Anomalous metallic phase in the one-dimensional Kondo lattice model

Hiroshi Wakameda, Naokazu Shibata

Department of Physics, Tohoku University, Sendai 980-8578, Japan
E-mail: hiroshi@cmpt.phys.tohoku.ac.jp

(Received September 30, 2013)

We analyze the ground state spin and charge correlation functions of the one-dimensional Kondo lattice model by employing the density matrix renormalization group method. With the use of the sine-square deformation analysis we find a paramagnetic metallic state which is characterized by a pairing of two holes in the conduction band with three localized spins.

KEYWORDS: Kondo-lattice, one-dimension, metallic ground state, DMRG

1. Introduction

The Kondo exchange interaction between the itinerant conduction electrons and the localized electrons is the origin of many interesting quantum phenomena. In the one-dimensional Kondo lattice model various types of insulating states, paramagnetic metallic states, and ferromagnetic metallic states are realized only by the Kondo exchange interaction [1, 2]. Such a variety of the ground states mainly comes from the competition between the Kondo effect and the RKKY interaction, where the Kondo effect screens the local magnetic moments while the RKKY interaction stabilizes them. In particular, the filling of the conduction band largely modifies the character of the RKKY interaction and this variable nature of the effective interaction further increases the diversity of the ground states. However, long-range nature of the RKKY interaction leads to long correlation length and in most cases detailed character of the ground state is strongly modified by the boundary conditions imposed on the system.

To remove such artifactual boundary effects, we use the sine-square deformation (SSD) analysis [3–5] and successfully suppress the discrete nature of the size effects. The remaining ideally small boundary effect makes spin and charge density oscillations in the ground state whose period is independent of the system size but uniquely determined by the filling of the conduction band and the Kondo exchange interaction. From the analysis on the intrinsic period of this oscillation, we identify a paramagnetic metallic state which is characterized by a pairing of two holes in the conduction band.

2. Model and method

The Hamiltonian of the one-dimensional Kondo lattice model is written as

$$H = -t \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + h.c.) + J \sum_i \mathbf{S}_i \cdot \mathbf{s}_i - \mu \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma},$$

where the first term is the nearest-neighbor hopping term of conduction electrons with $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) being the electron creation (annihilation) operator of spin $\sigma$ at the $i$-th site, and $J$ is the Kondo exchange interaction between the $S = 1/2$ localized $f$-spin $\mathbf{S}_i$ and the conduction electron spin $\mathbf{s}_i$. $\mu$ is the chemical potential.
The ground state wave function of the Hamiltonian is obtained by the density-matrix renormalization group (DMRG) method [6]. In this method we systematically include the important basis states and obtain results of large systems with controlled accuracy. In order to eliminate the boundary effects of finite system, we apply the SSD to the DMRG method. In the SSD analysis we gradually modify the energy scale of the Hamiltonian in real space, then use the resulting nearly zero energy edge states as buffer to realize the optimal bulk state in the main part of the system. The remaining small finite size effect and numerical error in the DMRG calculations are carefully examined and obtained results are finally used for analysis.

3. Result

Figure 1 shows the charge density oscillations of the ground state obtained by the DMRG method for $n_c = 0.4$ at $J/t = 0.9$ under the two boundary conditions: the usual open boundary conditions (OBC) and SSD. We clearly find that the average density for OBC around the center of the system $x \sim 0$ is slightly larger than 0.4, which is due to the reduction of the density at the both ends of the open system. Thus the slight increase of the density for OBC is size dependent and it seems to vanish in the limit of $L \to \infty$ as shown in Fig. 2 (a). By contrast, the size effect of the density oscillations for SSD is almost removed and the average density is always close to the bulk value of 0.4. This advantage of the SSD is clearly shown in the size independent period of the spin density oscillation shown in Fig. 2 (b) and Fig. 3. The period of the spin density oscillation obtained by SSD is also independent of the number of keeping states $m$ in the DMRG calculation. This fact also indicates that the period of the density oscillation is not an artifact of the DMRG analysis but an intrinsic character of the system. We note that the ideally small boundary effects under the SSD breaks SU(2) spin symmetry in the DMRG calculation, which seems to be recovered by increasing the number of keeping states $m$ in the DMRG calculation with the reduction of the amplitude of the spin density oscillation as shown in Fig. 3. Even in this case, $m$ and $L$ independent period of the spin density oscillation shows that the obtained period well characterizes the static spin-spin correlation function whose structure is determined by the low energy elementary excitations from the ground state.

To investigate the origin of this oscillation, we plot the relation between the period of the oscillation and the density of conduction electrons $n_c$ in Fig. 4. In this figure its period of the spin density
oscillation, $\lambda_s$, is represented by the wave number $2k_s$ through the relation $2k_s/(2\pi) = 1/\lambda_s$. If the ground state is characterized by a Tomonaga-Luttinger liquid of conduction electrons, $k_s$ should be the Fermi wave number $k_F$ of conduction electrons, which is proportional to the carrier density as $k_F = \pi n_c/2$. However, $2k_s$ obtained in the KLM is not proportional to the density of conduction electrons $n_c$ as shown in Fig. 4. In particular, $n_c$ dependence of $2k_s$ clearly changes at $n_c \sim 0.35$.

Fig. 2. (a) Size dependence of the average density $\langle n_{ci} \rangle$ around the center of the system for $n_c = 0.4$ at $J/t = 0.9$ under OBC and SSD. $L$ is the system size. (b) Size dependence of the wave number of spin density oscillation for $n_c = 0.4$ at $J/t = 0.9$. The total number of conduction electrons $N_c$ is 0.4$L$.

Fig. 3. Spin density oscillations for $n_c = 0.4$ at $J/t = 0.9$ under SSD. $m$ is the number of keeping states in the DMRG calculation. System size $L$ is 100.
Fig. 4. Inverse of the period of the spin density oscillation as a function of \( n_c \) at \( J/t = 0.7 \) obtained by SSD.

Fig. 5. Inverse of the period of the spin density oscillation as a function of \( n_c \) obtained by SSD. The number of keeping states in the DMRG calculation is 600. System size \( L \) is 100.

and \( n_{c2} \sim 0.386 \), and between the two densities \( 2k_s \) decreases with the increase in \( n_c \). In this region, \( 2k_s \) is well described by \( 2k_s = \pi(1 - n_c)/2 \), which is half the \( 2k_F \) of large Fermi surface, \( 2k_F = \pi(1 + n_c) = |\pi(1 + n_c) - 2\pi| \), where the Fermi surface includes both the conduction electrons and the localized spins. In the above equation, \(-2\pi\) is added to go back into the first Brillouin zone [7]. Outside the above region, \( k_s \) is neither \( k_F \) of large Fermi surface nor \( k_F^S \) of small Fermi surface, which includes only conduction electrons. Although the origin of this peculiar behavior is
unknown, \( n_c \) dependence of \( k_s \) is independent of the system size \( L \) and the accuracy of the DMRG as shown in Fig. 4. Indeed such odd periods of the spin correlation function have been obtained in standard DMRG calculations [8]. We thus think that the \( n_c \) dependence of \( k_s \) itself is not an artifact of the present calculation.

To see the stability of this anomalous ground state characterized by the oscillation of \( 2k_s = \pi(1 - n_c)/2 \), we next plot the results of different \( J \) in Fig. 5. We find the oscillation of \( 2k_s = \pi(1 - n_c)/2 \) at smaller \( n_c \) for smaller \( J \), but it is missing for \( n_c < 1/3 \). At \( n_c = 1/3 \), \( 2k_s^F = \pi n_c \) of the small Fermi surface is equivalent to the \( 2k_s \) of half the large Fermi surface \( \pi(1 - n_c)/2 \), that means the spin density of the ground state at \( n_c = 1/3 \) has six sites period as is previously shown in the DMRG and bosonization analyses [9, 10]. Even though the RKKY interaction plays an important role in the spin density oscillation, we need to consider the Kondo effect which binds conduction electrons and localized spins. Since the Kondo effect enhances the local singlet correlation, the local structure, which consists of three localized spins and one conduction electron, will be a characteristic component in the ground state around \( J/t \sim 0.5 \) where the RKKY interaction aligns three local spins ferromagnetically and the Kondo effect binds one electron within the three local spins. As a consequence, two holes in the conduction band are bound with each other to form composite particle. Since the number of the composite particle is half the number of holes in the conduction band, its Fermi wave number is identical to \( k_s \) of half the large Fermi surface which is obtained in a limited region of \( J \) with \( n_c > 1/3 \) where both the Kondo effect and RKKY interaction are important.

4. Summary

We have studied the ground state spin and charge density oscillations of the one-dimensional Kondo lattice model by using the DMRG method with the SSD analysis. From the intrinsic period of the density oscillation, we have identified a paramagnetic metallic state whose spin and charge density oscillations are characterized by half the large Fermi wave number, which suggests the pairing of two holes in three localized spins as a result of cooperative work of the RKKY interaction and the Kondo effect.

References