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Ground-state properties of the one-dimensional Kondo lattice at partial band filling

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We compute the magnetic structure factor, the singlet correlation function, and the momentum distribution of the one-dimensional Kondo lattice model at the density $\rho=0.7$. The density-matrix–renormalization-group method is used. We show that in the weak-coupling regime, the ground state is paramagnetic. We argue that a Luttinger-liquid description of the model in this region is consistent with our calculations. In the strong-coupling regime, the ground state becomes ferromagnetic. The conduction electrons show a spinless-fermion-like behavior.

The heavy-fermion materials display a variety of low-temperature states.[1] In some compounds, the Fermi-liquid state with huge quasiparticle mass is stable down to the lowest attainable temperatures. In others, the Fermi liquid becomes magnetic or superconducting or both. The magnetic structures vary from simple Néel antiferromagnetism through incommensurate order to ferromagnetism. This rich phenomenology arises from the interplay between a wide conduction-electron d band and a partially filled narrow f band of rare-earth actinide or lanthanide elements. One of the canonical models for the description of these systems is the Kondo lattice model (KLM).

After almost two decades of intense studies, the KLM is far from being completely understood.[2] Even for the simplest case of one dimension, a consensus is reached only for the half-filled case.[3] The model is an insulator. A spin gap and a charge gap open for all nonzero values of the Kondo coupling. In the metallic phase, Monte Carlo[4] and exact diagonalization[5] calculations have found that the KLM presents two phases. A paramagnetic (PM) state with Ruderman-Kittel-Kasaya-Yosida (RKKY) correlations is stable at low values of the Kondo coupling. The PM state evolves to a ferromagnetic (FM) ground state when the coupling becomes greater than a critical value. This FM phase is found to be numerically in accord with the results of strong-coupling expansion.[6] At very low densities, the model has a FM phase at all nonzero couplings.[7] The Monte Carlo study was, however, performed at finite temperature while the exact diagonalization one was restricted to a lattice of eight sites. Therefore, the trends displayed in these computations remain to be confirmed in the ground state of much longer chains. Using standard notations the KLM may be written as follows:

$$H=-t\sum_{is}(c_{is}^{\dagger}c_{i+1s}+h.c.)+J_K\sum_i \mathbf{S}_{ic}\cdot\mathbf{S}_{if}, \qquad (1)$$

where

$$\mathbf{S}_{ic}^{\alpha}=\frac{1}{2}\sum_{s,s'} c_{is}^{\dagger}\sigma_{ss'}^{\alpha}c_{is'}, \quad \mathbf{S}_{if}^{\alpha}=\frac{1}{2}\sum_{s,s'} f_{is}^{\dagger}\sigma_{ss'}^{\alpha}f_{is'} \qquad (2)$$

with the constraint that

$$\sum_s f_{is}^{\dagger}f_{is}=1 \qquad (3)$$

the letters c and f standing for conduction and localized electrons, respectively. We applied the density-matrix–renormalization-group (DMRG) technique[8] to this one-dimensional (1D) Kondo lattice. We chose a density $\rho=0.7$, typical of those found in 3D compounds. We believe that the properties displayed at this density will reflect the behavior of the model in the whole region of moderate doping. Although the physical range of J_K corresponds to small couplings, it is also interesting to study the strong-coupling regime in order to understand the behavior of the model in the whole range of parameters. We varied J_K from 0.25 to 10. In the DMRG, an iteration of the algorithm consists in adding two sites at each step. It can be immediately realized that there is a problem in keeping the electron density fixed during the iteration process. To get around such a problem, we constructed the reduced density matrix from the two states whose electron numbers bracket the desired density. In the DMRG method, the states are also labeled by the z component of the total spin. In the present study, we work in the subspaces having $S_T^z=0$ *and* $\pm\frac{1}{2}$. For more details, the reader is referred to a recent paper by Chen and one of us,[8,9] where the method has been successfully checked for the one-dimensional t-J model. The maximum lattice size we have reached is 75 with up to 180 states kept in the two external blocks. The truncation error of the Hilbert space at each iteration is around 7.10^{-4} at $J_K=0.5$ and less than 10^{-6} at $J_K=10$. We have computed the binding energy, the magnetic structure factor, the on-site conduction-electron-localized spin correlation and the electron momentum distribution. Our results confirm the conclusions of Monte Carlo[4] and exact diagonalization[5] studies. A paramagnetic state is stable in the small coupling regime. This state is characterized by a maximum in magnetic structure factor at $2k_{F_c}=\pi\rho$ and a singularity in the electron momentum distribution function at k_{F_c}. In the strong-coupling regime, the ground state is FM. The singularity of the conduction-electron momentum distribution is shifted to $2k_{F_c}$.

When calculating the ground-state energy, we have taken the average of the lowest states having ρ_1 and ρ_2 such that

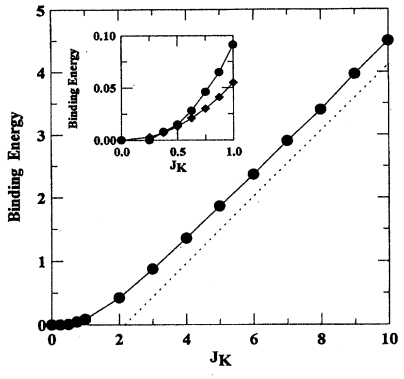

FIG. 1. The binding energy of the Kondo lattice E_B (circles) versus the Kondo coupling. The dashed line corresponds to the strong-coupling limit. In the inset E_B is compared with the binding energy of the one-impurity (diamonds) Kondo problem.

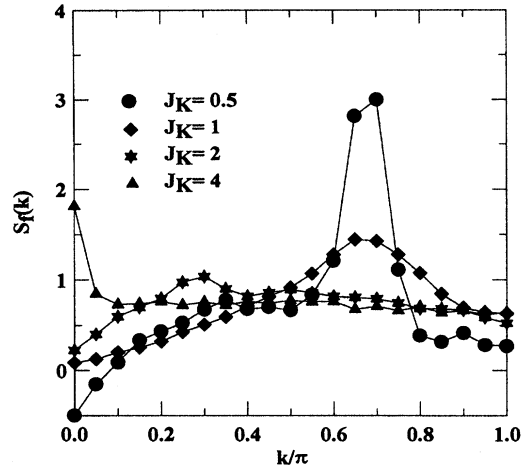

FIG. 2. The magnetic structure factor of the localized spins for $\rho=0.7$ at $J_K=0.5$ (circles), $J_K=1$ (diamonds), $J_K=2$ (stars), and $J_K=4$ (triangles).

$\rho_1 \leq \rho \leq \rho_2$ (see Ref. 9). This way, the ground-state energy per site of the noninteracting system can be reproduced up to four digits. In the $J_K=\infty$ case, the N_c conduction electrons form perfect on-site spin-singlets with the localized spins. The other $N-N_c$ f spins remain free. The system presents a $2^{(N-N_c)}$ fold spin degeneracy. When the coupling is strong but finite, the ground-state energy per site is very close to $-\frac{3}{4}J_K\rho$. The binding energy is defined as $E_B=[E_G(J_K=0,N)-E_G(J_K,N)]/N$, where $E_G(J_K,N)$ is the ground-state energy. At a given density ρ, E_B per site will be very close to $E_\infty=\frac{3}{4}\rho J_K+e_0$. The quantity $e_0=-4/\pi \sin[(\pi/2)\rho]$ is the energy per site of the noninteracting case. In Fig. 1, we show that our results are consistent with such an analysis. The convergence to E_∞ is very smooth. However, Fig. 1 also indicates that this picture breaks down around $J_K=2$. Below this value of the coupling, the system enters in the small coupling regime characterized by $\rho_F J_K<1$, ρ_F being the density of state at the Fermi level of the noninteracting Hamiltonian. For the one-impurity Kondo problem, the binding energy is given by $E_1=3t(\rho_F J_K)^2 Ln(2t)+4t \exp-(1/\rho_F J_K)$.[10] The nonanalytic part of E_1 defines the Kondo temperature T_K. In the inset of Fig. 1, we have compared E_B with E_1. One can see that E_B is greater than E_1. This enhancement of the binding energy of the lattice over the one-impurity case results from the intersite magnetic interaction. However, the latter conclusion does not necessarily mean that the Kondo temperature of the lattice is greater than T_K.

The magnetic properties of the KLM are studied by calculating the spin structure factors of the conduction electrons, $S_c(k)$ and of localized spins, $S_f(k)$. These quantities are defined here as follows:

$$S_{c,f}(k)=\frac{1}{N}\sum_{l,m}\langle \mathbf{S}_{l,c,f}\cdot\mathbf{S}_{m,c,f}\rangle \exp[i(l-m)k]. \quad (4)$$

At the first steps of the algorithm, ρ_1 and ρ_2 are significantly different from ρ and boundary effects are non-negligible. Thus, we started the calculation of the correlation functions when the lattice size was around 35. We have noticed that the value of the correlation functions are extremely sensitive to that of S_T^z. We have not taken the average as for the ground-state energy because when the lowest state corresponding to ρ_1 has $S_T^z=0$, that of ρ_2 is $S_T^z=\pm\frac{1}{2}$, and vice versa. We have used only the state with $S_T^z=0$. In order to reduce the effects due to the variation of the density during the iterations, we have started the calculation of the correlation functions at different lattice size around 35 and then taken the average. In agreement with previous studies, we have found that the structure factor shows the competition of PM and FM phases. For small J_K, both $S_f(k)$ (Fig. 2) and $S_c(k)$ (Fig. 3) have a maximum at $2k_{F_c}$. The strong spin correlation observed in $S_f(k)$ is due to the RKKY interaction. As the coupling is increased, this maximum flattens out. It completely disappears around $J_K=2$. We note that this result compares well with that of exact diagonalization and Monte Carlo

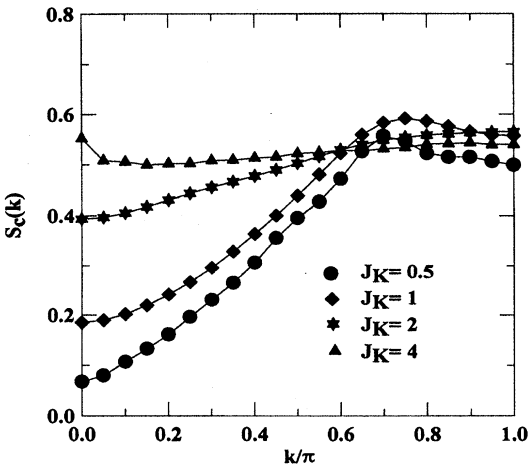

FIG. 3. The magnetic structure factor of the conduction electrons for $\rho=0.7$ at $J_K=0.5$ (circles), $J_K=1$ (diamonds), $J_K=2$ (stars), and $J_K=4$ (triangles).

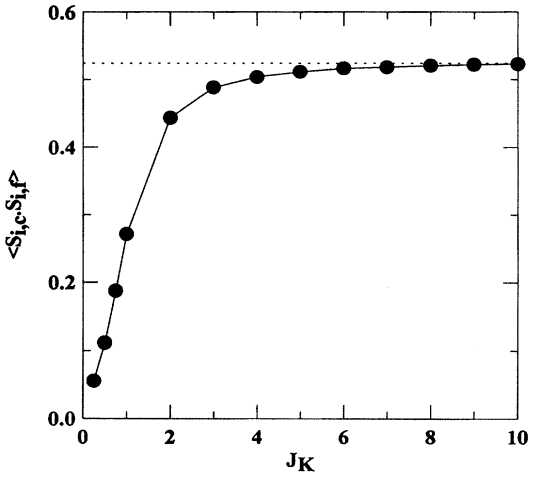

FIG. 4. The on-site conduction-electron-localized spin correlation versus the Kondo coupling. The dashed line corresponds to the strong-coupling limit.

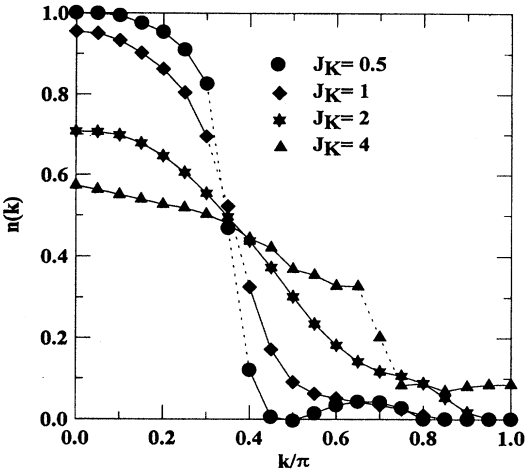

FIG. 5. The electron momentum distribution $n(k)$ for $\rho=0.7$ at $J_K=0.5$ (circles), $J_K=1$ (diamonds), $J_K=2$ (stars), and $J_K=4$ (triangles).

studies. When J_K is greater than this value, a new maximum arises at $k=0$. It has been shown that in the strong-coupling regime, the effective interaction between the f spins is ferromagnetic.[6] The maximum at $k=0$ of $S_c(k)$ can be seen as a consequence of small ferromagnetic correlations tracking those of the f spins.

The suppression of the RKKY correlations can be understood by the Kondo mechanism. When J_K is small, the on-site singlet correlation $\langle \mathbf{S}_{i,c}\cdot\mathbf{S}_{i,f}\rangle$ shown in Fig. 4, is different from that of perfect on-site singlets $-\frac{3}{4}\rho$. This is due to the nonlocal character of the Kondo singlets. This means that the singlet formed by an impurity and the conduction electrons has a spatial extension. Consequently, the RKKY interaction between impurities is favored. As the coupling is increased, the size of the singlet reduces. It rapidly approaches that of perfect on-site singlets. As a result, the RKKY mechanism is suppressed. However contrary to the conventional view of the KLM,[12] a global singlet state is unstable against a FM state in the strong J_K limit. In this limit, the local Kondo singlets are mobile. It is the underlying electron motion in reduced dimension that is responsible of the FM correlations.

Now, we turn to the discussion of the conduction electron momentum distribution $n(k)$. It has been argued that in the weak-coupling regime, the KLM may present a PM Luttinger liquid (LL) structure.[5] The LL behavior is characteristic of many one-dimensional interacting electron systems.[11] In the LL theory of PM systems, $S(k)$ has a maximum at $2k_{F_c}$ and $n(k)$ presents a singularity at k_{F_c}. The electron momentum distribution has the form that follows:

$$n(k)=n_{k_F}-C|k-k_F|^{\alpha}\ \mathrm{sgn}(k-k_F). \tag{5}$$

We cannot calculate accurately the value of the exponent α. But Fig. 5 clearly shows that the singularity is located at $k=k_{F_c}$ in the weak-coupling regime. The existence of this singularity is consistent with the presence of the maximum of $S_{c,f}(k)$. So, the description of the model in the weak-coupling regime in terms of LL is plausible. Further investigations of the excitation spectrum are necessary to get the full answer. At intermediate J_K, $n(k)$ is found to be very smooth so that it becomes hard to identify any singularity. At strong J_K however, the singularity now appears at $k=2k_{F_c}$ as in a spinless fermion system. We believe that this is due to the action of the Kondo coupling which suppress a double occupancy of the conduction electrons. It freezes the electron-spin degrees of freedom. The transition from a PM to a FM phase does not necessary mean that the LL description breaks down. It can be yet interpreted as a transition from a PM LL to a ferromagnetic LL.

Finally, we touch upon the question of the size of the Fermi surface in the PM phase. In the weak-coupling region, the KLM is an effective model of the periodic Anderson model (PAM). In the PAM the f electrons are mixed to the conduction electron through a hybridization term. The PAM is believed to have a large Fermi surface containing both conduction electrons and localized electrons. In the KLM, however, there is no hybridization between the two kind of particles. It is still a matter of debate whether or not the KLM has a large Fermi surface. A large Fermi surface supposes the existence of a maximum at $2k_{F_c}+\pi$ in the structure factor or of a singularity in the momentum distribution function at $k_{F_c}+\pi/2$. Our results do not show any significant feature at this wave number. There is yet the possibility that the singularity at the position of the large Fermi surface is very small.[13]

In conclusion, we have used the DMRG to study the KLM at the density $\rho=0.7$. We believe that the behavior of the model at this density is characteristic of the moderate doping region. In agreement with previous exact diagonalization and Monte Carlo calculations, we have shown that the model presents a transition around $J_K=2$. The weak-coupling region is PM. The magnetic structure factor has a maximum at $2k_{F_c}$. The electron momentum distribution function displays a singularity at k_{F_c}. We have argued that

this is consistent with the description of the model in terms of LL. The strong-coupling region is FM. In this phase, the singularity in the electron momentum distribution is shifted to $2k_{F_c}$. This can be interpreted as the presence of a ferromagnetic LL structure.

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