Variational Monte Carlo study of magnetic states in the periodic Anderson model

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Abstract. We study the magnetic states of the periodic Anderson model with a finite Coulomb interaction between $f$ electrons on a square lattice by applying variational Monte Carlo method. We consider Gutzwiller wavefunctions for the paramagnetic, antiferromagnetic, ferromagnetic, and charge density wave states. We find an antiferromagnetic phase around half-filling. There is a phase transition accompanying change in the Fermi-surface topology in this antiferromagnetic phase. We also study a case away from half-filling, and find a ferromagnetic state as the ground state there.

1. Introduction

In recent years, phase transitions characterized by change in Fermi-surface topology, called Lifshitz transitions [1], have been discussed as possible origin of some anomalies in heavy-fermion systems under a magnetic field and/or with magnetic order, for example, in YbRh$_2$Si$_2$ under a magnetic field [2–6].

Theoretically such a possibility of existence of a Lifshitz transition in $f$-electron systems has been investigated for a long time. In an antiferromagnetic phase, Fermi-surface reconstruction is found in the Kondo lattice model [7–10] and in the periodic Anderson model [11]. For states with finite magnetic polarization, i.e., under a magnetic field or in a ferromagnetic phase, there is a possibility of a half-metallic state where only one spin-band has a Fermi surface. A transition to the half-metallic state from other states accompanies a change in the Fermi-surface topology. Indeed, such transitions to the half-metallic state have been found in the Kondo lattice model [12–19] and in the periodic Anderson model [20–25].

In these studies, the Coulomb interaction $U$ between $f$ electrons is taken as $U \to \infty$ for the periodic Anderson model except for the studies of the transition to the half-metallic state by the slave-boson mean-field approximation [20, 22]. Note also that the Kondo lattice model is an effective model of the periodic Anderson model in the limit of $U \to \infty$. Thus, it is still not obvious whether the Fermi-surface reconstruction exits or not even for a finite $U$ beyond the slave-boson mean-field treatment.

In this paper, we investigate the Fermi-surface reconstruction in magnetic states of the periodic Anderson model with finite $U$ by applying variational Monte Carlo method. We consider both the antiferromagnetic and ferromagnetic states on an equal footing and compare them.
2. Model and method

The periodic Anderson model is given by

\[ \mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \epsilon_f \sum_{i\sigma} n_{fi\sigma} - V \sum_{i\sigma} (f_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_{k\sigma}) + U \sum_{i} n_{fi\uparrow} n_{fi\downarrow}, \tag{1} \]

where \( c_{k\sigma} \) and \( f_{k\sigma} \) are the creation operators of the conduction and \( f \) electrons, respectively, with momentum \( k \) and spin \( \sigma \). \( n_{fi\sigma} \) is the number operator of the \( f \) electron with spin \( \sigma \) at site \( i \). We consider a square lattice with nearest-neighbor hopping and the kinetic energy is given by \( \epsilon_k = -2t(\cos k_x + \cos k_y) \), where \( t \) is the hopping integral and we set the lattice constant unity. \( \epsilon_f \) is the \( f \)-electron level, \( V \) is the hybridization matrix element, and \( U \) is the onsite Coulomb interaction between \( f \) electrons.

The variational wavefunction is given by

\[ |\psi\rangle = P|\phi\rangle, \tag{2} \]

where \( P = \prod_i [1 - (1 - g)n_{fi\uparrow}n_{fi\downarrow}] \) is a projection operator with a variational parameter \( g \). \( |\phi\rangle \) is a one-electron part of the wavefunction. In the present study we choose the one-electron part as the ground state of the mean-field-like effective-Hamiltonian which we define in the followings.

For the paramagnetic or ferromagnetic state, we consider the following effective Hamiltonian:

\[ H_{\text{eff}} = \sum_{k\sigma} (c_{k\sigma}^\dagger f_{k\sigma}^\dagger) \begin{pmatrix} \epsilon_k & -\tilde{V}_\sigma \\ -\tilde{V}_\sigma & \tilde{\epsilon}_{f\sigma} \end{pmatrix} \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix}, \tag{3} \]

where \( \tilde{V}_\sigma \) is the effective hybridization matrix element and \( \tilde{\epsilon}_{f\sigma} \) is the effective \( f \)-level. They are variational parameters. For the paramagnetic state, they do not depend on spin \( \sigma \).

For the antiferromagnetic state, we consider the ordering vector \( Q = (\pi, \pi) \) in this study, and then, the effective Hamiltonian is given by

\[ H_{\text{eff}} = \sum_{k\sigma} (c_{k\sigma}^\dagger f_{k\sigma}^\dagger c_{k+Q\sigma}^\dagger f_{k+Q\sigma}^\dagger) \begin{pmatrix} \epsilon_k & -\tilde{V} & \sigma \tilde{\epsilon}_{cQ} & -\sigma \tilde{V} Q \\ -\tilde{V} & \tilde{\epsilon}_f & -\sigma \tilde{V} Q & \sigma \tilde{\epsilon}_{fQ} \\ \sigma \tilde{\epsilon}_{cQ} & -\sigma \tilde{V} Q & \epsilon_{k+Q} & -\tilde{V} \\ -\sigma \tilde{V} Q & \sigma \tilde{\epsilon}_{fQ} & -\tilde{V} & \tilde{\epsilon}_f \end{pmatrix} \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \\ c_{k+Q\sigma} \\ f_{k+Q\sigma} \end{pmatrix}, \tag{4} \]

where \( k \)-summation runs over the folded Brillouin-zone of the antiferromagnetic state. The parameters with tilde are variational parameters. \( \tilde{\epsilon}_{cQ} \) and \( \tilde{\epsilon}_{fQ} \) play roles like mean-fields. In addition, we consider \( \tilde{V} Q \) which denotes the site and spin depending part of the effective hybridization matrix element in the antiferromagnetic state.

For the charge-density-wave state, we can consider a similar effective Hamiltonian, but we find that the charge-density-wave state does not become the ground state within parameters we have investigated for. Thus, we show results only for the paramagnetic, ferromagnetic, and antiferromagnetic states in the following.

For each state, we evaluate energy by using the Monte Carlo method, and optimize the variational parameters which minimize energy. Then, we compare energy of these states and determine the ground state. Other physical quantities can also be calculated by using the optimized variational parameters.
3. Results

Now, we show the calculated results. In this study, we set $U = 8t$ and $V = t$. The calculations are done for a $12 \times 12$ lattice with antiperiodic-periodic boundary conditions.

First, we show the results around half-filling. We set the number of electrons per site $n = 276/12^2 = 1.917$. Figure 1 shows energy of antiferromagnetic (AF) and ferromagnetic (FM) states measured from that in the paramagnetic (PM) state $E_{PM}$ as functions of $\epsilon_f$. For the ferromagnetic states, we fix magnetization $m = n^↓ - n^↑$, where $n_\sigma$ is the number of $\sigma$-spin electrons per site. Here, we have chosen three values for the magnetization: $m = 0.083, 0.583, \text{and } 1$. The state with $m = 0.083$ is the half-metallic state for this filling, i.e., $m = n^↓ - n^↑ = 1 - (n - 1)^2/n$.

In a wide region, we find that the antiferromagnetic state is the ground state. At $\epsilon_f/t \gtrsim -0.1$, a weak ferromagnetic state with $m = 0.0083$ has the lowest energy, while the difference in energy is not visible on this scale. The energy gain of this ferromagnetic state is very small, and the stability of this state should sensitively depend on the choice of the variational wavefunction. In particular, this state may become unstable against the paramagnetic state if we revise the variational wavefunction. Thus, we simply ignore this ferromagnetic state here, and concentrate on the antiferromagnetic state. In the antiferromagnetic state, there is a bend in the energy at $\epsilon_f/t \simeq -1.3$. It indicates a first-order transition.

In Fig. 2, we show the antiferromagnetic moment $m_{AF}$ as a function of $\epsilon_f$. The antiferromagnetic moment is defined as $m_{AF} = \frac{1}{N} \sum_i e^{iQ \cdot r_i} (n^↓_i - n^↑_i)$, where $N$ is the number of lattice sites, $r_i$ is the position of site $i$, and $n_{i\sigma}$ is the expectation value of the number of electrons with spin $\sigma$ at site $i$. By decreasing $\epsilon_f$, $m_{AF}$ develops from zero around $\epsilon_f \simeq 0.1$. It seems a second-order phase transition. By decreasing $\epsilon_f$ further, we find a jump in $m_{AF}$ at $\epsilon_f/t \simeq -1.3$. It is a first-order phase transition as is already recognized in energy (Fig. 1).

Here, we call the antiferromagnetic phase with smaller $m_{AF}$ ($\epsilon_f/t \gtrsim -1.3$) AF1 and that with larger $m_{AF}$ ($\epsilon_f/t \lesssim -1.3$) AF2. For each phase, we can draw the Fermi surface by using

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**Figure 1.** Energy $E$ per site as functions of $\epsilon_f$ for $n = 1.917$, $U/t = 8$, and $V/t = 1$. Energy is measured from that in the paramagnetic state $E_{PM}$. 

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Figure 2. Antiferromagnetic moment as a function of $\epsilon_f$ for $n = 1.917$, $U/t = 8$, and $V/t = 1$. The Fermi surface in each phase is also shown. In the paramagnetic state, the shaded area indicates the momenta where the lowest band is occupied by electrons and the unshaded area indicates unoccupied states in the Brillouin zone. In the antiferromagnetic states, the shaded area indicates the momenta where both the first and second lowest bands are occupied and the unshaded area indicates the momenta where only the lowest band is occupied in the folded Brillouin zone.

The obtained variational parameters in the one-electron part (see insets in Fig. 2). In the paramagnetic state, there is a small hole pocket around ($\pi, \pi$) since it is near half-filling. In the present method, the paramagnetic state is always regarded as an itinerant $f$ state, that is, the $f$-electron state contributes to the volume of the Fermi surface. In the AF1 state, we obtain a hole pocket centered at (0,0). This Fermi surface can be obtained by simply holding the paramagnetic Fermi-surface. Thus, the AF1 states is naturally connected to the paramagnetic state, and in this sense, it is regarded as an itinerant $f$ state. In the AF2 state, the Fermi surface is different from that in AF1. The transition in the antiferromagnetic phase accompanies a change in Fermi-surface structure as in the previous studies [7–11]. The Fermi surface in AF2 can be obtained by ignoring one $f$ electron per site, that is, the Fermi surface is the same as that for the paramagnetic state with the electron number per site $n – 1$. It means that the AF2 state can be interpreted as a localized $f$ state.

Finally, we show the results away from half-filling. Figure 3 shows energy as functions of $\epsilon_f$ for $n = 1.5$. In contrast to the case around half-filling, the ferromagnetic state has lower energy than the antiferromagnetic state in a wide parameter region. We note that even at $\epsilon_f/t = -3$, the ferromagnetic state with $m \approx 0.9$ has lower energy than the antiferromagnetic state (not shown). We expect a half-metallic state $n\uparrow = 1$, i.e., $m = n\uparrow - n\downarrow = 2 - n = 0.5$, for $-1.5 \leq \epsilon_f/t \leq -1$. Such a half-metallic state has been discussed in the literature [12–25]. However, to determine magnetization $m$ for each parameter set, we need to calculate energy by changing $m$ with a smaller interval. It is now in progress, and we will discuss the details of the ferromagnetic state in the near future.
Figure 3. Energy $E$ per site as functions of $\varepsilon_f$ for $n = 1.5$, $U/t = 8$, and $V/t = 1$. Energy is measured from that in the paramagnetic state $E_{PM}$.

4. Summary
We have studied both the antiferromagnetic and ferromagnetic states of the periodic Anderson model with finite $U$ on an equal footing by applying variational Monte Carlo method. We find that the antiferromagnetic state is the ground state around half-filling for a deep enough $f$ level. There are two antiferromagnetic states: the AF1 state has itinerant $f$ character and the AF2 state has localized $f$ character. We find a first-order phase transition between them accompanying a change in the Fermi-surface topology, i.e., Lifshitz transition. We have also investigated a case away from half-filling, and we have found that the ground state is the ferromagnetic state. The details of this ferromagnetic state will be reported elsewhere.

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