Fermi surface reconstruction in the Kondo lattice model and the periodic Anderson model

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Abstract. We study the ground state properties of the Kondo lattice model (KLM) and the periodic Anderson model (PAM) in a two-dimensional square lattice with the variational Monte Carlo method. In addition to the conventional second-order antiferromagnetic transition, we find a novel type of quantum phase transition which induces the change of topology of the Fermi surface (Fermi surface reconstruction). The Fermi surface reconstruction is originated from the mechanism of the energy gain and is characteristic both of the KLM and of the PAM. We show the ground state phase diagrams of both models and discuss the relation to the recent experiments which have investigated the change of the Fermi surface.

1. Introduction
Recently, the change of the Fermi surface across the antiferromagnetic (AF) transition is observed in some heavy fermion compounds and attracts much attention. The de Haas-van Alphen (dHvA) experiment in CeRh$_2$Si$_2$ shows that the topology of the Fermi surface changes abruptly at the first-order AF transition [1]. The Hall-effect experiment in YbRh$_2$Si$_2$ indicates a discontinuous change of the Hall coefficient across the AF quantum critical point (QCP) [2]. These experiments challenge the conventional view of the AF transition in heavy fermion system. The novel types of theories for heavy fermion QCP have been proposed in recent years. They are based on the breakdown of the Kondo screening or the decoupling of conduction ($c$-) electrons and $f$-electrons [3, 4, 5]. However, the relation between the AF transition and the change of the Fermi surface have not been clarified yet.

2. Model and method
In this paper, we study the ground states of the Kondo lattice model (KLM) and the periodic Anderson model (PAM) to clarify the relation between the AF transition and the change of the Fermi surface. The KLM is expressed as

$$ H = \sum_{k\sigma} \varepsilon_k c_k^{\dagger} c_{k\sigma} + J \sum_{i} \mathbf{S}_i \cdot \mathbf{s}_i $$  \hspace{1cm} (1)

where $s_i$ and $S_i$ represent the $c$- and $f$-electron spins, respectively. $J (>0)$ denotes the AF exchange coupling between them and $\varepsilon_k = -2t(\cos k_x + \cos k_y)$ is the $c$-electron energy dispersion. In the following, we set $t = 1$ for energy unit. The $f$-electrons are completely localized ($n_f = 1$) and thus the $c$-electron density $n_c$ is a controlling parameter.
The PAM is expressed as

\[
H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + E_f \sum_{i\sigma} n_{i\sigma}^f + U \sum_i n_{i\uparrow}^f n_{i\downarrow}^f + V \sum_{i\sigma} (f_{i\sigma}^\dagger c_{i\sigma} + \text{h.c.)},
\]

where \(\varepsilon_k, E_f, U\) and \(V\) represent energy dispersion of \(c\)-electrons, energy level of \(f\)-electrons, on-site Coulomb interaction between \(f\)-electrons and hybridization between \(c\) and \(f\)-electrons, respectively. In the PAM, the number of \(f\)-electrons at each site is not fixed and thus the total electron density \(n = n_c + n_f\) is a controlling parameter. The variational Monte Carlo (VMC) method is used for the calculation of ground state energies and other physical quantities of these models.

We prepare the Gutzwiller-type trial wave functions for paramagnetic and AF states. They consist of a projection operator and a one-body part \(|\Phi\rangle\) which is obtained from the solution of a certain one-body Hamiltonian. For the KLM, the specific form is as follows,

\[
|\Psi_{\text{KLM}}\rangle = P_{n_f=1} |\Phi\rangle, \quad P_{n_f=1} = \prod_i \left[ (1 - n_f^i) (1 - n_f^i) + n_f^i (1 - n_f^i) \right].
\]

\(P_{n_f=1}\) keeps the \(f\)-electron number of each site exactly one. Since the \(f\)-electrons must be treated as localized spins in the KLM, this constraint is necessary for the accurate calculation. For the PAM, we use

\[
|\Psi_{\text{PAM}}\rangle = P_G^f |\Phi\rangle, \quad P_G^f = \prod \left( 1 - (1 - g) n_f^i n_f^i \right).
\]

\(P_G^f\) reduces the probability of double occupancy of \(f\)-electrons at the same site and \(g\) is a variational parameter. In this paper, we consider the case of \(U = \infty\) and thus we set \(g = 0\) in the following. We construct the one-body part \(|\Phi\rangle\) by diagonalizing the following Hamiltonian,

\[
H = \sum_{k\sigma} \begin{pmatrix} \sigma m & -\tilde{V} & 0 \\ -\sigma m & 0 & -\tilde{V} \\ -\tilde{V} & 0 & \tilde{E}_f - \sigma M \end{pmatrix} \begin{pmatrix} c_{A\kappa\sigma}^\dagger \\ c_{B\kappa\sigma}^\dagger \\ f_{A\kappa\sigma}^\dagger \\ f_{B\kappa\sigma}^\dagger \end{pmatrix},
\]

where \(\tilde{V}\) and \(\tilde{E}_f\) are “effective” hybridization and \(f\)-electron energy level. \(m\) and \(M\) are AF gaps in \(c\)- and \(f\)-electrons, respectively. These four variational parameters are optimized so as to give the lowest energy state. Note that in the KLM, actual \(c-f\) hybridization is absent since the \(f\)-electrons are completely localized. Instead, the role of \(\tilde{V}\) is reflected as the exchange energy gain. On the other hand, \(M\) stabilizes the local magnetic moment and works so as to gain the kinetic energy of \(c\)-electrons. In this way, the competition between the Kondo effect and the RKKY interaction is roughly described as the competition between \(\tilde{V}\) and \(M\).

We classify the trial states according to the shape of the Fermi surface and the band dispersion of the one-body part: (a) paramagnetic metal (PM), (b) AF metal with hole-like Fermi surface (AF\(_h\)), (c) AF metal with electron-like Fermi surface (AF\(_e\)) and (d) AF metal with \(\tilde{V} = 0\) (AF\(_S\)). The details are shown in our previous paper [6].

3. Kondo lattice model
First we show the results for the KLM. Figure 1 shows the ground state phase diagrams for \(n_c = 60/64 = 0.9375\) and \(n_c = 52/64 = 0.8125\). At \(n_c = 0.9375\), there are two types of quantum phase transition. As \(J\) decreases from the large value, the ground state changes from PM to AF\(_h\) at \(J_{AF}\). It is a conventional second-order (continuous) AF transition. The first Brillouin
Figure 1. Ground state phase diagrams of the KLM in a two-dimensional square lattice.

zone is folded and the lowest energy band is decoupled from the Fermi surface. However, the topology of the Fermi surface is unchanged compared with PM (hole-like Fermi surface). As $J$ decreases further, the state changes from AF$_h$ to AF$_e$ at $J_{FS}$. In this transition, the topology of the Fermi surface changes from hole-like to electron-like within the AF state. It is a novel type of first-order quantum phase transition and we call it “Fermi surface reconstruction”. The staggered magnetization of $f$-electrons discontinuously increases across this transition. Moreover, at $n_c = 0.8125$, AF$_h$ is not stabilized and the ground state changes directly from PM to AF$_e$ at $J_{AF+FS}$ as shown in Fig. 1(b). In this case, the AF transition and the Fermi surface reconstruction occur simultaneously and thus the first-order AF transition is realized. The Fermi surface reconstruction is originated from the change of the mechanism of the energy gain. In PM and AF$_h$, the hole-like Fermi surface which is favorable for the exchange energy gain is realized. In AF$_e$, on the other hand, the electron-like Fermi surface which is favorable for the kinetic energy gain is realized. In other words, the role of $\tilde{V}$ is dominant in PM and AF$_h$ while the role of $M$ is dominant in AF$_e$. We emphasize that even in AF$_e$, $\tilde{V}$ have small but finite value and therefore the breakdown of Kondo screening does not occur. The result of dynamical cluster approximation study also suggests the same kind of Fermi surface reconstruction [7].

4. Periodic Anderson model
Next we show the results for the PAM. In the PAM, the value of $E_f$ is important for the nature of AF transitions. We fix the total electron density $n = n_c + n_f = 1.8125$ and varies the value of $E_f$. The ground state phase diagrams are shown in Fig. 2. When $E_f = 0.0$, AF$_e$ is not stabilized and only the conventional AF transition occurs at $V_{AF}$. On the other hand, when $E_f = -0.2$, AF$_e$ appears for small values of $V$. As $E_f$ becomes lower, the region of AF$_e$ is greatly extended and finally covers the region of AF$_h$. In this way, the Fermi surface reconstruction observed in the KLM is also realized in the PAM for appropriate values of $E_f$. However, its detailed property is somewhat different from the case of the KLM. In the KLM, the $f$-electrons are completely localized and can not move. In the PAM, on the other hand, the $f$-electrons have itinerancy before and after the Fermi surface reconstruction, although their mobility is greatly suppressed on the AF$_e$ side. The average $f$-electron density $\langle n_f \rangle$ is discontinuously increased across the transition as shown in Fig. 2(d). We can say that the $f$-electrons change their character from itinerant to (almost) localized through the Fermi surface reconstruction. Similar results are shown in the study of cellular dynamical mean field theory for the three-dimensional case [8].
Figure 2. (a), (b), (c) Ground state phase diagrams of the PAM in a two-dimensional square lattice for different values of $E_f$. (d) $V$ dependences of average $f$-electron densities. Open symbols represent the second-order AF transition points $V_{AF} (PM \rightarrow AF_h)$.

5. Summary

In this paper, we have shown the existence of the novel type of quantum phase transition which is called “Fermi surface reconstruction” in the KLM and the PAM. It is originated from the competition between the Kondo screening and the RKKY interaction and our simple trial wave functions seem to capture the essence of this competition. For example, the results of dHvA experiments and band calculations for CeRh$_2$Si$_2$ suggest that the $f$-electrons are localized in the AF state while they are itinerant in the paramagnetic state. This picture is qualitatively consistent with our result for the PAM. We expect that the abrupt changes of the Fermi surface observed in some heavy fermion compounds are closely related to the Fermi surface reconstruction obtained in our results.

References

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