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Instability of the Fermi surface in the one-dimensional Kondo lattice

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Abstract

The key parameters that characterize the long wavelength behaviour of correlation functions, including the Fermi momenta and the correlation length, are calculated using the transfer matrix renormalization group for the one-dimensional Kondo lattice model. The Fermi momentum varies slowly at high temperatures, but changes sharply at low temperatures in association with the formation of the Kondo singlets. By comparison with the temperature dependence of the conduction electron density, we find that the long wavelength correlations of conduction electrons are strongly affected by the localized spins at low temperatures. At high temperatures, the conduction electrons behave as for a system with a small Fermi surface. However, at low temperatures, the Fermi momentum of the conduction electrons is altered by the coupling with the localized spins.

Investigations on heavy fermion systems have attracted great attention in the past two decades [1, 2]. In these systems, two kinds of electrons are involved: conduction electrons in outer unfilled orbitals and localized electrons in inner filled orbitals. The former form a conduction band in a periodic lattice, while the latter, weakly hybridized with the former, are highly correlated. The heavy fermions are realized in the Kondo regime where the mobility of the electrons in the inner orbitals is greatly reduced by a large level splitting. In a mixed valence regime with a relatively small level splitting, the periodic Anderson model (PAM) is an appropriate starting point [3]. In a Kondo regime, the low-energy physics of the periodic Anderson model can be effectively described by the Kondo lattice model (KLM) [4] up to the second order of perturbation [5].

In one dimension, the KLM has been studied using the exact diagonalization [6, 7], density matrix renormalization group [8] as well as other methods [9]. It was found that the 1D KLM

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consists of three phases [2]: a Kondo insulator phase at half-filling, a ferromagnetic (FM) metallic phase at low doping and strong coupling, and a paramagnetic (PM) metallic phase. The former two phases are relatively well understood. The ferromagnetic state is characterized by a non-zero magnetization. The Kondo insulator is a spin liquid with gapped spin and charge excitations. However, the PM metallic phase has been less clearly explored.

In the PM phase, an issue of great interest is whether the Fermi surface of the KLM is purely determined by the conduction electrons or contains the contribution from the localized spins. This is the so-called small or large Fermi surface problem. If only the conduction electrons have a contribution to the Fermi sea volume, then the Fermi momentum k_{F} is given by

$$k_{\mathrm{F}} = \frac{\pi}{2} n_{\mathrm{c}}, \tag{1}$$

where n_{c} is the conduction electron concentration per site. However, if we take the KLM as an effective model of the PAM in the strong coupling limit, we would also expect the localized spins to have a contribution to k_{F} since the conduction electrons are entangled with d electrons. In this case, the Fermi momentum is determined by both conduction and localized electrons:

$$k_{\mathrm{F}} = \frac{\pi}{2}(n_{\mathrm{c}} + n_{\mathrm{d}}) = \frac{\pi}{2}(n_{\mathrm{c}} + 1), \tag{2}$$

where $n_{\mathrm{d}} = 1$ is the number of localized spins at each site.

This problem of large or small Fermi momentum has been extensively studied in recent years. In particular, Shiba and Fazekas showed that the Fermi momentum is given by equation (2) from a variational calculation with a Gutzwiller-type trial wavefunction [9]. Their result was supported by a numerical analysis of the Friedel oscillations of an edge state on finite-lattice systems [10], and a number of other calculations [7, 8, 11]. However, all these studies were performed on finite lattice systems and there is a rather big uncertainty in the determination of the Fermi momentum. Recently, Yamanaka *et al* [12] showed rigorously that there is gapless excitation in the density–density channel at a momentum twice that given by equation (2). Their result implies that the Fermi surface is large. Although these investigations have been performed on this problem, numerical simulations without the finite lattice size effect are helpful.

The Fermi momentum is associated with low energy excitations. It determines the long wavelength behaviour of correlation functions of electrons. In a finite lattice system, the singular behaviour of the momentum distribution or other correlation functions of electrons at the Fermi surface is smeared out by the finite size effect. This is the difficulty in determining the value of Fermi momentum accurately from finite size calculations. To resolve this difficulty, we have calculated the single particle correlation function of the 1D KLM using the transfer matrix renormalization group (TMRG) method [13–15].

The TMRG is a finite temperature extension of the density matrix renormalization group (DMRG) method [16]. It can handle an *infinite* lattice system directly. With this method, one can calculate the Fermi momentum directly, without being bothered by the finite lattice size effect.

The Kondo lattice model is defined by the Hamiltonian

$$H_{\mathrm{K}} = \sum_i H_i \tag{3}$$

$$H_i = -t \sum_\sigma (c^\dagger_{i\sigma} c_{i+1\sigma} + \mathrm{h.c.}) + J \mathbf{S}^{\mathrm{c}}_i \cdot \mathbf{S}^{\mathrm{d}}_i, \tag{4}$$

where $c_{i\sigma}$ is the annihilation operator of conduction electrons. $\mathbf{S}^{\mathrm{c}}_i$ and $\mathbf{S}^{\mathrm{d}}_i$ are the spin operators for conduction and localized electrons, respectively. The exchange interaction between conduction and localized electrons is assumed to be antiferromagnetic ($J > 0$).

The TMRG is based on the Trottor–Suzuki decomposition and a quantum transfer matrix representation of the partition function:

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta H} = \mathrm{Tr}\, \mathcal{T}_M^{N/2} + \mathrm{O}(\varepsilon^2) \tag{5}$$

where $\varepsilon = \beta/M$ and N is the lattice length. A similar quantum transfer matrix representation of the partition function has been used to numerically study the integrable models [17–20]. The quantum transfer matrix $\mathcal{T}_M$ in equation (5) is a product of $2M$ local transfer matrices and is defined by the following equation:

$$\langle s^3|\mathcal{T}_M|s^1\rangle = \sum_{s^2}\prod_{i}^{N/2} \tau(s^3_{2i+1}s^3_{2i}|s^2_{2i+1}s^2_{2i})\tau(s^2_{2i}s^2_{2i-1}|s^1_{2i}s^1_{2i-1}), \tag{6}$$

where $s^\alpha = \{s^\alpha_1, \ldots, s^\alpha_N\}$ and s^α_i is a basis state at site i, including both localized spins and conduction electrons. The local quantum transfer matrix τ is defined by

$$\tau(s^{\alpha+1}_i s^{\alpha+1}_{i+1}|s^\alpha_i s^\alpha_{i+1}) = \langle s^{\alpha+1}_{i+1}, s^\alpha_{i+1}|\mathrm{e}^{-\varepsilon H_i}|s^\alpha_i, s^{\alpha+1}_i\rangle.$$

In the limit $N \to \infty$, it is readily shown that the partition function is determined purely by the largest eigenvalue of the quantum transfer matrix $\lambda_{\max}$:

$$Z|_{N\to\infty} = \lambda^{N/2}_{\max} + \mathrm{O}(\varepsilon^2). \tag{7}$$

Thus only the maximum eigenvalue needs to be evaluated for investigating thermodynamic quantities.

In the TMRG, it is straightforward to evaluate the thermal average of a local operator with the maximum eigenvector of $\mathcal{T}_M$. For instance, the average of the number of conduction electrons per site can be computed using the following formula:

$$n_{\mathrm{c}} = \lim_{N\to\infty} \mathrm{Tr}(\hat{n}_i \mathrm{e}^{-\beta H}) = \frac{1}{\lambda_{\max}} \left\langle \psi^{\mathrm{L}}_{\max}\right| \mathcal{T}_M(\hat{n}_i) \left|\psi^{\mathrm{R}}_{\max}\right\rangle, \tag{8}$$

where $\hat{n}_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$, and $\psi^{\mathrm{L}}_{\max}$ and $\psi^{\mathrm{R}}_{\max}$ are the maximum left and the right eigenvectors of $\mathcal{T}_M$, respectively. The matrix $\mathcal{T}_M(\hat{n}_i)$ is defined similarly to $\mathcal{T}_M$, except that one of the local transfer matrices in equation (6) is replaced by

$$\tau_n(s^{\alpha+1}_i s^{\alpha+1}_{i+1}|s^\alpha_i s^\alpha_{i+1}) = \langle s^{\alpha+1}_{i+1}, s^\alpha_{i+1}|\hat{n}_i \mathrm{e}^{-\varepsilon H_i}|s^\alpha_i, s^{\alpha+1}_i\rangle.$$

The TMRG can also be used to evaluate the correlation length as well as the characteristic wavevector of a correlation function. In particular, the Fermi momentum can be determined from the long range particle–particle correlation function. Similarly to n_{c}, it can be shown that the single-particle correlation function in the thermodynamic limit is determined by the following equation [14, 15]:

$$\langle c^\dagger_{i\sigma} c_{j\sigma}\rangle = \frac{\left\langle \psi^{\mathrm{L}}_{\max}\right| \mathcal{T}_M(c^\dagger_{i\sigma}) \mathcal{T}_M^{[j]-[i]-1} \mathcal{T}_M(c_{j\sigma}) \left|\psi^{\mathrm{R}}_{\max}\right\rangle}{\lambda^{[j]-[i]+1}_{\max}},$$

where $[i]$ is an integer equal to $i/2$ when i is even, and $(i+1)/2$ otherwise. $\mathcal{T}_M(c^\dagger_{i\sigma})$ and $\mathcal{T}_M(c_{j\sigma})$ are similarly defined as for $\mathcal{T}_M(\hat{n}_i)$. In the limit $|j-i| \to \infty$, the above equation can be simplified as

$$\langle c^\dagger_{i\sigma} c_{j\sigma}\rangle = A_{ij} \left(\frac{\lambda_\alpha}{\lambda_{\max}}\right)^{[j]-[i]}, \tag{9}$$

where

$$A_{ij} = \frac{\langle \psi^{\mathrm{L}}_{\max}|\mathcal{T}_M(c^\dagger_{i\sigma})|\psi^{\mathrm{R}}_\alpha\rangle\langle\psi^{\mathrm{L}}_\alpha|\mathcal{T}_M(c_{j\sigma})|\psi^{\mathrm{R}}_{\max}\rangle}{\lambda_{\max}\lambda_\alpha},$$

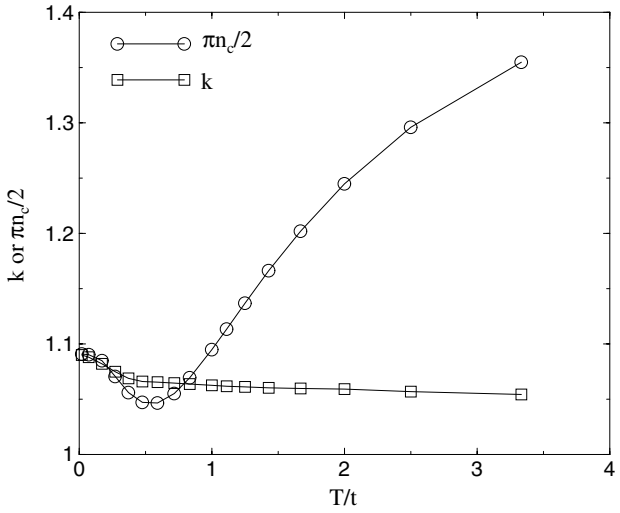

Figure 1. The characteristic wavevector k of the one-particle correlation function and $\pi n_c/2$ as a function of temperature for the 1D Hubbard model with $t = 1$, $U = 2$ and $\mu = -1$. $\varepsilon = 0.1$ and 200 states are retained in the TMRG iteration.

and λ_α is the next largest eigenvalue of $\mathcal{T}_M$ that satisfies the condition $A_{i,j} \neq 0$. $\psi_\alpha^{\mathrm{L,R}}$ are the corresponding eigenvectors of λ_α.

The maximum eigenvalue $\lambda_{\max}$ of $\mathcal{T}_M$ is always positive. However, λ_α is complex in general. Assuming $\lambda_\alpha = |\lambda_\alpha| \mathrm{e}^{2\mathrm{i}k}$, then the above correlation function has the following asymptotic form:

$$\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle_{|j-i|\to\infty} = A_{ij} \mathrm{e}^{-(\xi^{-1} - \mathrm{i}k)|j-i|}, \tag{10}$$

where ξ is the thermal correlation length

$$\xi^{-1} = \frac{1}{2} \ln \left| \frac{\lambda_{\max}}{\lambda_\alpha} \right| \tag{11}$$

and k is a characteristic wavevector of single particle excitations. At zero temperature, k is just the Fermi momentum k_{F} of the system, i.e.

$$k_{\mathrm{F}} = \lim_{T\to 0} \tfrac{1}{2} \arg(\lambda_\alpha) + n\pi, \tag{12}$$

where $n = 0$ or 1. Thus by evaluating the phase of λ_α at low temperatures, we can determine the Fermi momentum of the electrons.

The transfer matrix is asymmetric. The associated reduced density matrix is also asymmetric. This is a key difference between the TMRG and the zero temperature DMRG. Numerically, it is rather challenging work to evaluate λ_α since it is much more difficult to handle a non-symmetric matrix than a symmetric one, especially when a complex eigenvalue is evaluated.

The Fermi momentum is defined at zero temperature. To understand better how the characteristic wavevector k approaches the Fermi momentum at low temperatures, we have first evaluated the temperature dependence of k for the Hubbard model:

$$H = t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \mathrm{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{13}$$

In the Hubbard model, since there are only conduction electrons, equation (1) is expected to hold at zero temperature. Our numerical results, as shown in figure 1, do agree with this

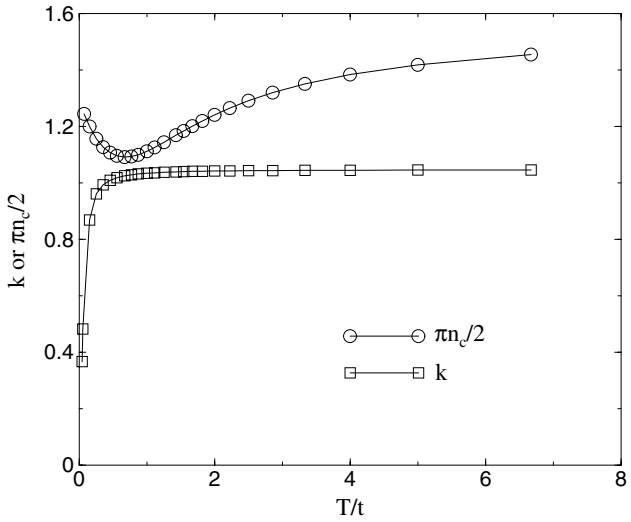

Figure 2. The characteristic Fermi wavevector of the single-particle correlation function k and $\pi n_c/2$ as functions of temperature for the KLM with $t = 1$, $J = 2$ and $\mu = -1$. $\varepsilon = 0.05$ and 150 states were retained in the TMRG iteration.

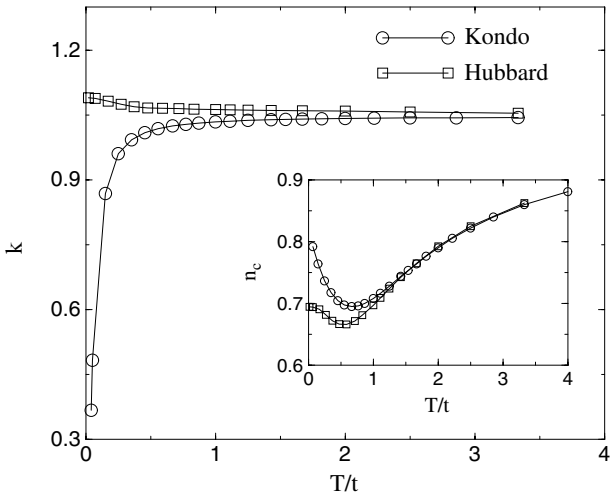

Figure 3. Comparison of the characteristic wavevector of the k as well as n_c for the KLM (with $t = 1$, $J = 2$ and $\mu = -1$) and the Hubbard model (with $t = 1$, $U = 2$ and $\mu = -1$).

conclusion. With fixed chemical potential, we find that the temperature dependence of n_c is different from that of k. In particular, the characteristic wavevector k is not proportional to the electron concentration at finite temperatures. The variation of k with temperature is much smaller than n_c, especially at high temperatures. However, at low temperatures, k tends to approach to $\pi n_c/2$, as expected.

Figure 2 shows the numerical results for the KLM. When $t = 1$ and $\mu = -1$, n_c and k show nearly the same temperature dependence as for the Hubbard model with the same t and μ, except at low temperatures. These similar behaviours are explicitly shown in figure 3. If only the high temperature results for k and n_c are considered, we would not see much difference

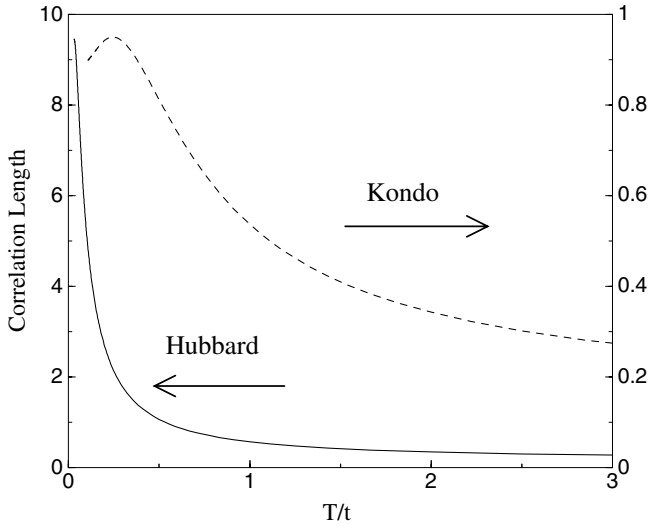

Figure 4. The correlation length as a function of temperature. The parameters of the Hubbard model and the KLM are the same as for figures 1 and 2, respectively.

between the KLM and the Hubbard model. This is not surprising since at high temperatures the conduction electrons are effectively decoupled with the localized spins for the KLM.

At low temperatures, the physics governing low-lying excitations is different in the two models. In the KLM, the coupling between conduction electrons and localized spins becomes stronger and stronger with decreasing temperature. This causes the formation of the Kondo singlet below the so-called Kondo temperature T_K. The sharp downturn of k in figure 2 is an indication of the onset of the Kondo physics. It shows that the Fermi momentum of the conduction electrons is altered by the formation of the Kondo singlets. This means that equation (1) is no longer valid in the zero temperature limit. Thus the long wavelength correlation of electrons is not governed by the low-lying excitation around the momentum determined by equation (1) in the Kondo lattice at low temperatures. However, due to technical difficulties, we are still unable to evaluate the wavevector k accurately down to very low temperatures and to give a firm confirmation of equation (2).

Figure 4 shows the correlation length as a function of temperature for both the KLM and the Hubbard model. For the parameters used, the correlation length of the KLM is much shorter than that for the Hubbard model. While the correlation length of the Hubbard model increases with decreasing temperature, it varies non-monotonically in the KLM. For the Hubbard model, the correlation length diverges at zero temperature. The monotonic increase of the correlation length with temperature as shown in this figure is consistent with this expectation. In accord with the sharp behaviour of the characteristic wavevector, a broad peak appears in the correlation length curve of the KLM. This peak is due to the competition between the kinetic energy and the formation of the Kondo singlets. This is an indication of the crossover from a kinetic energy dominant phase to a Kondo phase. At very low temperatures, the KLM is a Luttinger liquid and the correlation length of the KLM is expected to diverge. Our result does not show any sign of the divergency because the temperature we have studied is still not low enough.

In summary, the Fermi vector and the correlation length of the one-particle correlation function of the KLM are evaluated and compared with those of the Hubbard model, using the

transfer matrix renormalization group. Our results show that, at low temperatures, the Fermi volume of the KLM is strongly affected by the localized spins and determined not purely by the conduction electrons. At high temperatures, the local spins are decoupled with the conduction electrons and the Fermi volume is determined by the conduction electrons, similarly as for the Hubbard model. This is the first TMRG calculation for the complex eigenvalues of the transfer matrix. It shows that the TMRG is a powerful tool for determining the Fermi momentum and other parameters associated with low-lying excitations.

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