\langle S_f^z(0)\rangle} \tag{9}$$

so that with the first equation

$$G_{ff}(\mathbf{q},\omega)=-\frac{1}{\pi}\frac{\langle S_f^z(0)\rangle}{\omega+(J^2/N)\langle S_f^z(0)\rangle[\chi_c(0,0)-\chi_c(\mathbf{q},\omega)]}\ . \tag{10}$$

The poles of this susceptibility of the localized spins describe the spectrum ω_q of the spin waves. Independent of $\chi_c(\mathbf{q},\omega)$ it is guaranteed that $\omega_q\to 0$ for $\mathbf{q}\to 0$.

As an example, we consider here the case of a free-electron band energy $\varepsilon(\mathbf{k})=\mathbf{k}^2-\mu$. In the low-concentration limit this is certainly a good approach. For this case we obtain for $\chi_c(\mathbf{q},\omega)$ at $T=0$ K the following well-known expression:

$$\chi_c(\mathbf{q},\omega)=\frac{1}{32\pi^2 q}\sum_{s=\pm 1}s\left[(k_{Fs}^2-\tilde{k}_s^2)\ln\left|\frac{\tilde{k}_s+k_{Fs}}{\tilde{k}_s-k_{Fs}}\right|+2k_{Fs}\tilde{k}_s\right]\ , \tag{11}$$

with

$$\tilde{k}_s=[\omega+sq^2+J\langle S_f^z(0)\rangle/N]/2q\ ,$$

and k_{Fs} the Fermi momentum for the electrons depending on their spin ($\uparrow\to s=+1$ and $\downarrow\to s=-1$). This Fermi momentum depends on the spin direction, since the electron spin is coupled to the uniform background via $Js_z\cdot\langle S^z(0)\rangle$. This susceptibility is discussed in detail in Ref. 18. The spin-wave excitations are well defined for small q, where the dispersion of $\omega_{\mathbf{q}}$ is quadratic in leading order. However, this is not the case for q between $\sim|k_{F\uparrow}-k_{F\downarrow}|$ and $\sim|k_{F\uparrow}+k_{F\downarrow}|$, where the spin waves are damped due to electron-hole excitations. For $\mathbf{q}>|k_{F\uparrow}+k_{F\downarrow}|$ this damping disappears again.

The mean field $\langle S_f^z(0)\rangle$ contained in $G_{ff}(\mathbf{q},\omega)$ has to be determined self-consistently. For this purpose the following sum rule is applied:

$$\int d\omega\int d^3q\langle S_f^+(\mathbf{q},\omega)S_f^-(-\mathbf{q})\rangle=\frac{1}{2}+\frac{1}{N}\langle S_f^z(0)\rangle\ ,$$

which is easily obtained from the commutation relations for the spin operators. As mentioned above, this sum rule imposes some constraint on the spin-wave modes and leads to an effective coupling among them, which was neglected by the decoupling procedure in Eq. (6). The self-consistency equation corresponding to the fluctuation-dissipation theorem for $\langle S_f^+(\mathbf{q},\omega)S_f^-(-\mathbf{q})\rangle$ has the form

$$\frac{1}{2}=\frac{1}{N^2}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty}d\omega\coth\left(\frac{\beta\omega}{2}\right)\mathrm{Im}G_{ff}(\mathbf{q},\omega)\ . \tag{12}$$

Due to the damped spin-wave modes in the spectrum of $G_{ff}(\mathbf{q},\omega)$ it is in general rather difficult to evaluate this equation. Therefore, we will concentrate here on the calculation of the transition temperature T_c obtained from this equation by the limit $\langle S_f^z(0)\rangle \to 0$. For small values of $\langle S_f^z(0)\rangle$ the spin-wave dispersion ω_q is proportional to $\langle S_f^z(0)\rangle$. Thus it is easy to see that for temperatures close to T_c the electron susceptibility $\chi_c(q,\omega)$ can be replaced by $\chi_c(q,0)$. It is then very simple to perform the integration over ω, since the electron-hole damping does not play any role in this limit [it is of higher order in $\langle S_f^z(0)\rangle$]. We obtain

$$\frac{1}{2}=\frac{k_B T_c}{2J^2\pi^3}\int d^3q \frac{1}{\chi_c(0,0)-\chi_c(q,0)} , \tag{13}$$

where $\langle S_f^z(0)\rangle$ is set zero. This equation corresponds to that obtained from the Ruderman-Kittel-Kasuya-Yosida (RKKY) perturbation theory.

Under the assumption that $T_c \ll T_F$ (in the low-concentration limit this condition has to be considered more carefully, as we do below) we can use the zero-temperature form of $\chi_c(q,\omega)$. This condition can be satisfied for any $k_F>0$ by choosing the coupling constant $|J|$ small enough. (Note that $|J|$ much smaller than t corresponds to the physical limit obtained by the Schrieffer-Wolf transformation of the periodic Anderson model in lowest order.) Then the denominator of the integrand shows the limiting behavior

$$\chi_c(0,0)-\chi(q,0)=\frac{1}{(2\pi)^2}\times\begin{cases}\dfrac{q^2}{24k_F}+O(q^4) , & q\ll 2k_F\\ \dfrac{k_F}{2}+O(q^{-2}) , & q\gg 2k_F ,\end{cases} \tag{14}$$

and may be approximated by

$$\chi_c(0,0)-\chi(q,0)=\frac{1}{(2\pi)^2}\times\begin{cases}\dfrac{q^2}{24k_F} , & q<2\sqrt{3}k_F\\ \dfrac{k_F}{2} , & q>2\sqrt{3}k_F ,\end{cases} \tag{15}$$

where the boundary $2\sqrt{3}k_F$ is chosen to obtain a continuous functional dependence on q. Introducing a cutoff radius q_c for the upper boundary of the q integration ($q_c^2\sim$bandwidth) the integration in Eq. (13) leads to

$$k_B T_c=\frac{J^2}{16}\times\begin{cases}\left[48\sqrt{3}k_F^2+\dfrac{2}{3k_F}(q_c^3-24\sqrt{3}k_F^3)\right]^{-1} , & k_F<\dfrac{q_c}{2\sqrt{3}}\\ (24k_F q_c)^{-1} , & k_F>\dfrac{q_c}{2\sqrt{3}} .\end{cases} \tag{16}$$

In Fig. 6 the curve of $T_c(k_F)$ is plotted. The critical temperature has a pronounced maximum at $k_F^*\approx 0.2q_c$ with $k_B T_c\approx 0.012J^2/q_c^2$ (the zero-temperature limit is appropriate at this concentration if $J\ll q_c^2$). This corresponds to about $(k_F^*/q_c)^3\approx 0.8\%$ band filling. For small k_F it is like $k_B T_c=3J^2k_F/32q_c^3+O(k_F^2)$. In this case, T_c approaches the ordinary mean-field result, which is

$$k_B T_c=\frac{3(2\pi)^2J^2}{16q_c^3}\chi_c(0,0) . \tag{17}$$

The reason for this behavior is that the lower k_F the more ferromagnetically long-ranged the RKKY interaction among the localized spins is becoming. Thus the mean-field solution is becoming better as it is exact in the infinite range limit of the interaction. [Certainly, the condition $T_c \ll T_F$ must be violated for very small k_F, since $T_c \propto k_F$ in the zero-temperature approach but $T_F \propto k_F^2$. However, keeping the mean-field approach, it is easy to see how T_c vanishes as k_F goes to zero. The high-temperature static, homogeneous electron susceptibility $\chi_c(0,0;T)=k_F^3/6\pi^2k_B T$ leads to

$$k_B T_c=\left[\frac{J^2}{8q_c^3}\right]^{1/2}k_F^{3/2} , \tag{18}$$

for very small k_F, i.e., $T_c\propto\sqrt{n}$ with n as the density of electrons.] The extension of the mean-field regime is essentially determined by the range of the effective ferromagnetic interaction between the localized spins. Using the standard expression of the RKKY coupling constant for a parabolic band,

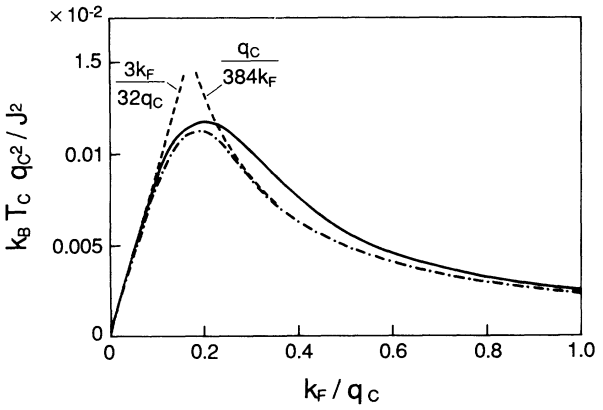

FIG. 6. Ferromagnetic transition temperature T_c vs k_F. The solid line shows the result of Eq. (13) evaluated numerically. The dashed-dotted line is the approximate result of Eq. (16). The dashed lines show the limiting behaviors where especially the one denoted by $3k_F/32q_c$ corresponds to the mean-field result.

$$J_{ij} \propto [\sin(2k_F r_{ij}) - (2k_F r_{ij})\cos(2k_F r_{ij})]/r_{ij}^4 ,$$

we find the first node in the spatial oscillation of the interaction at $r_{ij} \approx 2.9a$ for $k_F = k_F^* = 0.2q_c$ [the lattice constant a is defined by the volume of the first Brillouin zone, $4\pi q_c^3/3 = (2\pi/a)^3$]. Thus, the critical value k_F^* corresponds to the situation where only two shells of neighboring localized spins are ferromagnetically coupled.

Increasing the electron concentration beyond 0.8% leads to a further shortening of the ferromagnetic interaction range and to a strengthening of the antiferromagnetic coupling included in the RKKY oscillation. In this regime the system starts to deviate from the mean-field behavior strongly and the spin fluctuations become more effective to suppress the ferromagnetic order. Consequently the critical temperature decreases and tends eventually to $k_B T_c = J^2/384 k_F q_c$.

For simplicity we have introduced a parabolic band for the conduction electrons. This is certainly not sufficient if the electron concentration $n \gg 0.8\%$, and the behavior of T_c for a realistic band may deviate from that shown in Fig. 6. Furthermore, considering a more realistic electron band we have to take into account that for band filling close to half filling a spin-density-wave state would dominate over the ferromagnetic one. Thus, for higher concentration the ferromagnetic state has to compete with a spin-density-wave state, which depends on the actual structure of the electron band. The description of the change of the system from the ferromagnetic state to a spin-density-wave state with increasing number of conduction electrons is going beyond the scope of this paper (see Ref. 19 for a recent work on this problem using a variational method).

IV. CONCLUSION

The aim of the numerical studies presented in Sec. II is the extension of the rigorous result proved recently for the case of one conduction electron in a Kondo lattice. We have shown by exact diagonalization for the case of two conduction electrons in a finite 1D Kondo lattice with antiferromagnetic coupling ($J < 0$) that this system also tends to form a ground state with an incompletely saturated ferromagnetic order. From our result we believe that the Kondo-lattice model has a ferromagnetic ground state also in the thermodynamic limit for a certain range of low-carrier concentration. The interaction between the quasiparticles, which are electrons dressed with a spin-polarization cloud, plays a major part for the formation of a ferromagnetic state in a Kondo lattice containing more than one conduction electron. The fact that the particles in the Nagaoka problem interact only via a hard-core potential and not via an extended spin-polarization cloud may be the most important difference between this ($J \to -\infty$) and our problem (J finite). This may explain why the extension of the Nagaoka theorem to the thermodynamic limit is problematic.

In a 3D Kondo-lattice system the ferromagnetically ordered state may appear at finite temperatures. By studying the behavior of the critical temperature, we analyzed the effect of spin fluctuations on this ferromagnetic state. The result obtained in the Tyablikov-decoupling scheme shows that there are two distinct regimes. For electron concentrations below a critical value $\sim 0.8\%$ band filling, the spin fluctuations are suppressed and the simple mean-field approach gives a rather good description of the system. This fact can be traced back on the effective ferromagnetic coupling mediated by the conduction electrons between the localized spins, which becomes more long ranged as the electron concentration is decreased. On the other hand, if the concentration exceeds the critical value 0.8% spin fluctuations start to suppress the ferromagnetic order. Additionally, with increasing band filling, the actual band structure becomes more important and instabilities to other states may occur. Therefore, a ferromagnetic phase may exist only in a very restricted range of electron concentrations.

Discussing the possible realization of this type of ferromagnetic order in a certain material, we have to be aware that in the low-electron-concentration limit interband effects with lower completely filled bands can also lead to contributions for the magnetic correlation. The existence of a direct band gap to the lower band could support the creation of a ferromagnetic phase due to an additional enhancement of the ferromagnetic spin fluctuations, whereas an indirect band gap would lead to a competition between intraband ferromagnetic and interband spin-density-wave correlation tendency. For a semimetallic situation (slight overlap of two bands) nesting properties play a very important role possibly suppressing ferromagnetic ordering completely. These problems have certainly to be taken into account considering real physical systems with low conduction-electron concentration.

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[16]Recently, Trugman showed rigorously for this model that any finite number of holes do not form a bound state in the infinite-system-size limit. The numerical data plotted in Fig. 2 suggest that the same statement is true for the finite-J Kondo-lattice model with any finite number of carriers.

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