One-dimensional Kondo lattice model studied through numerical diagonalization

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The one-dimensional Kondo lattice model is studied by means of the numerical diagonalization method. By using massively parallel computations, we were able to study lattices large enough to obtain convergent results for electron densities $n \leqslant 2/3$. For such densities, an additional ferromagnetic region is found inside the paramagnetic phase. Also, a region is found where the localized spins participate in the low-energy dynamics together with the conduction electrons, thus resulting in a large Fermi surface. These results are an independent confirmation of previous density matrix renormalization group results.

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The Kondo lattice model (KLM) is one of the most important models for studying strongly correlated electron systems and has been the subject of intensive study since its introduction in 1977 by Doniach.[1] Strongly correlated electron systems is an important area of modern condensed matter physics, relevant to many phenomena; just to mention a few, high-temperature superconductivity and colossal magnetoresistance.[2] Other canonical models include the Hubbard and the periodic Anderson model.

The KLM describes the interaction of an array of localized moments with conduction electrons. The model is important from a theoretical point of view since methods developed for the Kondo lattice are expected to aid in formulating methods for other strongly correlated electron systems.[3,4] Further, the model is important due to its applicability to several classes of real materials.[5] It is an effective model for the heavy fermion and colossal magnetoresistance compounds.[6–10] The heavy fermion compounds are intermetallic compounds containing rare-earth or actinide elements, which have a very small energy scale at low temperatures. This leads to a large specific heat and spin susceptibility, which can be accounted for by quasiparticles with very large effective mass, hundreds to a thousand times the electron mass, thus earning their name, heavy fermions. The KLM is one of the simplest models which describes the heavy fermion compounds of a conduction electron band interacting with a lattice of localized f-electron spins, provided the Kondo coupling between the localized f-electrons and the conduction electrons is antiferromagnetic and small. Other studies of the KLM include Ref. 11, showing incommensurate spin ordering obtained previously in Refs. 12 and 13, and the possibility of dimer order at quarter filling[14] that has been refuted in Ref. 15.

The model is defined by the Hamiltonian

$$H = -t\sum_{\langle i,j\rangle}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma} + \text{H.c.}) + J\sum_{j}\mathbf{S}_{cj}\mathbf{S}_{j}, \qquad (1)$$

where t is the conduction electron hopping parameter, the Kondo coupling $J>0$ is measured in units of the electron hopping t, and $\langle i,j\rangle$ denotes nearest neighbors.

We denote by $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ the creation and annihilation operators of an electron with spin σ on site i. $\mathbf{S}_j$ denotes the spin-1/2 operators for the localized moments. The spin operators $\mathbf{S}_{cj}$ for the conduction electrons are defined as

$$\mathbf{S}_{cj} = \frac{1}{2}\sum_{\tau,\tau'} c_{j\tau}^{\dagger}\sigma_{\tau,\tau'}c_{j\tau'},$$

where the σ are Pauli matrices. Partial conduction band filling $n<1$ is assumed. Here, the filling is defined as $n = N_{\text{el}}/L$, where N_{el} is the number of electrons in a system of size L.

The one-dimensional KLM (henceforth we will omit the qualifier "one dimensional") has been studied for a long time and some of its properties are well established. For example, for large values of the exchange coupling, it has been shown that the model exhibits ferromagnetism.[8,16,17]

Previously, some authors have mentioned regions of ferromagnetic (FM) ordering inside the paramagnetic (PM) phase in the phase diagram. The authors of Ref. 18 found just one point with FM ordering and argued that this point is a finite size effect. In Ref. 19, the authors discarded a FM signal inside the PM phase. Our group, see Ref. 12, was the first to perform a detailed study of the additional FM phase and later, see Refs. 13 and 20, two more FM phases. It is worth mentioning that the term "additional" is here used in the sense that the "main" FM phase appears for large J, for which there is a rigorous result[8] that for any $n<1$ and $J\to\infty$ the ground state of the KLM has total spin $S^{\text{tot}} = (L - N_{\text{el}})/2$, i.e., $L - N_{\text{el}}$ localized spins are ferromagnetically ordered and the rest form singlets with the conduction electrons.

There is another question about the ground state properties of the KLM which still is under debate, namely, the so-called size of the Fermi surface (FS).[21] Do the localized spins participate in the low energy excitations together with the conduction electrons? If so, this would imply a large FS, with the Fermi vector determined by the density of both particles: $k_F = \pi(n+1)/2$. If not, then one would see a small FS with $k_F = \pi n/2$. On one hand, the $J=0$ case gives completely free conduction electrons with $k_F = \pi n/2$, and if the interaction with the localized spins does not change the volume inside the FS (which is the case for Fermi liquids), then we would obtain a small FS. On the other hand, the KLM is

the limiting case for the periodic Anderson model, which allows localized spins to move, and the natural answer is a large FS.

In this Brief Report, we wish to shed some light on these issues; first, whether there exist additional FM regions, and second, the role of localized spins in the low-energy dynamics of the system.

The results presented here were obtained through numerical diagonalization. They show strong evidence of the existence of an additional FM region inside the PM phase which demonstrate that for $n \geqslant 1/2$, though below the transition, *the interaction of the conduction electrons with localized spins results in a large FS.*

In 1993, Tsunetsugu *et al.*[18] studied the phase diagram by numerical diagonalization of lattices up to nine sites, which was quite an achievement at the time. By using massively parallel computation, we have been able to investigate larger lattices; large enough to look for the ferromagnetic regions found inside the paramagnetic phase for $n > 1/2$ in the density matrix renormalization group (DMRG) studies.[12,13,20]

We used Lanczos method of the numerical diagonalization and studied model (1) under open boundary conditions. This case has the advantage of having a complete spin degeneracy in the $J \to \infty$ limit, while periodic and antiperiodic boundary conditions partially lift this degeneracy by cyclic spin permutations. We used the parallel version of the ARPACK package[22] and our own code for the vector-sparse matrix (Hamiltonian) multiplication. With these tools, we were able to study systems of 11 sites and 8 electrons for which the Hamiltonian matrix has over 3×10^9 nonzero elements in a matrix of size over $1.24 \times 10^8 \times 1.24 \times 10^8$.

For Hamiltonian (1), the total spin S^{tot} and its z projection S_z^{tot} are the good quantum numbers and therefore the Hamiltonian matrix is block diagonal and inside each block S_z^{tot} stays the same. That is why one can use the (largest) block with S_z^{tot} taking the minimum value 1/2 or 0, depending on whether $L+N_{\text{el}}$ is odd or even, to study the properties of the KLM. So in our calculations, we first chose all the states with a given S_z^{tot}, found all nonzero elements of Hamiltonian (1), and then for a given J calculated the smallest eigenvalue, which is the energy of the ground state, and its corresponding eigenvector $|v\rangle$. Using $|v\rangle$, we determined other properties of the ground state, namely, S^{tot} and the spin-structure factor.

In order to find S^{tot}, we calculated the square of the total spin operator,

$$(\mathbf{S}^{\text{tot}})^2 = \mathbf{S}_+^{\text{tot}}\mathbf{S}_-^{\text{tot}} + (\mathbf{S}_z^{\text{tot}})^2 - \mathbf{S}_z^{\text{tot}}.$$

Note that bold symbols denote operators, whereas italics are used for scalars. We found S^{tot} by solving the equation

$$S^{\text{tot}}(S^{\text{tot}}+1) = \langle v|(\mathbf{S}^{\text{tot}})^2|v\rangle.$$

It is obvious that one would obtain an energy and S^{tot} greater than or equal to what we found for the block with the minimal S_z^{tot} if we did the same for a block of the Hamiltonian with any other S_z^{tot}.

Due to the finite size of the system, S^{tot} can take only discrete steps when changing J. That is why we took the transition coupling J_{crit} to be the half-sum of the most close J with different S^{tot}, and their half-difference as the error for a given J_{crit}.

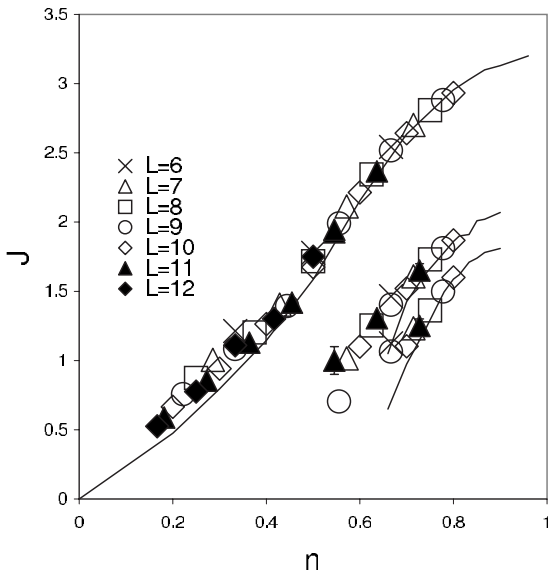

FIG. 1. The boundaries for different phases in the 1D KLM found with the numerical diagonalization method. The upper curve of symbols shows J above which S^{tot} takes the maximum value $S^{\text{tot}}=(L-N_{\text{el}})/2$ (Ref. 8). The symbols inside the paramagnetic region for $n \geqslant 2/3$ shows an additional ferromagnetic region with $S^{\text{tot}}=(L-N_{\text{el}})/2$. Above these symbols, the system has a large Fermi surface, and below, it has a small Fermi surface. For $6/11 \leqslant n < 2/3$ right below the FM-PM transition, the system has a large Fermi surface. The lower symbols are the transition points into the state with a small Fermi surface. The solid curves are the DMRG results from Ref. 13.

Figure 1 contains our results for J_{crit} and they add some new features to the results of Ref. 18. They agree well with the boundary of the PM-FM transition, but our results clearly demonstrate that there is an additional FM region inside the PM phase. For $n \geqslant 2/3$ and for any L, we found that below the PM-FM transition, the system becomes ferromagnetic again with maximum total spin in the ground state, i.e., $S^{\text{tot}}=(L-N_{\text{el}})/2$. When we lowered J even more, the system turned back into the PM state. This effect was also seen in Ref. 18 but discarded as an artifact. As proposed in Ref. 13, we believe that in this region, the double exchange mechanism causes the formation of the additional FM region.

The consistency of our results clearly suggests that this is not a finite size effect. First, as one can see, the results for $n=2/3$ for two different sizes $L=6$ and 9 coincide with good accuracy. Second, the results for different L and N_{el} form a reasonably good shape for the additional FM region. Third, the finite size scaling for $n=1/2$ in Fig. 2 shows the convergence of our results to the large-L DMRG result. We believe that as $L \to \infty$, our results of the additional FM region will converge to the DMRG results shown in Fig. 1 as a solid curve. Here, we use only a simple scaling ansatz of the form $c_0+c_1L^{\lambda}$ and take the average values of the fillings nearest one half for odd L.

We studied the spin structure factor (SSF) for localized spins as well. The SSF is defined as

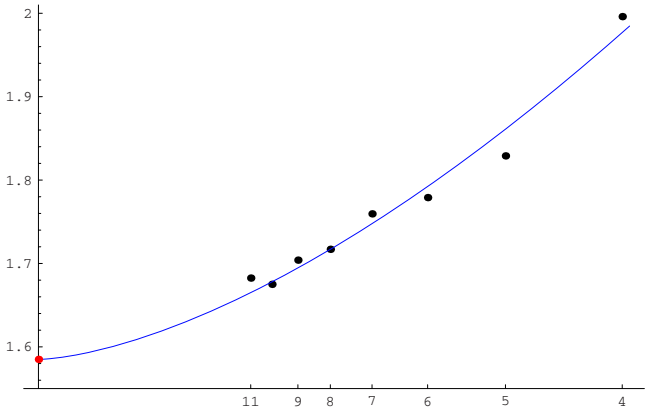

FIG. 2. (Color online) The finite-size scaling for J_{crit} for $n=1/2$. The dots for the odd L are obtained as a half-sum of the closest n's. The point on the y axis is the infinite-size scaling point from the DMRG calculations of Ref. 13. The curve was found through a Gaussian fit of $1.585+cL^{-\lambda}$ giving $c=3.459$ and $\lambda=1.571$.

$$S(q)=\left|\left\langle v\left|\sum \mathbf{S}_l\mathbf{S}_k e^{iq(l-k)}\right|v\right\rangle\right|. \tag{2}$$

We detected three regions where the system behaved differently. In the first region, $n<1/2$, the maximum of the SSF changes position at the point of the FM-PM transition and from the position at $q=0$ (in the FM region) moves to $q=2k_F=\pi n$ in the PM phase [see Fig. 3(a)]. The second region is at $1/2<n<2/3$. In this region, right below the FM-PM transition, the system has a large FS [the maximum of the SSF is at $q=2k_F^*=\pi(1-n)$]. When J decreases, the maximum of the SSF changes position to one which characterizes a small FS (the maximum of the SSF is at $q=2k_F=\pi n$) [see Fig. 3(b)] or the system becomes ferromagnetic until $J=0$. The latter, we believe, is a finite size effect. As an argument for this we look at the case when the filling is $n=0.6$: for $(L,N_{\mathrm{el}})=(5,3)$ below the upper curve in Fig. 1, we saw a PM-FM transition with decreasing J, and the system stayed ferromagnetic until $J=0$, but for $(L,N_{\mathrm{el}})=(10,6)$, the picture becomes clear—instead of the PM-FM transition, we see a change in the properties of the paramagnetic state. The shift of the maximum of the SSF was first discussed in Ref. 12 and is a sign of the fact that J becomes so small that the localized moments do not contribute to the dynamics of the conduction electrons any longer. The interaction of the localized moments takes a Ruderman-Kittel-Kasuya-Yosida (RKKY) form with the maximum of the SSF at $q=2k_F=\pi n$. This region has to be studied by other means since the numerical diagonalization methods are restricted to relatively small system sizes. The behavior of the SSF in the last region, $n\geqslant 2/3$, differs from that of the previous ones. In this region, there is an additional FM region inside the PM phase. Above this region, the SSF indicates a large FS, and below, a small FS for any system size studied. The additional maximum of the SSF at $q=0$ seen in Fig. 3(c) for small J seems to be a finite size effect, but our system sizes were too small to draw any conclusions from them.

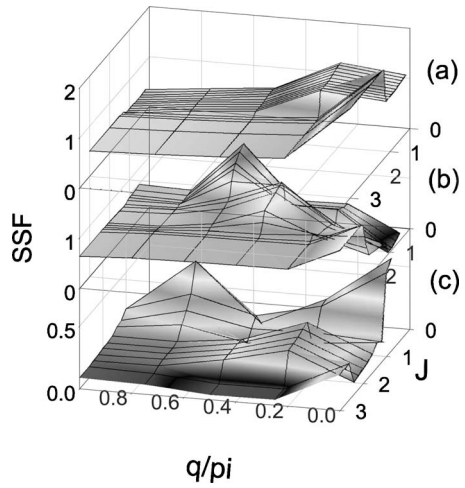

FIG. 3. The spin-structure factor (SSF) for different n. (a) $L=8$, $N_{\mathrm{el}}=3$, (b) $L=10$, $N_{\mathrm{el}}=6$, and (c) $L=9$, $N_{\mathrm{el}}=6$. The maximum of the SSF at $q=0$ for large J is a sign of the ferromagnetic ordering. The maximum of the SSF at $q=\pi(1-n)$ in (b) and (c) proves that below the FM-PM transition the system has a large Fermi surface. The maximum of the SSF at $q=\pi n$ is resulting from the scattering of the conduction electrons on the localized spins and has an RKKY form.

It is interesting that in the previous studies[12,13,20] as well as in the present Brief Report, we were not able to see an additional FM region for $n<2/3$. We believe that this is not a numerical problem, but rather a characteristic of model (1). A possible explanation for smaller n could be that the double exchange cannot provide an energy gain large enough to form an FM ordering. However, this energy can still cause a spin polaron formation, i.e., a bound state of kink and antikink domain walls. For $n<1/2$, as well as for the low-J region with $n>1/2$, the energy of the polaron excitation becomes too large and spin polarons do not contribute to the low-energy dynamics of the system and it behaves like an RKKY liquid (see Ref. 13).

To conclude, we have studied the one-dimensional Kondo lattice model by means of the numerical diagonalization method using massively parallel computation. In the phase diagram, we have found an additional ferromagnetic region inside the paramagnetic phase for conduction band filling $n>2/3$. Further, we have investigated the spin structure factor for the localized spins to determine the size of the Fermi surface and found a region in the phase diagram with a large Fermi surface. Both of these issues have been under debate. Our results, which are based on exact data, are in agreement with the previous density matrix renormalization group results,[12,13,20] and are a strong independent confirmation of these.

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