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# Friedel oscillations in the one-dimensional Kondo lattice model

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The paramagnetic metallic phase of the one-dimensional Kondo lattice model is studied by the density matrix renormalization group method. We observe charge and spin Friedel oscillations. They reflect the long-range charge-charge and spin-spin correlation functions. The observed oscillations are consistent with a Tomonaga-Luttinger liquid. From the period of the oscillations it is concluded that the Fermi surface is large, including both the conduction electrons and the localized spins, $k_F=\pi(1+n_c)/2$, where $n_c$ is the density of conduction electrons. [S0163-1829(96)04043-X]

Electron density oscillations as a response to a local perturbation provide a clue to understanding electronic states of a system. Response to an impurity potential is known as Friedel oscillations. The period of the oscillations is given by the diameter of the Fermi surface which is defined by the singular points in the momentum distribution function. As a local perturbation it is also possible to use a magnetic impurity. Then spin density oscillations are induced. Since these oscillations are the origin of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, the Friedel oscillations are responsible for the magnetically ordered structure of rare earth metals.

Generally speaking, a key to understanding the physics of heavy fermion systems is the competition between the RKKY interaction and the Kondo screening effect of the magnetic moments. The Kondo lattice model is one of the canonical models for heavy fermions and much effort has been devoted to elucidate the properties of the model. Recently the ground state phase diagram of the Kondo lattice model was completed in one dimension.[1,2] There are three phases in one dimension: a ferromagnetic metallic, a paramagnetic metallic, and an insulating spin liquid phase.

Our concern in the present paper is the metallic phase of the one-dimensional Kondo lattice model. In one dimension it has been established that most interacting metallic systems belong to the universality class of Tomonaga-Luttinger liquids.[3] The asymptotic forms of charge- and spin-correlation functions are

$$\langle n(x)n(0)\rangle = K_\rho/(\pi x)^2 + A_1\cos(2k_F x)x^{-1-K_\rho} + A_2\cos(4k_F x)x^{-4K_\rho}, \quad (1)$$

$$\langle \mathbf{S}(x)\cdot\mathbf{S}(0)\rangle = 1/(\pi x)^2 + B_1\cos(2k_F x)x^{-1-K_\rho}, \quad (2)$$

where $k_F=\pi\rho/2$, with $\rho$ being the density of charge carriers, is the Fermi momentum and $K_\rho$ is the correlation exponent.[4] In the above equations logarithmic corrections to the $2k_F$ correlations have been omitted. The momentum distribution function around $k_F$ shows a power law singularity $n_k \sim 1/2 - \mathrm{sgn}(k-k_F)|k-k_F|^\alpha$ with $\alpha=(K_\rho+1/K_\rho-2)/4$. The anomalous power law decays of the correlation functions naturally reflect themselves in the Friedel oscillations: the asymptotic form of the charge density oscillations induced by an impurity potential is

$$\delta\rho(x) \sim C_1\cos(2k_F x)x^{(-1-K_\rho)/2} + C_2\cos(4k_F x)x^{-2K_\rho} \quad (3)$$

as a function of the distance $x$ from the impurity.[5–7] Analogously, the spin density oscillations induced by a local magnetic field behave as

$$\sigma(x) \sim D_1\cos(2k_F x)x^{-K_\rho}. \quad (4)$$

Concerning the one-dimensional Kondo lattice model the paramagnetic metallic state is expected to belong to the class of Luttinger liquids. However, in this case the position of the Fermi points is already a nontrivial problem since the model consists of two components with completely different characters, the conduction electrons and the localized spins.

There are two different points of view concerning the above question. If the interaction between the conduction electrons and the localized spins is strictly zero, it is clear that the singularity in the momentum distribution function of the conduction electrons is determined only by the number of conduction electrons. Thus, if the singular points are not affected by the interaction, $k_F=\pi n_c/2$ is expected. On the other hand, a different answer is obtained by identifying the Kondo lattice model as an effective model for the periodic Anderson model. In the periodic Anderson model the con-

 

duction electrons and the $f$ electrons are mixed with each other through the hybridization matrix elements. Therefore it is naturally expected that $k_F$ is determined by the total density of both the conduction electrons and the $f$ electrons; $k_F=\pi(1+n_c)/2$.

In order to draw a conclusion on whether the Luttinger sum rule includes localized spins or not, it is necessary to deal with large-size systems because the Luttinger liquid is characterized by the long-range correlations and the singularity in the momentum distribution function is clearly defined only in the infinite system. For this purpose the density matrix renormalization group (DMRG) method developed by White[8] is most promising since in the DMRG we can study long chains and obtain results with only small systematic errors, which can be estimated from the eigenvalues of the density matrix.

In this paper, we calculate the Friedel oscillations of the one-dimensional Kondo lattice model by using the DMRG. The charge density oscillations are induced naturally by open boundary conditions and the spin density oscillations are introduced by applying local magnetic fields at both ends. From the period of the Friedel oscillations we can determine the Fermi momentum. Surprisingly the Friedel oscillations are compatible with the large Fermi surface $k_F=\pi(1+n_c)/2$ in spite of the fact that the charge degrees of freedom are completely suppressed for the $f$ electrons in the Kondo lattice model.

The Hamiltonian we use in the present study is the usual one-dimensional Kondo lattice model,

$$H=-t\sum_{i\sigma}\ (c_{i\sigma}^{\dagger}c_{i+1\sigma}+\ \text{H.c.})+J\sum_{i\mu}\ S_i^{\mu}s_i^{\mu}, \qquad (5)$$

where $c_{i\sigma}^{\dagger}$ $(c_{i\sigma})$ is the creation (annihilation) operator of a conduction electron at the $i$th site, and $s_i^{\mu}=(1/2)\Sigma_{\sigma\sigma'}c_{i\sigma}^{\dagger}\tau_{\sigma\sigma'}^{\mu}c_{i\sigma'}$, with $\tau_{\sigma\sigma'}^{\mu}$ $(\mu=x,y,z)$ being the Pauli matrices, are the spin density operators of the conduction electrons. The spin densities are coupled to the localized spins $S_i^{\mu}$ through an antiferromagnetic exchange coupling $J$.

Here we briefly summarize the phase diagram of this model.[1,2] At half filling, $n_c=1$, the ground state is a spin singlet with a gap for excitations.[9–12] Away from half filling the ground state is ferromagnetic in the strong coupling limit.[13,14] The ferromagnetic ground state is continuously connected to the low carrier density limit, $n_c\to 0$, where the ferromagnetic state survives even in the limit of weak exchange couplings. The paramagnetic metallic ground state exists only for weak couplings for finite carrier densities. The phase boundary between the ferromagnetic state and the paramagnetic state had been determined by the numerical exact diagonalization of finite clusters, and it was shown that the critical value $J_c$ goes up with increasing the carrier density.[2]

To treat large systems with sufficient accuracy, small truncation errors in the DMRG calculation are necessary. Since the truncation errors decrease with increasing $J$, we chose $n_c=4/5$ for the calculation of Friedel oscillations, where the paramagnetic state remains up to $J_c=3.0t$. At this filling there is a small additional ferromagnetic region below $J_c=3.0t$. It has already been reported in previous exact diagonalization studies at slightly different carrier concentration $n_c=0.75$.[2] Our DMRG results for clusters of size $N=10$ and 20 confirm the existence of this ferromagnetic region between $J=1.6t$ and $J=1.8t$ at $n_c=4/5$. The total spin of the ferromagnetic state is the same as that for strong coupling, and the phase transitions are caused by simple level crossings between the two lowest states with $S=0$ and $S=N(1-n_c)/2$. We calculate Friedel oscillations in the two paramagnetic states at $J=2.5t$ and $J=1.5t$.

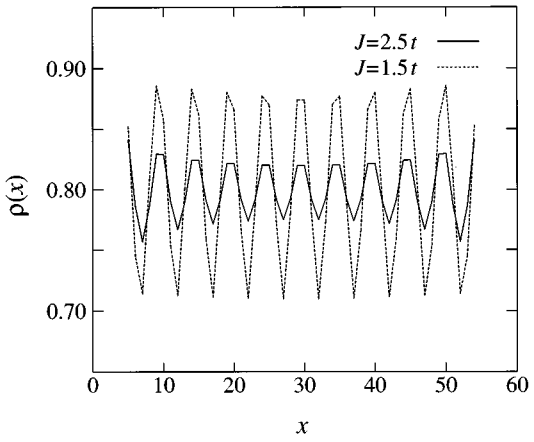


FIG. 1. Charge density oscillations of the Kondo lattice model. The system size is 60 sites and the carrier density is $n_c=4/5$. The solid line and the broken line correspond to $J=2.5t$ and $J=1.5t$, respectively. Typical truncation errors in the DMRG calculations are $1\times10^{-6}$ for $J=2.5t$ and $3\times10^{-6}$ for $J=1.5t$.

We first consider the paramagnetic state at $J=2.5t$. The charge density oscillations induced by the open boundary conditions are presented in Fig. 1 by the solid line. As expected, long-range oscillations characteristic of a Luttinger liquid are induced by the boundary conditions. Since the weak decay of the oscillations makes it difficult to determine the correlation exponents $K_\rho$ by the present system size, we focus our attention mainly on the period of the oscillations. The Fourier components of the oscillations, presented in Fig. 2, show a clear single peak at $q=2\pi/5$. The single peak at this wave number is natural in the strong coupling limit where the conduction electrons and the localized spins form local singlets, leading to complete spin-charge separation. In this case we can treat the charge part as spinless fermions whose correlation functions are characterized by its single $2k_F$ structure given by $2\pi(1-n_c)$. The peak at $q=2\pi/5$ corresponds to the $2k_F$ structure of the spinless fermions which is equivalent to $4k_F$ structure of the original fermions. The result of Fig. 1 means that the charge density oscillations at $J=2.5t$ are already well characterized by the nature of the strong coupling region.

From the above results, it is not possible to draw a conclusion about whether the Fermi surface includes the localized spins, because $4k_F=2\pi(1+n_c)=2\pi n_c(\text{mod } 2\pi)$. In order to see the contribution of the localized spins we next calculate spin density oscillations. If the $2k_F$ structure is found in the spin density Friedel oscillations reflecting the spin-spin correlations of Luttinger liquids, it may be possible to argue whether the Fermi surface includes the localized spins or not: if the localized spins contribute to the Fermi surface a $2k_F=\pi/5$ structure should appear but if it does not

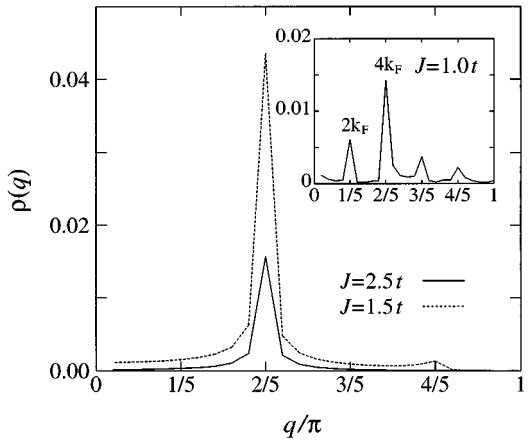


FIG. 2. Fourier components of the charge density oscillations. The system size is 60 sites and the carrier density is $n_c=4/5$. The solid line and the broken line correspond to $J=2.5t$ and $J=1.5t$, respectively. The Fourier transformation is carried out by using the central 50 sites. The inset shows the result for $J=1.0t$, for which typical truncation errors are $4\times10^{-5}$.

a $4\pi/5$ structure appears. To induce the Friedel oscillations of spin density, we apply local magnetic fields, $H_{\rm local}=2h(S_1^z-s_1^z-S_N^z+s_N^z)$ to the spins and conduction electrons at the boundary sites. These local magnetic fields with opposite directions for the two boundary spins induce oscillations that are odd with respect to reflection. This feature has been used to confirm the convergence of the DMRG.

The spin density oscillations are presented in Fig. 3 by the solid line and their Fourier components are shown in Fig. 4. We clearly see long range oscillations with $q=\pi/5$. They are consistent with a Luttinger liquid prediction, Eq. (4), if we assume the large Fermi surface where both the conduction electrons and the localized spins contribute to the Fermi volume:

$$k_F=\frac{\pi}{2}(1+n_c). \tag{6}$$

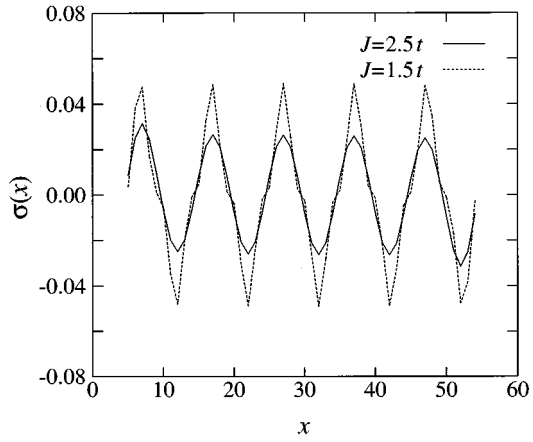


FIG. 3. Spin density oscillations of the Kondo lattice model. The system size is 60 sites and the carrier density is $n_c=4/5$. The solid line and the broken line correspond to $J=2.5t$ and $J=1.5t$, respectively. The strength of the local magnetic field $h$ is $0.1t$. Typical truncation errors in the DMRG calculations are $1\times10^{-6}$ for $J=2.5t$ and $3\times10^{-6}$ for $J=1.5t$.

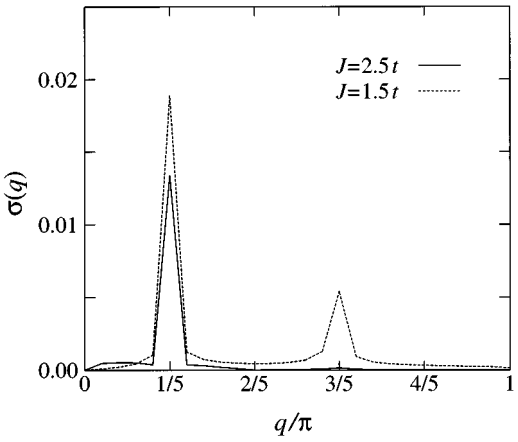


FIG. 4. Fourier components of the spin density oscillations. The system size is 60 sites and the carrier density is $n_c=4/5$. The solid line and the broken line correspond to $J=2.5t$ and $J=1.5t$, respectively. The Fourier transformation is carried out by using the central 50 sites.

Now we proceed to the paramagnetic metallic phase in the weak coupling region. The result of the charge density oscillations at $J=1.5t$ is presented in Fig. 1 by the broken line. In this case, too long-range oscillations are induced and their period is the same as $J=2.5t$. The similarity is also seen in the Fourier components shown in Fig. 2 by the broken line. For these coupling strengths we cannot see a peak at $q=2k_F=\pi/5$. This means the amplitude of the $2k_F$ oscillations of the charge density is still negligible even in the case of $J=1.5t$. However, as is shown in the inset of Fig. 2, we find clear $2k_F$ oscillations in addition to the dominant $4k_F$ oscillations at a smaller coupling $J=1.0t$ which is consistent with the general form of the Luttinger liquids.

For the spin density at $J=1.5t$, the oscillations and their Fourier components are presented in Fig. 3 and Fig. 4, respectively, by the broken lines. Although a small structure is also found at $q=3\pi/5$, the dominant component is at $q=\pi/5$. The structure at $q=3\pi/5$ is considered to be induced by the coupling mode of the spin density oscillations with $q=\pi/5$ and the charge density oscillations with $q=2\pi/5$ whose amplitude is larger than that of $J=2.5t$. Since the structure at $q=3\pi/5$ decreases rapidly with an increasing system size compared with the structure at $q=\pi/5$, we observe that it is not an intrinsic property of the infinite system. Combined with the results of the charge density oscillations it is concluded that the paramagnetic state at $1.5t$ is also characterized by the Luttinger liquid with the large Fermi surface.

At representative values for the exchange coupling constant $J=2.5t$ and $J=1.5t$, we have seen that the paramagnetic metallic phases of the Kondo lattice model show Friedel oscillations characteristic of a Luttinger liquid with a large Fermi surface. Similar results are obtained at different concentrations of conduction electrons, $n_c=2/3$, $J=2.0t$ and $n_c=6/7$, $J=1.7t$. These results are consistent with the previous work on the $t$-$t'$ Kondo lattice model for which it was shown exactly that its strong coupling limit is described by a Luttinger liquid with the large Fermi surface.[15] Therefore it is natural to conclude that the paramagnetic metallic phase of the Kondo lattice model has a large Fermi surface in general.

This conclusion is consistent with a variational Monte Carlo study using Gutzwiller projected hybridization form.[16] This conclusion is also consistent with the bosonization study by Fujimoto and Kawakami.[17] Although their work was recently criticized by White and Affleck,[18] it should be noted that the model used by the latter authors is different from the usual Kondo lattice model.

The DMRG method has made it possible to observe the Friedel oscillations corresponding to the large Fermi surface in the paramagnetic phase of the weak coupling region. However, it is still difficult to see them in the weak coupling limit $J<t$, where the length scale of the Luttinger liquid properties clearly exceeds the system size studied in the present work. Calculations on longer systems and the determination of the correlation exponent $K_\rho$ are important areas for future investigation.

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