The finite-temperature density-matrix renormalization-group method is applied to the one-dimensional Kondo lattice model near half filling to study its thermodynamics. The spin and charge susceptibilities and entropy are calculated down to $T = 0.03t$. We find two crossover temperatures near half filling. The higher crossover temperature continuously connects to the spin gap at half filling, and the susceptibilities are suppressed around this temperature. At low temperatures, the susceptibilities increase again with decreasing temperature when doping is finite. We confirm that they finally approach the values obtained in the Tomonaga-Luttinger (TL) liquid ground state for several parameters. The crossover temperature to the TL liquid is a new energy scale determined by gapless excitations of the TL liquid. The transition from the metallic phase to the insulating phase is accompanied by the vanishing of the lower crossover temperature.

The Kondo insulator is a typical strongly correlated insulator and develops a spin gap at low temperatures [1]. The half-filled Kondo lattice (KL) model has been studied as its theoretical model, particularly in one dimension (1D) by both numerical and analytical approaches [2,3]. The ground state of this model is shown to have both spin and charge gaps, $\Delta_s$, $\Delta_c$, and strong correlation effects appear in their difference [4]. The spin gap is always smaller than the charge gap, and for small exchange coupling $J$ the spin gap is exponentially small, $\Delta_s \sim \exp(-1/\alpha \mu J)$ [2,3], while the charge gap is linear in $J$ [4,5].

At finite temperatures, the spin gap characterizes unique temperature dependence of the excitation spectrum. With increasing temperature, the structure of the charge gap in the dynamic charge structure factor and the quasiparticle density of states disappears at $T \sim \Delta_s$, much lower than $\Delta_c$, although the latter is the energy scale of charge excitations at $T = 0$ [3,6]. This feature is also seen in the temperature dependence of the charge susceptibility, which drastically decreases below $T \sim \Delta_s$ [7,8]. As for the spin susceptibility, it decreases exponentially with the energy scale of $\Delta_s$, as expected [1,9].

When a finite density of carriers are doped, the 1D KL model belongs to another universality class. The ground state and the low energy excitations are described as a Tomonaga-Luttinger (TL) liquid [10,11]. In contrast to the half filled case, the ground state has gapless excitations in both spin and charge channels. Consequently the spin and charge susceptibilities are finite at $T = 0$ and determined by the velocities of the collective excitations, $\chi_s = 1/(2\pi v_s)$ and $\chi_c = 2K_c/(\pi v_c)$ where $K_c$ is the Luttinger-liquid parameter [12,21], whereas $\chi_s = 0$, $\chi_c = 0$ at half filling due to the gap.

In the present paper we study thermodynamics of the 1D KL model near half filling, i.e. in the vicinity of metal-insulator transition. Thermodynamic quantities are calculated by the finite-temperature density-matrix renormalization-group (finite-$T$ DMRG) method [22,23], and we find that the spin gap at half filling appears as a crossover temperature such that the susceptibilities are suppressed around there. We also find a new lower crossover temperature which is the energy scale of the gapless excitations of the TL liquid ground state. This is sensitive to the hole doping, and the transition from the metallic phase to the insulating phase corresponds to the vanishing of the lower crossover temperature.

The Hamiltonian we use in the present study is the 1D KL model described as

$$H = -t \sum_{i,s}(c^\dagger_{i,s}c_{i+1,s} + \text{H.c.}) + J \sum_{i,s,s'} \frac{1}{2} \sigma_{ss'} c^\dagger_{is} c_{is'},$$

where $\sigma_{ss'}$ are the Pauli matrices and $S_i = \sum_{s,s'} \frac{1}{2} \sigma_{ss'} f^\dagger_{is} f_{is'}$ is the localized spin at site $i$. The model has hoppings $-t$ ($t > 0$) for only nearest neighbor pairs. The density of conduction electron $n_e$ is unity at half filling, and hole doping ($n_e = 1 - \delta$) is physically equivalent to electron doping ($n_e = 1 + \delta$) due to the particle-hole symmetry.

In order to study thermodynamics we employ the finite-$T$ DMRG method [22,23]. By iteratively increasing the Trotter number of the quantum transfer matrix, we can obtain the eigenvector for the largest eigenvalue with desired accuracy. Thermodynamic quantities are directly calculated from this eigenvector, and the extrapolation in the system size is not needed [24]. This method was first applied to the quantum spin systems and shown to be reliable down to the low temperature $T = 0.01J$ [24,25]. This method is free from statistical errors and the negative sign problem, which are advantages compared with the quantum Monte Carlo method.

To obtain thermodynamic quantities with fixed hole density $\delta = 1 - n_e$, we need chemical potential $\mu$ at each temperature. This requires many DMRG calculations at different fixed chemical potentials: for each $J$ we use 36 sets of $\mu$ with a typical interval $\Delta \mu = 0.025t$. The number of states used in the present study is typically 54 and corresponding truncation error is $10^{-3}$ at the lowest temperature $T = 0.03t$ with the Trotter number 60.
The $T$-dependence of the chemical potential for several $\delta$'s is shown in Fig. 1 for $J = 1.6t$ and $1.2t$. Note that the chemical potential at half filling is always zero due to the particle-hole symmetry. At high temperatures, $\mu$ is similar to the value for the free conduction electrons and indicates metallic behavior. At low temperatures, however, a significant increase in $|\mu|$ appears for small $\delta$. In the limit of $T = 0$, $\mu$ approaches $T = 0$ value and this clearly shows the presence of the quasiparticle gap $\Delta_{qp}$ as shown in Fig. 1. Previous $T = 0$ DMRG calculations show that $\Delta_{qp} = 0.7t$ for $J = 1.6t$ and $0.47t$ for $J = 1.2t$, which is consistent with the present calculation. In the following, we calculate thermodynamic quantities for fixed $\mu$'s and convert them for fixed $\delta$'s using these data of $\mu(\delta,T)$.

Temperature dependence of spin susceptibility $\chi_s(T)$ is plotted in Fig. 2 for $J/t = 1.6$ and $1.2$ at $0 \leq \delta \leq 0.2$. At high temperatures $\chi_s$ is asymptotically determined by the sum of the Curie term of the localized spins, $1/(4T^2)$, and the Pauli susceptibility, $\chi_{Pauli}$, of the free conduction electrons. This is actually seen in the inset of Fig. 2(a). For $\delta \leq 0.2$, the change in the density of states of the free conduction band due to hole doping is within $5\%$ leading to little change in $\chi_{Pauli}$, and it is reasonable that the $\delta$-dependence of $\chi_s$ is small at high temperatures.

With decreasing temperature the spin susceptibility increases owing to the Curie term of the localized spins, but around $T \sim \Delta_s$, the spin susceptibility starts to be suppressed as in the $\delta = 0$ case. Previous $T = 0$ DMRG calculations show that $\Delta_s = 0.4t$ for $J = 1.6t$, and $\Delta_s = 0.16t$ for $J = 1.2t$. These behaviors suggest that the spin gap at $\delta = 0$ persists as the crossover temperature characterizing the suppression of $\chi_s$ even away from half filling.

With further decreasing temperature, $\chi_s$ sharply increases again when doping is finite, whereas it exponentially decreases at half filling with the energy scale of $\Delta_s$. The increase in $\chi_s$ seems to be proportional to $\delta$ at low temperatures. In order to see this $\delta$-dependence in more detail, we plot the difference in $\chi_s$ between $\delta > 0$ and $\delta = 0$ divided by $\delta$. As shown in Fig. 3 for $J = 1.6t$, the universal behavior is observed at low temperatures indicating $\chi_s(T, \delta) \sim \chi_s(T, \delta = 0) + \delta/(4T)$. This means that the doped holes induce almost free spins of $S = \frac{1}{2}$ with density $\delta$.

In the limit of $T \to 0$, the thermodynamic properties are determined by the gapless collective excitations of the TL liquid, and the spin susceptibility is given by the spin velocity $v_s$ as $\chi_s = 1/(2\pi v_s)$. Thus there must be a crossover temperature where $\chi_s(T)$ deviates from $\chi_s(T) \sim \chi_s(T, \delta = 0) + \delta/(4T)$ towards $1/(2\pi v_s)$. This crossover temperature is expected to be proportional to $v_s$, because it is the energy scale of the spin excitations. One can estimate this crossover temperature from $\chi_s$ at $T = 0$ through the relation $\nu_s = 1/(2\pi \chi_s)$.

The $\chi_s(T=0)$ are plotted in Fig. 4 for $J = 2.0t$. They are calculated by the zero-temperature DMRG method with open boundary conditions via the size dependence of the lowest spin excitation energy, $\Delta E(L) = \pi v_s/L$. The $T = 0$ susceptibility is very sensitive to the
hole doping $\delta$ and diverges in the limit of $\delta \to 0$. It reflects the behavior that the spin velocity as a characteristic energy scale vanishes. Thus the crossover temperature to the TL liquid phase may correspondingly vanish as $\delta \to 0$. The $\delta$-dependence of $\chi_s$ seems to be exponential in the present calculation, but we will discuss this point again later.

The crossover to the TL liquid is more clearly seen in the charge susceptibility, $\chi_c$. The charge susceptibility is defined as the change in the conduction electron density due to a small shift of chemical potential, $\chi_c = \partial n_c/\partial \mu = -\partial \delta/\partial \mu$. The results for $J = 1.6t$ and $1.2t$ are shown in Fig. 5.

At high temperatures, $\chi_c$ is almost the same as that of free conduction electrons and proportional to $1/T$. With decreasing temperature, $\chi_c$ for small doping is suppressed around $T \sim \Delta_s$, as for $\chi_s$. The suppression of $\chi_c$ at $\delta = 0$ is due to the development of the charge gap. Below $T \sim \Delta_s$, the correlation length of the localized spins becomes longer than the charge correlation length, and this induces an internal staggered magnetic field for the conduction electrons through the Kondo coupling. When the charge excitations are concerned, their time scale is much shorter than that for the spin excitations ($\propto \Delta_s^{-1}$), and the staggered field may be considered as almost static. This staggered field induces a unit-cell doubling for the conduction electrons and a finite gap appears at the Fermi energy of the otherwise free conduction electrons. Since this behavior is induced by the development of long-range spin correlations, it becomes noticeable only below $T \sim \Delta_s$, rather than $\Delta_c$. The present results show that contributions to $\chi_c$ from the small number of holes are small at temperature $T \sim \Delta_s$ and the suppression is visible near half filling.

With further decreasing temperature, the temperature dependence of $\chi_c$ at $\delta > 0$ differs from the $\delta = 0$ case as for $\chi_s(T)$. $\chi_c$ at half filling becomes exponentially small below $T \sim \Delta_s$ with the energy scale of the quasiparticle gap, $\chi_c \sim \exp(-\Delta_{qp}/T)$, but for finite $\delta$, $\chi_c$ sharply increases. The increase of $\chi_c$ at low temperatures seems to be larger for smaller $\delta$. This behavior near half filling is consistent with the doping dependence of $\chi_c$ at $T = 0$, which is obtained by the zero-temperature DMRG method. At $T = 0$, $\chi_c$ is given by the difference in the chemical potential $\chi_c = 2/L(\mu(L, N_c + 1) - \mu(L, N_c - 1))$, where $2\mu(L, N_c + 1) = E_g(L, N_c + 2) - E_g(L, N_c)$ and $E_g(L, N)$ is the ground state energy of $N$ conduction electrons in the system of length $L$. The results are shown in Fig. 6, which actually shows that the $\chi_c$ increases with decreasing $\delta$ and it seems to diverge in the limit of $\delta \to 0$.

The divergent behavior of $\chi_c$ corresponds to the vanishing charge velocity as the characteristic energy of the TL liquid as $\delta \to 0$. The $\delta$-dependence of $\chi_c$ is close to $1/\delta$ and different from the exponential dependence observed.
However, for small $\delta$, the $T$-dependence is small even at temperatures $T \sim 0.05t$. The remaining entropy is consistent with the entropy of free spin-$\frac{1}{2}$ carriers with density $\delta$. This implies that the characteristic energy scale for gapless excitations of the TL liquid is small near half filling and the $T$-linear dependence will be seen at further low temperatures $T \ll 0.05t$.

In conclusion, we have applied finite-$T$ DMRG method to the one-dimensional Kondo lattice model away from half filling, and found two crossover temperatures which characterize thermodynamics near half filling. One is the spin gap at half filling and the other is the characteristic energy of collective excitations in the TL-liquid ground state. The energy scales of the TL liquid becomes smaller with approaching half filling and seems to vanish in the limit of $\delta \to 0$.

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