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Shibata, Naokazu
Nishino, Tomotoshi
Ueda, Kazuo
Ishii, Chikara

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Spin and charge gaps in the one-dimensional Kondo-lattice model with Coulomb interaction between conduction electrons

Naokazu Shibata
Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan
and Department of Physics, Faculty of Science, Science University of Tokyo, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162, Japan

Tomotoshi Nishino
Department of Physics, Graduate School of Science, Tohoku University, Sendai 980, Japan

Kazuo Ueda
Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan

Chikara Ishii
Department of Physics, Faculty of Science, Science University of Tokyo, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162, Japan
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The density-matrix renormalization-group method is applied to the one-dimensional Kondo-lattice model with the Coulomb interaction between the conduction electrons. The spin and charge gaps are calculated as a function of the exchange constant J and the Coulomb interaction U_c. It is shown that both the spin and charge gaps increase with increasing J and U_c. The spin gap vanishes in the limit of $J\rightarrow 0$ for any U_c with an exponential form, $\Delta_s \propto \exp[-1/\alpha(U_c)J\rho]$. The exponent, $\alpha(U_c)$, is determined as a function of U_c. The charge gap is generally much larger than the spin gap. In the limit of $J\rightarrow 0$, the charge gap vanishes as $\Delta_c=\frac{1}{2}J$ for $U_c=0$ but for a finite U_c it tends to a finite value, which is the charge gap of the Hubbard model.

Recently the insulating phase of the Kondo-lattice model (KLM) has been extensively studied in relation to the Kondo insulators.[1] In contrast to the strong-coupling limit where various properties are easily understood from the local bases, the weak-coupling limit has not yet been fully understood. Since the KLM with weak exchange coupling is an effective model of the symmetric periodic Anderson model with strong Coulomb interaction, the weak-coupling region of the KLM is important to understanding the strongly correlated insulating phase. For the one-dimensional case it has been established that both spin and charge gaps exist for any exchange coupling. The excitation gaps vanish in the limit of vanishing exchange coupling.[2,3] Since the gaps are tiny in the weak-coupling regime, it is no longer justified to neglect Coulomb interaction between the conduction electrons.

In this article we determine the spin and charge gaps in the entire region of the exchange constant taking account of the Coulomb interaction between the conduction electrons U_c. The excitation gaps are obtained precisely by employing the density-matrix renormalization-group (DMRG) method. Among other things, we find that U_c actually stabilizes the Kondo spin liquid phase, resulting in monotonic increase of both the spin and charge gaps as a function of U_c.

The model we consider in this article is the following one-dimensional KLM with Coulomb interaction (KLMC):

$$H=-t\sum_{i\sigma}\ (c^{\dagger}_{i\sigma}c_{i+1\sigma}+\ \text{H.c.})+J\sum_{i\mu}\ S^{\mu}_{i}\sigma^{\mu}_{i}$$

$$+U_c\sum_{i}\ (c^{\dagger}_{i\uparrow}c_{i\uparrow}-\tfrac{1}{2})(c^{\dagger}_{i\downarrow}c_{i\downarrow}-\tfrac{1}{2}), \qquad (1)$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator of a conduction electron at the ith site, and $\sigma^{\mu}_{i}=(1/2)\Sigma_{\sigma\sigma'}c^{\dagger}_{i\sigma}\tau^{\mu}_{\sigma\sigma'}c_{i\sigma'}$ with the Pauli matrices $\tau^{\mu}_{\sigma\sigma'}$ ($\mu=x,y,z$) are the spin-density operators of the conduction electrons. In the second term S^{μ}_{i} represents a localized f-spin operator with $S=1/2$. Concerning the kinetic energy of the conduction electrons we consider only the hopping processes between the nearest-neighbor sites, t. This model was considered by Yanagisawa and Harigaya in connection with the ferromagnetic ground state in the strong-coupling limit of the one-dimensional KLM away from half filling.[4] Here we are interested in the half-filling case where the total number of conduction electrons is equal to the number of lattice site: $N\equiv\Sigma_{i\sigma}c^{\dagger}_{i\sigma}c_{i\sigma}=L$. It is needless to say that this Hamiltonian is reduced to the Hubbard model in the limit of vanishing exchange interaction, $J\rightarrow 0$, and to the usual KLM for $U_c=0$.

For the case of $U_c=0$ extensive studies on the spin and charge gaps have already been done. First Tsunetsugu *et al.* showed numerically that the ground state is singlet and the spin gap always exists for any finite exchange by using exact diagonalization combined with finite-size scaling.[2] They have concluded that the J dependence of the spin gap has a similar form as the Kondo temperature of the single impurity Kondo model but the exponent is larger than that of single impurity case, the lattice enhancement effect. Subsequently, semiclassical analysis based on the nonlinear σ model obtained by mapping from the one-dimensional KLM was carried out by Tsvelik.[3] He showed that the spin gap exists for any J in consistent with the above results with some logarithmic correction in the exponent. For the charge gap, on the

other hand, a J-linear behavior is suggested by Nishino and Ueda. By using exact diagonalization of the one-dimensional periodic Anderson model up to eight sites, they observed that the charge gap is proportional to $1/U$ in the region of strong Coulomb interaction which means J-linear dependence in the corresponding weak-coupling region of the KLM ($J=8V^2/U$).[5] It follows that the ratio between the charge and spin gaps Δ_c/Δ_s diverges in the limit of vanishing exchange constant. Yu and White applied the DMRG method to the KLM.[6] Their results for larger clusters have confirmed the diverging behavior of Δ_c/Δ_s in the region of weak exchange coupling. For an asymmetric case, however it is also pointed out the ratio remains finite.[7]

In spite of these progresses, the results in the region of weak exchange coupling are still not accurate enough to determine precisely the functional form of the gaps due to the smallness of clusters used in these numerical studies. For example, the exponent of the spin gap has not yet been determined with sufficient accuracy and the linear J dependence of the charge gap remains to be a plausible scenario. In order to determine functional forms of these gaps it is essential to treat large clusters systematically so that we can extrapolate the gap energies to the bulk limit. For this purpose the DMRG method developed by White[8] is efficient because the number of the states used to construct the wave function does not increase with increasing the system size. Naturally the truncation of the states introduces numerical errors, but the errors may be estimated by the eigenvalues of the density matrix which are truncated off. Thus it is possible to increase the system size within a given accuracy.

In the previous DMRG calculation by Yu and White,[6] the number of states kept for each block is 180 and the number of the maximum system size is 24. However the lattice sizes are too small to fix the J dependence of the spin and charge gaps. For this purpose we use the finite system algorithm of the DMRG method with open boundary conditions keeping up to 300 states for each block and increase the system size up to 80.

In contrast to the infinite system algorithm, the finite system algorithm gives more accurate results, but the extrapolation to the infinite system is necessary. The extrapolation to the infinite may be done in the following way. Since the lowest excited state generally corresponds to the bottom of an excitation spectrum which can be expanded in terms of k^2, we expect finite-size scaling is of the form of L^{-2} for large systems. It means the gap energy of the large systems behaves as

$$\Delta(L)=\Delta(\infty)+\beta L^{-2}+O(L^{-4}). \tag{2}$$

We determine the gap energy of the bulk system by using this scaling when data for available system sizes already follows the scaling form. When a gap is tiny, for example, the spin gap of $J=0.6t$ and $U_c=0$, the scaling form is not yet clear for the system size available. In such a case the upper and lower bounds are estimated by L^{-2} and L^{-1} scaling, respectively, because the size dependence of the gap for smaller systems is close to L^{-1} rather than L^{-2}.

First we discuss the spin gap. It is obtained from the difference of the ground-state energies in the subspace of total S^z being zero and one with the same total electron number L, $E_g(S^z=1,N=L)-E_g(S^z=0,N=L)$. The $SU(2)$ symmetry in the spin space guarantees the energy difference is the same as the spin gap in the subspace of total S^z being zero.

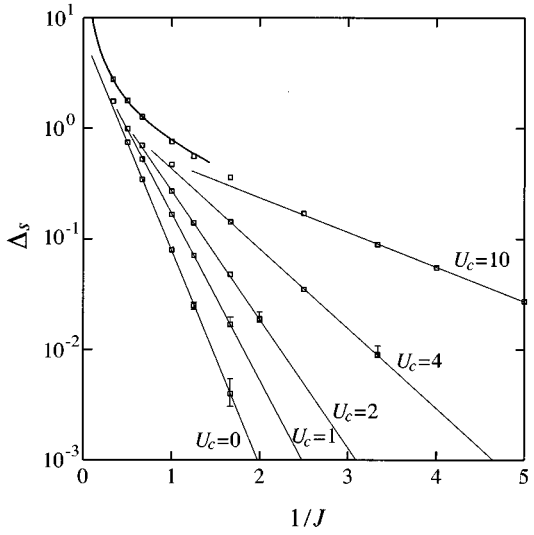

FIG. 1. Spin gap of the one-dimensional Kondo lattice model with Coulomb interaction. The thick curve represents the result of the perturbation theory in terms of t/J for $U_c=10t$. Typical truncation error in the DMRG calculation is 10^{-6} for $J=1$. Error bars are estimated from L^{-1} and L^{-2} scaling. Gap energies, exchange constant J, and Coulomb interaction U_c are in units of t.

Before proceeding to the analysis of the results it is worth reminding the Kondo impurity model. In the Kondo impurity model all physical quantities are scaled by single energy scale $T_K\sim D\ \exp(-1/\rho J)$ which is known as the Kondo temperature. Here $\rho=1/2\pi t$ is the density of states of the conduction band at the Fermi level. The simplest extension to the lattice problem is to include an enhancement of the exponent owing to intersite correlations. Then the spin gap is expected to behave as

$$\Delta_s\propto\exp\left(-\frac{1}{\alpha\rho J}\right), \tag{3}$$

where the α is the enhancement factor. The Gutzwiller approximation predicts an enhancement factor of 2.[9] As a matter of fact, Tsunetsugu *et al.* have estimated that the enhancement factor α is in the range of $1\leqslant\alpha\leqslant 5/4$ by using a finite-size scaling based on exact diagonalizations for the systems up to $L=10$.

The first task of the present study is to determine this enhancement factor more precisely. For this purpose we plot logarithm of the spin gaps as a function of $1/J$. Figure 1 shows the results extrapolated to the bulk limit using data of $L=6,8,12,18,24,40$. From this figure we obtain the exponent $\alpha=1.4(1)$ for the case of $U_c=0$. There are some ambiguities in the extrapolation to the bulk limit for a tiny gap. However within the present accuracy we do not observe any logarithmic correction to the exponent which is predicted by the semiclassical approach.[3]

Now we proceed to the effect of the Coulomb interaction between conduction electrons. As is well known, one of the most important effect of the Coulomb interaction for low-energy properties is the mass enhancement, which may be

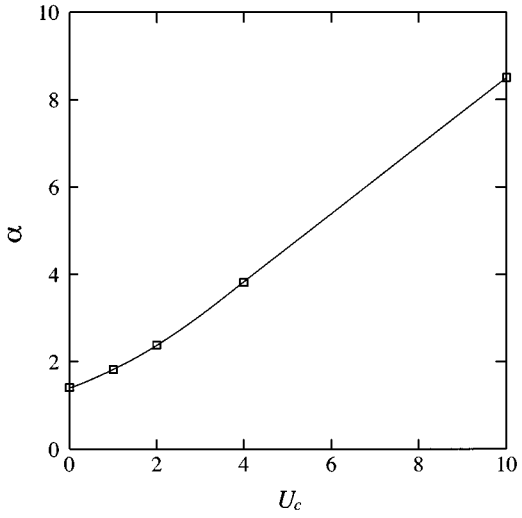

FIG. 2. U_c dependence of the exponent of the spin gap. Coulomb interaction U_c is in units of t.

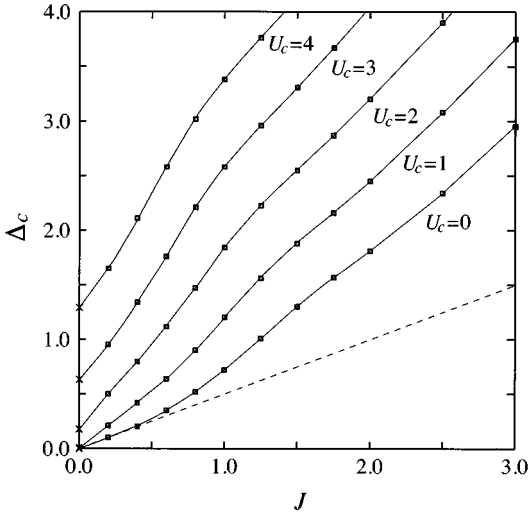

FIG. 3. Charge gap of the one-dimensional Kondo lattice model with Coulomb interaction. Results on the vertical axis are obtained from the exact solution of Lieb-Wu. Typical truncation error in the DMRG calculation is 10^{-6} for $J=1$ and 10^{-4} for $J=0.2$, which is a dominant source of numerical errors since the finite-size scaling, Eq. (2), is well obeyed. Gap energies, exchange constant J, and Coulomb interaction U_c are in units of t.

represented by an effective density of states at the Fermi energy, ρ^*. Thus in the weak-coupling region it is natural to extend the form of Eq. (3) to finite U_c by allowing U_c dependence of the exponent, $\alpha(U_c)$. In Fig. 1 it is seen that the numerical data are nicely fitted by this form. The exponent α is determined for various U_c. As shown in Fig. 2 the exponent α increases with increasing U_c and the asymptotic behavior is linear in U_c.

In the limit of strong Coulomb interaction ($U_c/t\to\infty$) the KLMC is mapped to the Heisenberg chain coupled with localized f spins. Since the effective coupling of the Heisenberg chain is given by $J_{\rm eff}=4t^2/U_c$, we can compare the present spin gap with that of the spin system. From Fig. 2 we find the asymptotic behavior of the exponent is $\alpha=0.78U_c/t+0.7$. It means that the spin gap of the above spin system behaves as $\Delta_s\sim\exp(-2J_{\rm eff}/J)$. In order to check this form we have analyzed the numerical data for the spin system obtained by Igarashi *et al.*[10] and found good agreement. Thus we conclude that the spin gap of the KLMC always vanishes exponentially in the limit of weak exchange coupling for any Coulomb interaction, U_c, and the exponent α increases monotonically with increasing U_c.

In the strong-coupling region of J, we may use the perturbation theory with respect to t/J also in the presence of finite Coulomb interaction U_c. After straightforward calculation we get the following result for the spin gap:

$$\Delta_s=J-\frac{4t^2}{\frac{1}{2}J+U_c}+\frac{2t^2}{\frac{3}{2}J+U_c}. \tag{4}$$

The solid curve in Fig. 1 represents this result for $U_c=10t$ which shows that our numerical data for the spin gap is well reproduced by the perturbation result down to $J\sim t$. From Eq. (4) one can see that the derivative of the spin gap with respect to U_c is always positive, $\partial/(\partial U_c)\Delta_s>0$, for any positive U_c and J. From these observations in both the strong- and weak-coupling regions we can conclude that the spin gap increases with increasing Coulomb interaction for any antiferromagnetic exchange J.

The charge gap is obtained by $E_g(S^z=0,N=L+2)-E_g(S^z=0,N=L)$. Owing to the hidden $SU(2)$ symmetry in the charge space, the energy difference is the same as the charge excitation gap in the subspace of total electron number fixed to L.[5]

Before discussing the charge gap we first notice the relation between the charge gap Δ_c and the quasiparticle gap $\Delta_{\rm qp}$ which is defined by $E_g(S^z=\pm 1/2,N=L\pm 1)-E_g(S^z=0,N=L)$. In the strong-coupling limit, $J/t\to\infty$, it is evident that the charge gap is twice the quasiparticle gap because the energy required to create the lowest charge excited state is the same as the energy cost to add two additional electrons owing to the $SU(2)$ symmetry in the charge space. In the second order perturbation in t/J, one can show that the interaction between the two additional electrons is repulsive, leading to only a phase shift. Therefore, the charge gap is given by the sum of two quasiparticle gap $\Delta_{\rm qp}$ in the bulk limit:

$$\Delta_c=2\Delta_{\rm qp}. \tag{5}$$

A similar argument is also valid for the periodic Anderson model.[5] Validity of this relation is checked by the present DMRG calculation and we have confirmed this relation in the entire region of the exchange constant J. On the other hand the spin gap is determined by the lowest bound state of a quasielectron and a quasihole.

Let us start from the case of $J=0$ where exact results are known. In this limit the KLMC is reduced to the Hubbard model which is exactly solved by Lieb and Wu for the one-dimensional case.[11] The asymptotic form of the charge gap is $\Delta_c\propto\sqrt{U_c t}\,\exp(-1/\rho U_c)$ for small U_c, and $\Delta_c\propto U_c-4t$ for large U_c. Figure 3 shows the charge gap extrapolated to the infinite system from the data for $L=6,8,12,18,24,40$. These

results for finite J are consistent with the exact results which are denoted by crosses on the vertical axis.

For $U_c=0$, the charge gap of the Hubbard model vanishes. In this case an important question is how the charge gap opens for finite J. As is shown in the previous work by Nishino *et al.* the charge gap is much larger than the spin gap in the weak-coupling regime.[5] It implies that the correlation length for the spin degrees of freedom is much longer than the charge correlation length. Therefore, for the discussion of the charge gap it is justified to assume that the spin-spin correlation length is infinitely long. Under the assumption of the infinite spin correlation length, one can get the charge gap which is linear in J with its coefficient 1/2

$$\Delta_c=\frac{J}{2}. \tag{6}$$

This linear dependence in J is actually seen in the present DMRG calculations shown in Fig. 3. For the case of $J=0.2t$ and $U_c=0$ we have additionally calculated a larger system of $L=80$ and we get the charge gap of $0.1t$ from the extrapolation. We may take this fact as a numerical confirmation of the coefficient of 1/2. It should be stressed again that this type of mean-field theory is not justified for the discussion of the spin gap.

From Fig. 3 we also find that the charge gap increases with increasing Coulomb interaction U_c. In the strong-coupling regime, we get the following result for the charge excitation gap within the second order perturbation:

$$\Delta_c=\frac{3}{2}J+U_c-2t+\frac{5t^2}{\frac{3}{2}J+U_c}-\frac{3t^2}{J}. \tag{7}$$

From the result it is clear that the charge gap is a increasing function of U_c for large J. Thus it is concluded that the charge gap increases with increasing Coulomb interaction U_c for any exchange constant J similarly as the spin gap.

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