Ground State Properties of Randomly-Doped Kondo Lattice Model

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Abstract. We study the ground state properties of a Kondo lattice model with random configuration of \( f \) electrons, as a function of \( f \)-electron density \( n_f \). We show that the strength of on-site screening (averaged exchange energy per \( f \) electron) shows a rapid decrease at a certain value of \( n_f^{CO} \). For \( n_f > n_f^{CO} \), the correlation between \( f \) electrons gradually grows and the system is expected to change from local Fermi liquid to heavy Fermi liquid.

1. Introduction

Heavy-fermion materials are characterized by a large effective mass of electrons and their ground states are often called heavy Fermi liquid. When the magnetic ions with \( f \) electrons are substituted by the non-magnetic ones, e.g., Ce→La, the system gradually changes from heavy Fermi liquid (dense limit) to local Fermi liquid (single-impurity limit) [1, 2, 3, 4]. However, the details of this crossover are quite different in each compound. For example, in \( \text{Ce}_x\text{La}_{1-x}\text{Pb}_3 \), the resistivity shows local-Fermi-liquid behavior even at \( x \simeq 0.8 \) [2]. It is an interesting fact that the single-impurity picture is valid even for a rather “dense” region. On the other hand, the situation is rather complex in \( \text{Ce}_x\text{La}_{1-x}\text{CoIn}_5 \) [5]. Between the local Fermi liquid and heavy Fermi liquid, there is an intermediate region where the temperature scale that characterizes the Fermi liquid is greatly suppressed. The detailed properties of this region has not been clarified so far.

With these facts in mind, we study the ground state properties of Kondo lattice system with random configuration of \( f \) electrons. The variational Monte Carlo (VMC) method is used for calculation. We prepare random configurations of \( f \) electrons and calculate the physical quantities for each configuration. After that we take an average of them and obtain the result. Although a large amount of different configurations are necessary, this calculation procedure is considered to treat the effect of randomness more precisely than the coherent potential approximation that is often used for disordered system.

2. Model and method

We study the ground states of a Kondo lattice model (KLM) with random configuration of \( f \) electrons. We call sites with and without \( f \) electrons \( A \) and \( B \) sites, respectively. The Hamiltonian is expressed as

\[
H = \sum_{k\sigma} \varepsilon_k c_k^{\dagger} c_{k\sigma} + J \sum_{i \in A} \mathbf{S}_i \cdot \mathbf{s}_i
\]
where \( s_i \) and \( S_i \) represent the \( c \) - and \( f \) -electron spins, respectively. \( J(>0) \) denotes the antiferromagnetic exchange coupling between them and \( \varepsilon_k = -2t(\cos k_x + \cos k_y) \) is the \( c \) -electron energy dispersion. The \( f \) electrons are completely localized and treated as localized spins.

To investigate the ground state properties of (1), we use the VMC method. We prepare the Gutzwiller-type trial wave function \( |\Psi\rangle \) for a trial state. It consists of a projection operator \( \hat{P}_f \) and a one-body part \( |\Phi\rangle \) that is obtained from the solution of a certain one-body Hamiltonian. The specific form is as follows,

\[
|\Psi\rangle = \hat{P}_f |\Phi\rangle, \quad \hat{P}_f = \prod_{i \in A} \left[ \hat{n}_{i1}^{f} (1 - \hat{n}_{i1}^{f}) + \hat{n}_{i1}^{f} (1 - \hat{n}_{i1}^{f}) \right].
\]

(2)

\( \hat{P}_f \) keeps the \( f \) -electron number of each \( A \) site exactly one. Since the \( f \) electrons must be treated as localized spins in the KLM, this constraint is necessary for the accurate calculation [6]. The one-body part \( |\Phi\rangle \) is obtained by diagonalizing the periodic Anderson model with \( U = 0 \) in a real-space representation. For a case of \( 2 \times 2 = 4 \) sites, the explicit form is as follows,

\[
H' = \sum_{\sigma} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ c_{3\sigma} \\ c_{4\sigma} \\ f_{1\sigma} \\ f_{2\sigma} \\ f_{3\sigma} \\ f_{4\sigma} \end{pmatrix}^\dagger \begin{pmatrix} 0 & -\tilde{t}_{12} & -\tilde{t}_{13} & 0 & \tilde{V}_1 & 0 & 0 & 0 \\ -\tilde{t}_{21} & 0 & 0 & -\tilde{t}_{24} & 0 & \tilde{V}_2 & 0 & 0 \\ -\tilde{t}_{31} & 0 & 0 & -\tilde{t}_{34} & 0 & 0 & \tilde{V}_3 & 0 \\ 0 & -\tilde{t}_{42} & -\tilde{t}_{43} & 0 & 0 & 0 & 0 & \tilde{V}_4 \\ \tilde{V}_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \tilde{V}_2 & 0 & 0 & 0 & 0 & \tilde{E}_{f1} & 0 \\ 0 & 0 & \tilde{V}_3 & 0 & 0 & 0 & 0 & \tilde{E}_{f3} \\ 0 & 0 & 0 & \tilde{V}_4 & 0 & 0 & 0 & \tilde{E}_{f4} \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ c_{3\sigma} \\ c_{4\sigma} \\ f_{1\sigma} \\ f_{2\sigma} \\ f_{3\sigma} \\ f_{4\sigma} \end{pmatrix}.
\]

(3)

\( \tilde{t}_{ij} \) are transfer integrals from \( i \) to \( j \) site. \( \tilde{V}_i \) and \( \tilde{E}_{f_i} \) are “effective” hybridization and \( f \) -electron energy level for \( i \) site. To avoid the occupancy of \( f \) electrons at \( B \) sites, we set \( \tilde{E}_{f_i} = \infty \) for \( i \in B \). \( \tilde{t}_{ij} \), \( \tilde{V}_i \) and \( \tilde{E}_{f_i} \) \( (i \in A) \) are variational parameters and optimized so as to minimize the variational energy. Here, we set \( \tilde{t}_{ij} = \tilde{t}, \tilde{V}_i = \tilde{V} \) and \( \tilde{E}_{f_i} = \tilde{E}_f \) for simplicity. Then we calculate various physical quantities with the optimized wave function.

3. Results
In the following, we show the numerical calculation of averaged exchange energy per \( f \) electron,

\[
E_{ex}/n_f = - \left\langle \frac{1}{n_f} \sum_{i \in A} S_i \cdot s_i \right\rangle_{\text{rand}}
\]

(4)

where \( \langle \cdots \rangle_{\text{rand}} \) denotes the random average. This quantity is always positive and corresponds to the strength of on-site screening per \( f \) electron. The system size for calculation is \( 10 \times 10 \) and we take 40 patterns of random configurations. Figure 1 shows the \( f \) -electron density \( n_f \) dependence of \( E_{ex}/n_f \) for the case of \( J/t = 3.0 \) and \( n_c = 0.48 \). \( n_f \to 0 \) corresponds to the dilute limit and \( n_f = 1 \) corresponds to the usual KLM. We can observe the peak structure for small \( n_f \) but it is considered to be an artifact of a finite size effect. Indeed, we have checked the size dependence up to \( 16 \times 16 \) and found that this peak structure disappears as the system size increases. For larger value of \( n_f \), on the other hand, we cannot find a remarkable size dependence. \( E_{ex}/n_f \) is almost constant for \( n_f < n_f^{CO} \) and begins to decrease at \( n_f = n_f^{CO} \). Around this density, the screening clouds extend rapidly and reaches the neighboring sites. Through the contact of screening clouds, the correlation between \( f \) electrons begins to increase and the effective mass
is expected to be enhanced. We consider that it is an origin of “heavy” Fermi liquid. Here, we compare the picture of so-called “exhaustion problem” [7] in the strong-coupling limit with our result. In the strong-coupling limit, $J/t \to \infty$, each $c$ electron forms an on-site singlet pair with the localized $f$-electron spin. When $n_f < n_c$, all localized spins form singlet and remaining $c$ electrons become carrier. On the other hand, when $n_f > n_c$ ($c$ electrons are “exhausted”), unscreened localized spins exist and they behave as effective fermions with a reduced band width. In other words, holes with large effective mass become carrier in this condition. It is considered to be a simple picture for a heavy Fermi liquid. These two metallic states have different characters and separated by the special density of $n_f = n_c$, where the system has a gap of order $J/t$ and becomes insulator. For a finite value of $J/t$, this insulating state is not expected but it is possible that the character of metallic state changes at $n_f \approx n_c$ [8, 9]. According to our calculation, the change occurs at $n_f^{CO} \approx 0.38$, away from $n_c = 0.48$. In this condition, the spread of screening cloud is already beyond the lattice spacing and the region of heavy Fermi liquid extends for $n_f < n_c$.

On the other hand, we find $n_f^{CO} \approx n_c$ for $J/t = 3.0$ and $n_c = 0.84$ (not shown here). Although the value of $J/t$ is the same, the case of $n_c = 0.84$ is closer to the strong-coupling case than the case of $n_c = 0.48$ because the screening cloud is almost localized as the strong-coupling picture.

From these results, we consider that the crossover from local Fermi liquid to heavy Fermi liquid occurs at $n_f = n_f^{CO}$. For $n_f < n_f^{CO}$, the screening of localized spins occurs individually and the correlation between $f$ electrons are weak. For $n_f > n_f^{CO}$, on the other hand, the $c$ electrons are “exhausted” and the screening clouds extend to the neighboring sites and the correlation between $f$ electrons becomes large. It is considered to be an origin of large effective mass. The dynamical mean-field study by Pruschke et al. for the periodic Anderson model [10] shows that the effective mass is strongly enhanced for $n_c < n_f \sim 1$ (they fix $n_f$ and change $n_c$). It is also due to the “exhaustion” of $c$ electrons and consistent with our proposal.

Figure 1. $n_f$ dependence of strength of on-site screening for $J/t = 3.0$ and $n_c = 0.48$. Dotted line shows $n_f = n_c = 0.48$. 

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3
4. Summary
In this paper, we have studied the ground state properties of the KLM with random configuration of \( f \) electrons. The VMC method in real space is used for calculations. We have found that the strength of on-site screening shows rapid decrease at \( n_f = n_f^{\text{CO}} \). We expect that the change from local Fermi liquid to heavy Fermi liquid occurs at \( n_f = n_f^{\text{CO}} \).

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