Thermodynamic properties of the one-dimensional Kondo insulators studied by the density matrix renormalization group method

Naokazu Shibata, Beat Ammon, Matthias Troyer, Manfred Sigrist and Kazuo Ueda
Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan
1 Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland
Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-01, Japan
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Thermodynamic properties of the one-dimensional Kondo lattice model at half-filling are studied by the density matrix renormalization group method applied to the quantum transfer matrix. Spin susceptibility, charge susceptibility, and specific heat are calculated down to $T = 0.1t$ for various exchange constants. The obtained results clearly show crossover behavior from the high temperature regime of nearly independent localized spins and conduction electrons to the low temperature regime where the two degrees of freedom couple strongly. The low temperature energy scales of the charge and spin susceptibilities are determined and shown to be equal to the quasiparticle gap and the spin gap, respectively, for weak exchange couplings.

The Kondo lattice model (KLM) is a simple theoretical model for heavy Fermions which consists of two different types of electrons; the localized spins whose charge degrees of freedom are completely suppressed, and the conduction electrons that propagate as carriers in extended orbitals. Both the conduction electrons and the localized spins do not interact among themselves, however, the exchange interaction between them leads to correlations and yields various interesting physical phenomena.

Recent studies on the one-dimensional KLM has shown that this model is always insulating at half-filling. This insulating phase has different excitation gaps for the spin and charge channels. The spin gap defines the energy cost needed for the lowest spin excitation which changes the total spin quantum number. The charge gap defines that for the lowest pure charge excitation which changes the total carrier number by two keeping the spin quantum numbers fixed.

The spin gap of this insulating phase has been extensively studied both analytically and numerically. It has been shown that the spin gap $\Delta_s$ has similar $J$-dependence to that of the Kondo temperature $T_K$ for the single impurity Kondo model. The numerical studies show $\Delta_s \propto \exp(-1/\alpha \rho J)$, where $\rho$ is the density of state at the fermi level and $\alpha$ is the lattice enhancement factor. The lattice enhancement factor was recently determined to be $\alpha = 1.4$ by the density matrix renormalization group (DMRG) method. The similarity between the Kondo temperature and the spin gap suggests that the origin of the spin gap is due to some sort of singlet formation between the conduction electrons and the localized spins which is the essence of the Kondo effect. The difference appears in the coefficient $\alpha$ in the exponent, which is due to collective singlet formation of conduction electrons with many localized spins in the lattice.

For the charge gap, on the other hand, linear $J$-dependence ($\Delta_c = J/2$) has been obtained for weak exchange couplings. This $J$-dependence may be understood by the strong antiferromagnetic correlations among localized spins that generate a staggering internal magnetic field on conduction electrons which is proportional to the exchange constant. It should be noted that the correlation length of the spin degrees of freedom is much longer than the charge correlation length. Therefore the above arguments are justified in spite of the fact that there is no magnetic long range order.

The qualitatively different nature of the spin and charge gaps is a consequence of quantum mechanical many body effects among the conduction electrons and localized spins, and is a unique feature of this strongly correlated insulating phase.

In the present paper we will study how such interplay between the conduction electrons and the localized spins appears in the temperature dependence of various thermodynamic quantities. To discuss the thermodynamic properties we use the finite temperature density matrix renormalization group method (finite-$T$ DMRG). We calculate spin and charge susceptibilities and specific heat for various exchange constants. We will show clear crossover behavior between high and low temperature regimes. In the high temperature regimes the localized spins and the conduction electrons are only weakly coupled, while in the low temperature regime they couple strongly. Characteristic energy scales in the low temperature regimes are identified as the spin gap and the quasiparticle gap for the spin and charge degrees of freedom, respectively.

The Hamiltonian we use here is the one-dimensional KLM described by

$$H = -t \sum_{is}(c_{i\uparrow}^\dagger c_{i+1s} + c_{i+1s}^\dagger c_{is}) + J \sum_i S_{ci} \cdot S_{ci}$$

(1)

where the operator $c_{is}$ ($c_{is}^\dagger$) annihilates (creates) a conduction electron at site $i$ with spin $s (=\uparrow, \downarrow)$ ($S_{ci}^\mu = (1/2) \sum_{s,s'} c_{i\mu}^s \sigma_{ss'}^{\mu} c_{is'}$). The hopping matrix element is given by $t$ and $J$ is the antiferromagnetic exchange cou-
pling between the conduction electron spins \( \mathbf{S}_c \) and localized spins \( \mathbf{S}_l \), both being spin 1/2 degrees of freedom. The density of conduction electrons is unity at half-filling.

In order to calculate thermodynamic quantities we use the density matrix renormalization group method [9] applied to the quantum transfer matrix. Recently this method of finite-\( T \) DMRG was successfully applied to the one-dimensional quantum spin systems to calculate thermodynamic quantities. [10] The present study is the first application of the finite-\( T \) DMRG to a system with Fermionic degree of freedom.

In the following we briefly outline the method. We define the transfer matrix

\[
T_n(M) = [e^{-\beta h_{2n-1,2n}/M} e^{-\beta h_{2n,2n+1}/M}]^M
\]

where \( M \) is the Trotter number. Here the Hamiltonian \( H \) is decomposed into two parts \( H_{\text{odd}} = \sum_{n=1}^{L/2} h_{2n-1,2n} \) and \( H_{\text{even}} = \sum_{n=1}^{L/2} h_{2n,2n+1} \) such as \( [h_{2n-1,2n}, h_{2n',2n''}] = [h_{2n,2n+1}, h_{2n',2n''}] = 0 \). First we diagonalize the transfer matrix with a small \( M \) to obtain the maximum eigenvalue \( \lambda \) and corresponding eigenvector. Next we calculate generalized density matrix from the obtained eigenvector. By diagonalizing the density matrix, we chose important basis states which have large eigenvalues for the representation of the transfer matrix. Using these basis states we increase the Trotter number \( M \) of the transfer matrix within the fixed number of basis states and continue the above procedure until we get the Trotter number sufficient for a given temperature \( T \). The free energy of the infinite system is directly obtained from the maximum eigenvalue \( \lambda \) of the transfer matrix: \( F = -(T/2) \ln \lambda \). The spin and charge susceptibilities, and specific heat are obtained by numerical derivatives of the free energy.

The following calculations are performed by the infinite system algorithm of the finite-\( T \) DMRG keeping 40 states per blocks. [9] The truncation error in the finite-\( T \) DMRG calculation is typically \( 10^{-3} \) and \( 10^{-2} \) at the lowest temperature with the Trotter number \( M = 50 \). To check the results we have compared the obtained spin and charge susceptibilities to those calculated by the Quantum Monte Carlo simulations for \( J/t = 1.6 \). [11] The overall structure agrees well, but low temperature part of our results are more reliable. For example, the estimated spin gap energy \( 0.7t \) in Ref. 11 is not consistent with \( 0.4t \) obtained by the standard zero-temperature DMRG [9], while it is consistent with the present result \((0.45 \pm 0.1) t \) obtained by the finite-\( T \) DMRG.

We first show the temperature dependence of the uniform spin susceptibility. The spin susceptibility is obtained from the change of the free energy by a small magnetic field \( h \): \( \delta F = \chi_s h^2/2 \). The results for \( J/t = 0, 1.0, 1.2, 1.6 \) and 2.4 are shown in Fig. 1. In the limit of \( J/t = 0 \), both the localized spins and conduction electrons are uncorrelated. The susceptibility is given by the sum of the Curie term of localized spins and the Pauli term of free conduction electrons. In this system the contribution of the Pauli susceptibility of the free electrons (shown in Fig. 1) is relatively small, and the total susceptibility of \( J/t = 0 \) is dominated by the Curie term of the localized spins, which diverges in the limit of \( T = 0 \).

With introducing the exchange coupling, low temperature part of \( \chi_s \) sharply decreases with decreasing the temperature. This drastic change is due to the formation of the spin singlet state between the localized spins and conduction electrons whose energy scale is given by the spin gap for small exchange constant. The spin gap \( \Delta_s \) obtained by the zero temperature DMRG is 0.08\( t \) for \( J = 1.0t \), which is consistent with the characteristic temperature at which \( \chi_s \) starts to decrease.

![FIG. 1. Spin susceptibility of the half-filled one-dimensional Kondo lattice model. The truncation error in the finite-\( T \) DMRG calculation is typically \( 10^{-3} \) and \( 10^{-2} \) at the lowest temperature.](image)

This characteristic temperature separates high temperature region where \( \chi_s \) increases with decreasing the temperature, and low temperature region where the susceptibility drops rapidly with decreasing temperature. This temperature is expected to be determined by the competition between the thermal fluctuations and the singlet correlations. Since the exchange interaction stabilizes the singlet correlation between the localized spins and conduction electrons, the crossover temperature increases with enhanced exchange coupling.

In order to determine the energy scale at low temperatures more precisely we estimate the activation energy by fitting the obtained susceptibility. The estimated activation energy for the spin susceptibility is summarized in Table I for \( J/t = 1.6t, 2.4t, \) and \( 3.0t \). Here we can compare this energy scale with quasiparticle gap and spin gap, both responsible for the magnetic excitation. The quasiparticle gap and spin gap are obtained by the standard zero temperature DMRG method.

In Table I we see that the lower one of the quasiparticle gap and the spin gap determines the low temperature energy scale of the spin susceptibility. This is consistent with the general form of the susceptibility that is formally written as
According to the above equation the low temperature behavior is determined by the energy difference between the ground state and the lowest excited state which is active for magnetic field.

Next we consider the charge susceptibility. The charge susceptibility χ_c is obtained from the change of free energy by a small shift of chemical potential μ. δF = χ_cμT^2/2. In the present calculation we use the fact that the chemical potential is zero at half-filling owing to the SO(4) symmetry of the model. [7]

Calculated χ_c for J/t = 0, 1.0, 1.2, 1.6 and 2.4 are shown in Fig. 2. For J/t = 0, χ_c does not show diverging behavior at low temperatures in contrast to χ_s. In the limit of T = 0 χ_c is equal to the density of state of conduction electrons that is 1/π. This is natural since the charge degrees of freedom is solely governed by the conduction electrons. Since there is no correlation between up-spin and down-spin conduction electrons for J/t = 0, χ_c/4 is equal to the spin susceptibility of the free conduction electrons. The slight increase in χ_c in the low temperature region is a characteristic feature of the one-dimensional system where the density of states diverges at the band edge.

![Figure 2: Charge susceptibility of the half-filled one-dimensional Kondo lattice model.](image)

Switching on the exchange coupling, χ_c decreases rapidly at low temperatures. Similarly to χ_s, this is due to the singlet formation between the conduction electrons and the localized spins. With increasing the exchange coupling, decrease in χ_c appears at higher temperature. This is consistent with the behavior of the charge gap (quasiparticle gap), which is enhanced with increasing the exchange coupling.

To determine the energy scale at low temperatures, we estimate activation energy for the charge susceptibility. By fitting χ_c with an exponential function, activation energy Δ_χ_c is obtained as listed in Table I for J/t = 1.6t, 2.4t, and 3.0t. From this table it is concluded that the quasiparticle gap always determines the low temperature energy scale of the charge susceptibility. Since the charge gap is twice the quasiparticle gap, the lowest excitation that is responsible for the charge excitations is always the quasiparticle gap.

Finally, we consider the specific heat. The specific heat is calculated from the second derivative of the free energy; C = −Tδ^2F/δT^2. The results for J/t = 0, 1.0, 1.2, 1.6 and 2.4 are shown in Fig. 3.

At J/t = 0 the specific heat of this model is given by the sum of the delta function at T = 0 that originates from the localized spins and the specific heat of free conduction electrons. By including the exchange coupling, they are combined to make a two-peak structure. The peak at higher temperatures is almost independent of the exchange constant, and similar to the structure of the free conduction electrons. The peak at lower temperatures strongly depends on the exchange constant. The peak shifts toward higher temperatures and becomes broader with increasing J/t. This behavior is consistent with that of the spin susceptibility whose peak also shifts toward higher temperatures and becomes broader with increasing J/t.

Further increasing the exchange coupling, large excitation gap which is comparable to the hopping matrix element t opens for both spin and charge sectors. The ground state is close to the collection of the local singlets, and the specific heat has a single peak structure. (See J/t=2.4 in Fig. 3)

| J/t   | Δ_χ_s | Δ_χ_c | Δ_s | Δ_qp |
|-------|-------|-------|-----|------|
| 1.6t  | 0.45t ± 0.1t | 0.6t ± 0.1t | 0.4t | 0.7t |
| 2.4t  | 1.2t ± 0.1t | 1.0t ± 0.1t | 1.1t | 1.1t |
| 3.0t  | 1.6t ± 0.1t | 1.4t ± 0.1t | 1.8t | 1.5t |

TABLE I: Activation energy obtained from the spin and charge susceptibility, Δ_χ_s, and Δ_χ_c, and the quasiparticle gap Δ_qp and the spin gap Δ_s of the one-dimensional Kondo lattice model. The charge gap is twice the quasiparticle gap; Δ_c = 2Δ_qp.
In conclusion we have successfully applied the finite-$T$ DMRG to the one-dimensional Kondo lattice model at half-filling. Temperature dependence of the spin and charge susceptibility as well as the specific heat are calculated down to $T = 0.1t$. Compared with the quantum Monte Carlo simulations, an advantage of the finite-$T$ DMRG is that it is free from statistical errors and numerical errors in the calculations are under control to certain extent by keeping sufficient number of basis states. More importantly it is, in principle, free from the negative sign problem which practically invalidates the quantum Monte Carlo simulations for frustrated spin systems and most of Fermionic systems.

The subtle interplay between the localized spins and the conduction electrons are clearly seen in the temperature dependence of the susceptibilities and the specific heat. The low-temperature energy scale of the spin susceptibility is determined by the smaller one of the spin gap and the quasiparticle gap. Thus, the spin gap is the low energy scale in the weak coupling regime. On the other hand, the low energy scale for the charge susceptibility is always determined by the quasiparticle gap, which is half of the charge gap. Effects of both the spin gap and the charge gap are seen in the specific heat.

The present study is the first one where the finite-$T$ DMRG is applied to a system with Fermions. Existence of the excitation gap at half-filling is favorable for convergence of numerical calculations. Of course it is an interesting future problem to apply the finite-$T$ DMRG to the Kondo lattice model away half-filling where the ground state is a Tomonaga-Luttinger liquid with gapless spin and charge excitations [12,13].

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