Ferromagnetism of the one-dimensional Kondo-lattice model: A quantum Monte Carlo study

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The one-dimensional Kondo-lattice model is investigated using quantum Monte Carlo and transfer-matrix techniques. In the strong-coupling region ferromagnetic ordering is found even at large band fillings. In the weak-coupling region the system shows a Ruderman-Kittel-Kasuya-Yosida-like behavior.

In recent years the Kondo-lattice model (KLM) has been investigated to describe the physics of the so-called heavy-fermion systems.[1,2] The question was addressed whether this simple model could account for the rich variety of phases found in heavy-fermion materials, paramagnetism, antiferromagnetism, as well as superconductivity. However, as a typical model of strongly correlated electron systems it could be analyzed by only few approximate treatments[3,4] and has still resisted to give clear insight into the various possible ground states. It would be of particular interest to understand the phase diagram of the KLM. In this work we will tackle this problem by using quantum Monte Carlo techniques for the one-dimensional KLM. The results found here partially contradict the phase diagrams given by Ref. 2 obtained by variational methods.

The KLM consists of a lattice of L localized spins ($S_{i,f}=\frac{1}{2}$; $1,\ldots,L$) coupled to a single band of conduction electrons (creation operator $c^{\dagger}_{i,\sigma}$; $i=1,\ldots,L$; $\sigma=\uparrow,\downarrow$). It is described by the Hamiltonian

$$H=-t\sum_{\sigma=\uparrow,\downarrow}\sum_{i=1}^{L}(c^{\dagger}_{i,\sigma}c_{i+1,\sigma}+\text{H.c.})+J\sum_{i=1}^{L}\mathbf{S}_i\cdot\mathbf{S}_{i,f}\ , \tag{1}$$

$$\mathbf{S}_i=\tfrac{1}{2}(c^{\dagger}_{i,\uparrow}c^{\dagger}_{i,\downarrow})\boldsymbol{\sigma}\begin{pmatrix}c_{i,\uparrow}\\ c_{i,\downarrow}\end{pmatrix}\ , \tag{2}$$

where $\boldsymbol{\sigma}$ are the usual Pauli matrices. The first term denotes the hopping of conduction electrons between nearest-neighbor sites. The second term is an antiferromagnetic ($J>0$) exchange coupling between localized spins and conduction electrons. For small J/t the model can be derived from the periodic Anderson model in its strong-coupling limit.[5]

The behavior of the KLM is understood only for some limiting cases. At half-band filling the ground state is a spin singlet.[6] The nature of this singlet changes from localized singlet pairs in the limit $J/t\to\infty$ to a collective singlet at smaller values of J/t. A spin gap has been found at intermediate values of J/t using quantum Monte Carlo methods[7] and for the entire range of the coupling using exact diagonalization.[8] On the other hand, in the case of only one conduction electron the ground state of the system is known to be an incompletely saturated ferromagnet.[9] The same behavior has been found for two particles and large values of J/t.[10] Questions arising immediately are the following: What is the ground state of the system away from these special cases, where are the boundaries of the ferromagnetic region? Contrary to expectations from Ruderman-Kittel-Kasuya-Yosida (RKKY) mechanisms, our results show ferromagnetic ordering in the strong-coupling region even for very large fillings.[11] In the weak-coupling limit a RKKY-like behavior is observed at intermediate temperatures.

We have employed a generalization of the standard quantum Monte Carlo world-line algorithm (WLA) and quantum transfer-matrix algorithm (TMA).[12] The standard checkerboard WLA has to be extended to add the localized spins.[13] There is no hopping in the localized band, therefore the only local move we have to add is one that can exchange an up (down) spin in the conduction band with a down (up) spin in the localized band at any point of the checkerboard. This move accounts for the exchange interaction between the two bands. A global move that can change the spin of a world line allows for fluctuations in the total magnetization. The systematic error due to the finite Trotter time step $\Delta\tau$ is controlled by extrapolating from results for $\Delta\tau t=0.25$ and $\Delta\tau t=0.5$. The usual zero winding number boundary conditions are used.

Due to the fermionic degrees of freedom there is a sign problem. This sign problem is most severe at values of $J\sim t$ and near fillings of $\rho=\frac{2}{3}$, where $\rho=N/L$ and N is the number of conduction electrons. For larger or smaller values of J/t and for a filling of $\rho=\frac{1}{3}$ the sign problem is not too severe to make Monte Carlo simulations impossible.

To study the magnetic properties of the KLM we have measured the charge and spin structure factors and susceptibilities. The structure factors are defined as the Fourier transforms of the real-space correlations. For the conduction band we have, for the charge and spin structure factors,

$$S_{\text{charge}}(q)=\frac{1}{L}\sum_{j,k}^{L}e^{iq(j-k)}(n_{j,\uparrow}+n_{j,\downarrow})(n_{k,\uparrow}+n_{k,\downarrow})\ , \tag{3}$$

$$S_{\text{spin},c}(q)=\frac{1}{L}\sum_{k,j}^{L}e^{iq(j-k)}(n_{j,\uparrow}-n_{j,\downarrow})\times(n_{k,\uparrow}-n_{k,\downarrow})=\frac{4}{L}\sum_{j,k}^{L}e^{iq(j-k)}S^z_jS^z_k\ . \tag{4}$$

In the same manner we define the spin structure factor for the localized spins:

$$S_{\mathrm{spin},f}(q)=\frac{4}{L}\sum_{j,k}^{L}e^{iq(j-k)}S^z_{j,f}S^z_{k,f}\ . \tag{5}$$

The static susceptibility can be calculated as

$$\chi(q)=\frac{1}{L}\int_0^\beta d\tau\sum_{j,k}^{L}e^{iq(j-k)}\mathrm{Tr}[(S^z_j+S^z_{j,f})e^{-\tau H}\times(S^z_k+S^z_{k,f})\times e^{-(\beta-\tau)H}]\ , \tag{6}$$

where β is the inverse temperature $1/T$.

Simulations have been performed on lattices of $L=12$, 18, and 24 sites, at band fillings of $\rho=\frac{1}{3}$, $\frac{2}{3}$, and temperatures down to $\beta t=32$. Coupling constants $J/t=0.2$, 0.5, 1, 2, 4, and 10 have been investigated. Within the error bars of our results we cannot see any finite-size corrections. From this we conclude that the results show properties of the thermodynamic limit. In the figures we only show the data for the largest reasonable sizes allowed by the sign problem.

In the strong-coupling region we observe a tendency toward ferromagnetic ordering at both fillings. The spin structure factor of the localized spins and the susceptibility both show a clear peak at $q=0$ [Figs. 1 and 2(a)]. Furthermore, the $q=0$ component of the susceptibility is the fastest diverging one when lowering the temperature. We note that this ferromagnetic ordering found at large band fillings of $\rho=\frac{1}{3}$ and $\frac{2}{3}$ is not expected from the RKKY mechanism but is a *new* characteristic of the strong-coupling region. Also, a slight tendency toward ferromagnetic ordering can be observed in the spin structure factor of the conduction band [Fig. 2(b)]. Double occupancy of a site is strongly suppressed as it costs energy of the order of J, leading to an effective on-site repulsion. Therefore, the charge structure factor is essentially that of spinless fermions, showing a $4k_F$ structure (Fig. 3).

To get more insight into the magnetic properties we have studied the temperature dependence of the static uniform susceptibility $\chi(q=0)$ for $J/t=4$ and $\rho=\frac{1}{3}$ (Fig. 4). We have simulated systems of $L=6$, 12, 18, and 24 sites by the Monte Carlo method and the $L=6$ site system with the TMA. Special care is necessary for $L=6$ because the ground state is completely different depending on the boundary condition. It has been shown using

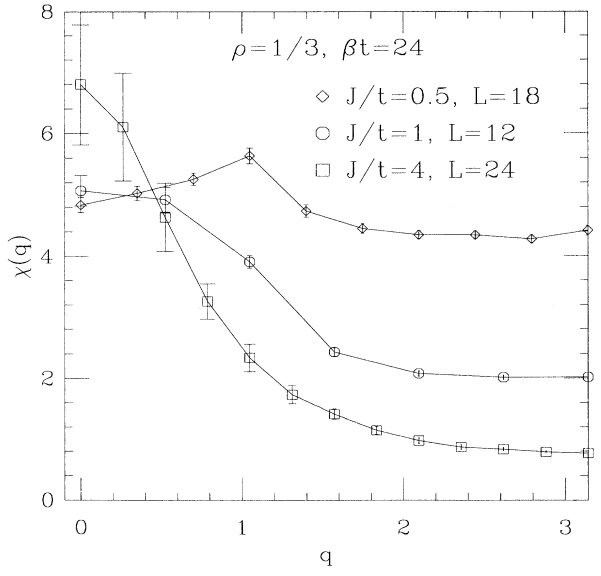

FIG. 1. Static uniform susceptibility for the Kondo lattice model at $\rho=\frac{1}{3}$ and J/t ranging from 0.5 to 4. The temperature is $\beta t=24$. At this filling $2k_F=\pi/3$.

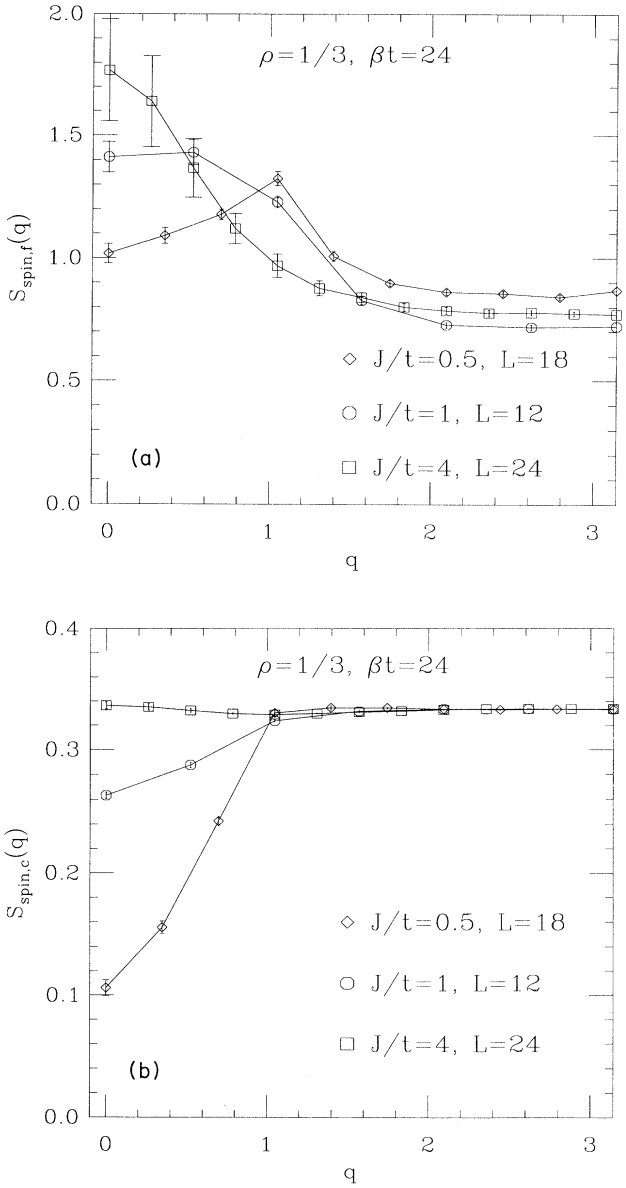

FIG. 2. Spin structure factors for (a) the localized spins and (b) the conduction band for the same parameters as in Fig. 1.

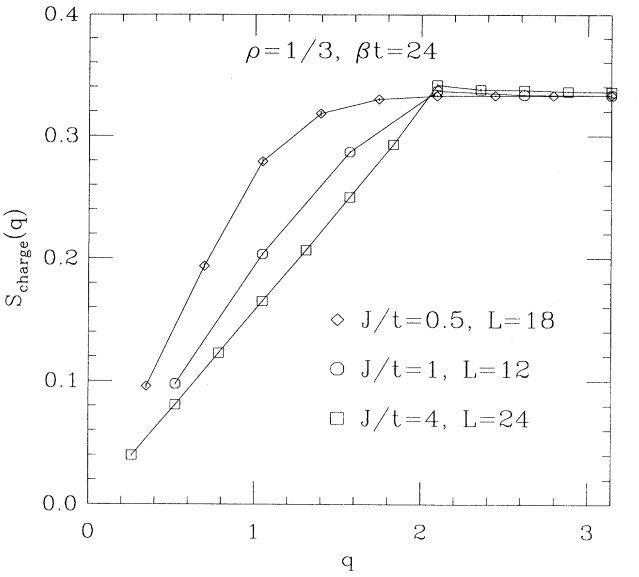

FIG. 3. Charge structure factors for the same parameters as in Fig. 1.

exact diagonalization that the ground state is a spin singlet for periodic boundary conditions, while it is an incompletely saturated ferromagnet for antiperiodic boundary conditions.[10] At $J/t=4$ the ground-state energy of the ferromagnetic state is lower than that of the singlet state. We have calculated $\chi(T)$ both for periodic and antiperiodic boundary conditions in the canonical ensemble using the TMA. In the high-temperature regime $\chi(T)$ can be obtained for an infinite-size system in the grand canonical ensemble by using the $M=1$ approximation (M is the Trotter number) in the TMA.[12]

At high temperatures the susceptibility is the sum of that of a free conduction electron system and that of free localized spins $T\chi=\frac{1}{4}(1+\rho-\rho^2/2)$. When the temperature is lowered to about $T\approx J$, the conduction electrons start to lock into singlets with localized spins and the susceptibility reduces to about the value for the remaining spin degrees of freedom $T\chi\approx\frac{1}{4}(1-\rho)$. Lowering the temperature even further, the spins start to order ferromagnetically, leading to an increase in $T\chi$ and possibly a divergence in an infinite-size system.

At small values of J/t, a completely different behavior can be observed. The effective on-site repulsion is smaller, leading to an increase in the $2k_F$ component of the charge structure factor. The charge structure factor resembles that of nearly free electrons. At the same time the $q=0$ component of the conduction electron spin structure factor and susceptibility is reduced while a cusp emerges at $2k_F$. In the localized spins a $2k_F$ structure is induced by the conduction electrons. This behavior may be called RKKY liquid. At lower temperatures the $2k_F$ peaks in the spin structure factors become more pronounced while at the same time the $q=0$ component is suppressed. From this we conclude that, in the temperature regime of our simulations ($\beta t\approx 32$), the system is dominated by the RKKY interaction. It does not show a heavy-fermion behavior. In a heavy-fermion system the conduction band and the band of localized spins are expected to hybridize. This would result in a single heavy-fermion band with a filling of $\rho+1$, characterized by a wave vector $k_f'=(\rho+1)\pi/2$.

A problem arising in the small J/t region is that the effective coupling gets very small. Although the temperature of the Monte Carlo simulations is well below the

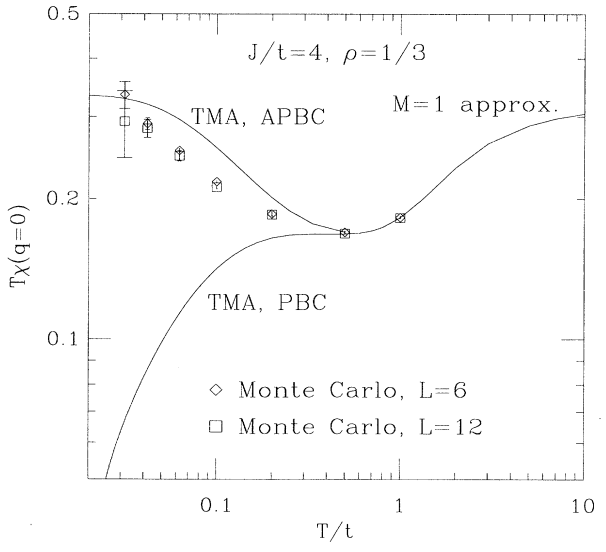

FIG. 4. Temperature dependence of the static uniform susceptibility for a filling of $\rho=\frac{1}{3}$. The solid lines show the $M=1$ approximation for high temperatures and the transfer matrix (TMA) results for periodic (PBC) as well as antiperiodic (APBC) boundary conditions. Monte Carlo data for $L=6$ and 12 sites and zero winding boundary conditions are included. Due to the sign problem the results for larger lattices have much larger error bars. They show no qualitatively different behavior.

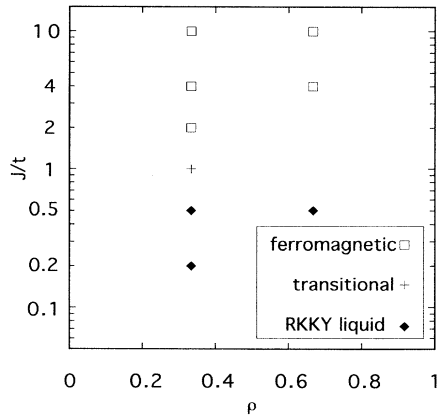

FIG. 5. Phase diagram of the Kondo-lattice model. The Monte Carlo simulations have been performed at the points shown here. The different symbols denote points with ferromagnetic, transitional, and RKKY liquid behaviors.

Fermi temperature, it is still orders of magnitude above the single impurity Kondo temperature T_K. $T_K \approx 10^{-5}$ (10^{-9}) at $J/t=0.5$ and $\rho=\frac{1}{3}$ ($\frac{2}{3}$). This makes it hard to get information on the ground state of the system from Monte Carlo simulations.

In Fig. 5, we summarize the results of our Monte Carlo simulations. At large values of J/t we find ferromagnetic ordering. There the $q=0$ component of the susceptibilities is the dominant and fastest diverging one. From our result we conclude that the ferromagnetic state is stable for a much wider region of the phase diagram than suggested in Ref. 2. In the small J/t region the system shows a RKKY liquid behavior, where the $q=2k_F$ component of the susceptibilities and spin structure factors are the dominant ones. At $J/t=1$ and $\rho=\frac{1}{3}$, the system shows a transitional behavior. Probably this point is near the phase boundary.[14]

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[14]An open question is whether the behavior we can observe using Monte Carlo techniques is the ground-state behavior or is there a crossover to a different state at lower temperatures. Further investigations are necessary.