Dynamic correlations in doped 1D Kondo insulator - Finite-T DMRG study -

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The finite-T DMRG method is applied to the one-dimensional Kondo lattice model to calculate dynamic correlation functions. Dynamic spin and charge correlations, $S_i(\omega)$, $S_c(\omega)$, and $N_c(\omega)$, and quasiparticle density of states $\rho(\omega)$ are calculated in the paramagnetic metallic phase for various temperatures and hole densities. Near half filling, it is shown that a pseudogap grows in these dynamic correlation functions below the crossover temperature characterized by the spin gap at half filling. A sharp peak at $\omega = 0$ evolves at low temperatures in $S_i(\omega)$ and $N_c(\omega)$. This may be an evidence of the formation of the collective excitations, and this confirms that the metallic phase is a Tomonaga-Luttinger liquid in the low temperature limit.

Heavy fermion systems have attracted much attention for more than a decade because of their enormous mass renormalization and diverse ground states including unconventional superconductivity. The periodic Anderson model (PAM) and the Kondo lattice model (KLM) are their canonical models, and their properties have intensively been investigated. In the framework of the PAM, hybridized band picture with strong renormalization is widely accepted for a scenario of the formation of heavy quasiparticles. The formation of heavy quasiparticles is not only crucial for the understanding of the Kondo effect, but also provides invaluable information on dynamics, although the precise behavior of the dynamic correlation functions and the characteristic temperature of pseudogap formation is highly dependent on the model parameters.

In the present work we calculate temperature and doping dependence of the dynamic correlation functions and clarify the character of these crossovers. It will be shown that the higher crossover temperature $T^*_1$ corresponds to the characteristic temperature of pseudogap formation in the dynamic spin and charge structure factors. At the same time a sharp peak structure appears at $\omega = 0$, indicating the formation of the collective excitations of the TLL at low temperatures. The lower crossover temperature $T^*_2$ may correspond to the coherence temperature of these collective excitations.

The Hamiltonian of the 1D KLM is described as

$$H = -t \sum_{i,s} (c^\dagger_{i,s} c_{i+1,s} + H.c.) + J \sum_{i,s,s'} \mathbf{S}_i \cdot \frac{1}{2} \mathbf{\sigma}_{ss'} c^\dagger_{i,s} c_{i,s'}$$

(1)
with standard notations. The density of conduction electron $n_c$ is unity at half filling, and hole doping ($n_c = 1 - \delta$) is physically equivalent to electron doping ($n_c = 1 + \delta$) due to particle-hole symmetry.

Dynamic correlation functions of local quantities can be calculated at finite temperatures for infinite-size systems by the DMRG method applied to the quantum transfer matrix. Imaginary-time correlation functions are first calculated from the eigenvector of the maximum eigenvalue of the quantum transfer matrix, and then they are analytically continued to real frequency using the maximum entropy method. The advantages of this method are that the finite-temperature methods do not need the extrapolation on the system size. This approach was first applied to the insulating phase of the 1D KLM and the many-body nature of the gap formation is revealed. The present study is the first application to a metallic phase. In our calculations we usually keep 50 states in the finite-T DMRG procedure with the Trotter number 60.

We have calculated temperature dependence of several dynamic correlation functions. The results of the local spin dynamics of the f-spins, $S_f(\omega) = \int dq S_f(q, \omega)$, are shown for $J/t = 1.6$ and $\delta = 0.2$ in the inset of Fig. 1. Note that the complete suppression of charge fluctuations for $f$-spins imposes the sum rule, $\int d\omega S_f(\omega) = 1/4$, independent of $J$, $\delta$ and $T$. We can see that a peak structure appears around $\omega \sim \Delta_s = 0.4t$ at $T \leq 0.2t$, and similar peak structure is also observed for different Kondo coupling $J/t = 1.2$ at $T \leq 0.06t$, where $\Delta_s = 0.16t$. Based on these results, we may conclude that the characteristic temperature of the peak formation is scaled by the higher crossover temperature $T^*_F$ determined by $\chi_s(T)$. At the same time another peak structure grows at $\omega = 0$, when $\delta$ is finite. It suggests the formation of the collective spin excitations of the TLL at low temperatures. We expect that the low energy part finally approaches $|\omega|^Nc$, which is predicted by the TLL theory at $T = 0$.

The doping dependence of $S_f(\omega)$ is shown at the low temperature $T = 0.04t \ll \Delta_s$ in the main panel of Fig. 1. With increasing $\delta$, the peak intensity at $\omega = 0$ grows, while the intensity around $\omega = \Delta_s$ is reduced as a consequence of the sum rule discussed before. We have checked that the peak intensity at $\omega = 0$ is 0.25$\delta$ within a few percent. The energy scale estimated from the peak width around $\omega = 0$ at $T = 0.04t$ is smaller than the lowest temperature in our calculations. This means the weight around $\omega = 0$ yields nearly free spin degrees of freedom with density $0.25\delta$ down to around this temperature $T \sim 0.04t$. This is consistent with the behavior of the static spin susceptibility, $\chi_s = \delta/(4T)$, observed at low temperatures.

In contrast to $S_f(\omega)$ the $\omega = 0$ peak is small in the conduction-electron spin correlations, $S_c(\omega) = \int dq S_c(q, \omega)$, as shown in Fig. 2. This shows that the low-energy part of the spin degrees of freedom of the conduction electrons are nearly exhausted to form spin singlet with f-spins and thus a clear peak is formed at $\omega = \Delta_s$. Therefore, the low energy spin dynamics is mostly dominated by the f-spin degrees of freedom. However, the intensity of the peak around $\omega \sim \Delta_c$ is less than 1/3 of the corresponding peak in $S_f(\omega)$ and over a half of the total weight extends over higher frequencies $t \leq \omega \leq 5t$. This

![FIG. 1. Dynamic spin correlations of the f-spins in the 1D KLM. $\Delta_s = 0.4t$ is the spin gap at $\delta = 0$.](image1)

![FIG. 2. Dynamic spin correlations of the conduction electrons.](image2)

![FIG. 3. Dynamic charge correlations. $\Delta_c = 1.4t$ is the charge gap at $\delta = 0$.](image3)
means that although the low energy part is dynamically coupled with \( f \)-spins, the majority part of the conduction spin degrees of freedom have another energy scale of almost the band width \( \sim 4t \gg \Delta_s \) when the Kondo coupling is small \( J < 4t \). This shows that only the conduction electrons close to the Fermi level screen the \( f \)-spins as pointed out by Nozières. \[2\] Rather surprisingly, even though the screening by conduction electrons is not complete, the intensity at \( \omega = 0 \) in \( S_\tau(\omega) \) is almost \( \delta / 4 \), just like the \( J = \infty \) case, where each conduction electron screens one \( f \)-spin. This shows the importance of the \( f \)-\( f \) spin correlations for the formation of the Kondo singlet state.

The doping dependence of the dynamic charge correlations, \( N_\epsilon(\omega) = \int \frac{dq}{2\pi} N_\epsilon(q, \omega) \), is shown in Fig. \[3\]. At half filling, the charge excitations are exponentially suppressed below the crossover temperature \( T_1^* \) at \( \omega < \Delta_s \). \[26\] Upon hole doping, a sharp peak appears at \( \omega = 0 \) as in \( S_\tau(\omega) \). This indicates the formation of collective charge excitations of the TLL as discussed for \( S_\tau(\omega) \). The peak intensity increases with \( \delta \), and this means that the effective carrier density of the TLL is strongly renormalized from \( n_c = 1 - \delta \). The renormalization of carrier is naturally explained in the limit of strong \( J \), where each conduction electron forms a local singlet with the \( f \)-spin on the same site. In this limit, effective carriers are introduced by hole doping, and their main component is the unscreened \( f \)-spins with density \( \delta \), \[21\] as discussed for \( S_\tau(\omega) \). The TLL theory predicts that the low-energy asymptotic form of \( N_\epsilon(\omega) \) is \( \omega^{[\min(K_s, 4K_c - 1)]} \) near \( \omega = 0 \), and we expect that the \( \omega = 0 \) peak finally approaches this form in the low temperature limit.

We now consider crossover behavior of the quasiparticle density of states, \( \rho(\omega) \). Figure \[4\] shows the temperature dependence at \( \delta = 0.2 \) and \( J/t = 1.6 \). We can see that a pseudogap develops just above the Fermi level \( \omega = \mu \) below \( T/t \sim 0.4 \). Similar behavior is observed also for \( J/t = 1.2 \) below \( T/t \sim 0.15 \). Based on these results, we may conclude that the characteristic temperature of pseudogap formation is scaled by \( T_1^* \) defined from \( \chi_s(T) \). This conclusion is consistent with the results obtained at half filling. \[31, 32\]

The crossover behavior around \( T_1^* \) may be explained as follows. Below \( T_1^* \), thermal fluctuations of the \( f \)-spins are substantially suppressed, since the temperature is lower than the characteristic energy scale of the \( f \)-spin excitations \( \Delta_s \). When \( \delta \) is small, the characteristic time scale of the dominant part of the \( f \)-spins is given by \( \Delta_s^{-1} \), and this is much longer than the time scale of quasiparticle propagation \( \tau_{qp} \), since \( \tau_{qp} \) may be determined by the inverse of bare hopping energy and charge gap, \( t^{-1} \) and \( \Delta_s^{-1} \). Therefore, concerning the quasiparticle excitations, the \( f \)-\( f \) spin correlations may be assumed to be static. Because of their staggered nature in space, these almost static \( f \)-\( f \) spin correlations induce the opening of a gap in \( \rho(\omega) \). Of course, as shown in \( S(\omega) \) and \( N(\omega) \), both the \( f \)-spins and the conduction electrons have a slow dynamics when \( \delta \) is finite, and therefore the gap discussed here is not a real gap but rather a pseudogap for finite \( \delta \). Thus the pseudogap develops below \( T_1^* \).

![FIG. 4. Temperature dependence of the quasiparticle density of states.](image)

![FIG. 5. Doping dependence of the quasiparticle density of states. Quasiparticle gap at \( \delta = 0 \) is \( \Delta_{qp} = 0.7t \).](image)

We next consider doping dependence to study small structures in \( \rho(\omega) \) near the Fermi level \( \omega = \mu \). The results for \( J/t = 1.6 \) at \( T/t = 0.04 \) are shown in Fig. \[5\] at various dopings. The pseudogap becomes more prominent with approaching half filling, where the clear quasiparticle gap, \( \Delta_{qp} = 0.7t \), exists. The sharp peak structure just below \( \omega = \mu \) also grows with decreasing \( \delta \) and seems to continuously connect to the gap edge structure at \( \delta = 0 \).

The nature of the structure near the Fermi level is not fully understood yet. One possible scenario is the mean-field type argument assuming the \( f \)-spin helical SDW order with wave number \( 2k_F = \pi(1 - \delta) \). Band mixing induces gap opening at \( k = \pi(\pm 1 + \delta)/2 \), and two new van-Hove (vH) divergent singularities appear in each of the two hybridized bands. The Fermi level sits between these two new singularities in the lower hybridized band, as far as \( \delta \) is small. A slightly different scenario is that the gap is induced by the short-range \( f \)-\( f \) spin correlations with wave number \( \pi \). Then, there appears only one vH singularity in each band. The peak-like behavior observed in Fig. \[5\] may be identified as the lower vH singularity in
the first scenario, while in the second one it is a consequence of the shift of the Fermi level towards the top of the lower band as $\delta \to 0$. However, it is not straightforward to describe the behavior of $\rho(\omega)$ just above the Fermi level in terms of these pictures. Another quite different scenario is that this peak is due to the Kondo singlet formation and reminiscence of the Kondo resonance. This may also be expressed as the renormalized characters of the two crossovers in the paramagnetic metallic phase. Below the first crossover temperature $T^*_1$, it has been shown that a pseudogap develops in the density of states and dynamic correlation functions, and $S_1(\omega)$ and $S_2(\omega)$ both show a peak structure around $\omega = \Delta_\omega$ as in the half-filling case. At the same time a peak structure appears at $\omega = 0$ in $S_1(\omega)$ and $N_\omega(\omega)$, and its intensity increases with hole density $\delta$. The $\omega = 0$ peak indicates that as a consequence of local Kondo singlet formation effective carriers are strongly renormalized to have density $\delta$ and small energy scale. The increase of the peak intensity with $\delta$ is naturally explained in the limit of strong $J$, where effective carriers of the TLL are the unscreened $f$-spins whose density is $\delta$. We note that this is consistent with the large Fermi surface. Below the second crossover temperature $T^*_2$, the interaction between the effective carriers becomes relevant and the renormalized carriers are expected to evolve into a TLL. This is supported by several sets of the present results.

[FIG. 6. Doping dependence of the quasiparticle density of states. Quasiparticle gap at $\delta = 0$ is $\Delta_{qp} = 0.47t$.]

the thermodynamics in the 1D KLM. Which shows that $T^*_2$ is lower for smaller $\delta$ and vanishes as $\delta \to 0$.

To summarize we have calculated dynamic quantities at various temperatures and hole densities, and clarified characters of the two crossovers in the paramagnetic metallic phase. Below the first crossover temperature $T^*_1$, it has been shown that a pseudogap develops in the density of states and dynamic correlation functions, and $S_1(\omega)$ and $S_2(\omega)$ both show a peak structure around $\omega = \Delta_\omega$ as in the half-filling case. At the same time a peak structure appears at $\omega = 0$ in $S_1(\omega)$ and $N_\omega(\omega)$, and its intensity increases with hole density $\delta$. The $\omega = 0$ peak indicates that as a consequence of local Kondo singlet formation effective carriers are strongly renormalized to have density $\delta$ and small energy scale. The increase of the peak intensity with $\delta$ is naturally explained in the limit of strong $J$, where effective carriers of the TLL are the unscreened $f$-spins whose density is $\delta$. We note that this is consistent with the large Fermi surface. Below the second crossover temperature $T^*_2$, the interaction between the effective carriers becomes relevant and the renormalized carriers are expected to evolve into a TLL. This is supported by several sets of the present results.

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