Study of Charge-Density-Wave Instability in Heavy Electron Systems

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Abstract. In this article an extended periodic Anderson model, including correlations between conduction and localized electrons, is studied with dynamical mean field theory and continuous-time quantum Monte Carlo method. In particular, we clarify how the antiferromagnetic phase, observed in the ordinary periodic Anderson model, changes into the charge-density-wave phase which emerges in a strong coupling region.

1. Introduction

Heavy fermion behavior can be found in lanthanide or actinide compounds where interesting phenomena are observed such as unconventional superconductivity, metamagnetism, Kondo insulators and so on. In heavy fermion systems, the effective mass of electrons can be thousands times heavier than that of free electrons and the hybridization between itinerant orbital and strongly correlated localized orbital plays an essential role in description of the system. To study these systems, the periodic Anderson model, which has the above feature, is often used.

In some compounds, however, correlations between conduction \(c\)-electrons and localized \(f\)-electrons are also important. In CePd\(_2\)Si\(_2\) and CeIn\(_3\), antiferromagnetism is suppressed with increasing pressure and the superconducting phase appears near the antiferromagnetic (AF) quantum critical point (QCP)[1]. In these compounds, a mechanism forming Copper pairs is related to AF fluctuations. On the other hands, the pairing mechanism in CeCu\(_2\)Si\(_2\) and CeCu\(_2\)Ge\(_2\) cannot be understood only in terms of AF fluctuations. In CeCu\(_2\)Si\(_2\) and CeCu\(_2\)Ge\(_2\), with increasing pressure, the AF phase is suppressed and the superconducting phase appears. However, the transition temperature of the superconducting phase has a maximum far from AF-QCP. Moreover, in CeCu\(_2\)(Si\(_0.9\)Ge\(_{0.1}\))\(_2\), two superconducting domes are found in the \(P\)-\(T\) phase diagram[2]. To understand these phenomena, Miyake and his collaborators have extended the periodic Anderson model by taking into account local interaction between \(c\)- and \(f\)-electrons and proposed that a mechanism for the unconventional superconducting phases is related to valence fluctuations[3]. Numerical calculations, such as density matrix renormalization and dynamical mean field theory (DMFT) with exact diagonalization, also indicate that the \(c\)-\(f\) correlations cause a valence transition (VT). Another example showing the importance of the \(c\)-\(f\) correlation is Yb\(_{0.38}\)In\(_{0.62}\)Cu\(_4\). This compound exhibits a metamagnetic behavior accompanied by volume expansion with lowering temperature. Motivated by this phenomenon, Watanabe et al. have proposed that the metamagnetism is caused by the VT which is induced by the cooperation of \(c\)-\(f\) correlation and magnetic field[4].
From these facts, the c-f electron correlation has received much attention and many groups have studied this effect intensively. Recently, it has been proposed that c-f correlations also enhance fluctuations of charge density wave (CDW) in the weak coupling region[6] and its instability is confirmed in the strong coupling region by our previous study[7]. However, the relation between this phase and the AF phase, stabilized in the ordinary periodic Anderson model, is unclear.

Thus, in this article, we study how the AF phase changes into the CDW phase with increasing c-f correlation. We analyze this system by using DMFT[8] combined with continuous time-quantum Monte Carlo method, which enables us to study the system with high accuracy[9, 10]. This paper is organized as follows. First, the model and method are explained in the next section. We discuss the effect of interorbital correlation on heavy fermion systems in sec. 3, which is followed by a brief summary in sec. 4.

2. Model and Methods

We consider the extended periodic Anderson model including the c-f correlations. The Hamiltonian is given by

\begin{equation}
H_{\text{E-PAM}} = -t \sum_{<i,j>,\sigma} c_i^{\dagger} \sigma c_j + H_{\text{loc}}
\end{equation}

\begin{equation}
H_{\text{loc}} = \epsilon_f \sum_{i,\sigma} n_f^i + V \sum_{i,\sigma} (c_{i\sigma} \sigma f_{i\sigma} + \text{h.c.}) + U_{ff} \sum_i n_f^i n_f^i + U_{cf} \sum_{i,\sigma,\sigma'} n_c^i n_f^i,
\end{equation}

where \(c_{i\sigma} (f_{i\sigma})\) is annihilation operator of \(c\)-\(f\)-electron at site \(i\) in spin state \(\sigma = \uparrow, \downarrow\). The c-electrons are itinerant with hopping integral \(t\) while f-electrons are localized with energy \(\epsilon_f\). The hybridization between c- and f-electrons at the same sites is represented by \(V\). Correlations between f-electrons (between c-and f-electrons) are represented by \(U_{ff} (U_{cf})\).

To analyze this model, DMFT is employed. In DMFT, the lattice problem is mapped onto an effective impurity problem which has to be solved self-consistently. For simplicity, we assume the lattice structure to the Bethe lattice, and this lattice structure simplifies the self-consistent equation to the following equation[8],

\begin{equation}
\left[ g_{\sigma}^{-1}(i\omega) \right]_{cc} = i \omega + \mu - \left( \frac{D}{2} \right)^2 [G_{\sigma}(i\omega)]_{cc},
\end{equation}

where \(D\) is the half-band width of the conduction band. The \(g_{\sigma}(i\omega)\) is the Green’s function of the effective bath, and \(G_{\sigma}(i\omega)\) is the full Green’s function in the impurity model. Long-range ordered phases are treated with sublattice method. The order parameter of the AF (CDW) phase is defined by \(m_{c(f)} = \frac{1}{2} \left( n_{c(f)} - n_{c(f)}^d \right) \left( \rho = \frac{1}{2} \sum_{\sigma} \left| \langle n_{\sigma}^c - n_{\sigma}^f \rangle \right| \right)\). In the following, we set \(D = 1\) as energy unit and fix the temperature at \(T = 0.02\). For simplicity, we analyze the particle hole symmetric case. Namely we set \(\mu = U_{cf}\) and \(\epsilon_f = -U_{ff}/2\), where \(\mu\) is chemical potential.

3. Correlation effects between conduction and localized electrons

Let us first analyze the order parameters. The order parameters for the AF and CDW phase are shown in Fig. 1. The AF order parameter at \(U_{cf} = 0.5\) is plotted in Fig. 1(a). As seen in this figure, c- and f-electrons are magnetized by RKKY interaction. Note that a paramagnetic phase in \(V \lesssim 0.3\) is different from the paramagnetic phase in \(V \gtrsim 0.425\). In \(V \lesssim 0.3\), the magnetic moments are suppressed by temperature, while in \(V \gtrsim 0.425\), the moments are suppressed by the Kondo effect. This behavior is qualitatively the same as in the ordinary periodic Anderson...
model, i.e. $U_{cf} = 0$ case. However, in the strong $U_{cf}$ region, this antiferromagnetic phase is replaced by the CDW phase. In Fig. 1(b), the order parameters for each phase at $V = 0.1$ are plotted as a function of the $c$-$f$ correlation.

In Fig. 1(b), we can observe how the system changes its character under strong $c$-$f$ correlation. As seen from this figure, if the correlation is weak, the system has no long range order. Note, however, that this paramagnetic phase is due to temperature effects, and the AF phase is considered to be stabilized in the lower temperature region. If $c$-$f$ correlation becomes stronger, the AF phase is stabilized even at $T = 0.02$. With increasing $c$-$f$ correlation further, the AF phase is suppressed and the CDW phase emerges in the strongly correlated region. Sketches of these phases are shown in Figs. 1(c) and (d). The origin of this CDW phase may be the competition between $f$-electron interaction and hybridization. It is confirmed that strong hybridization suppresses the CDW phase. As mentioned above, the AF phase is affected by the temperature particularly in the region $V/D \lesssim 0.25$. The detailed discussions on the temperature effects will be given elsewhere[11].

![Figure 1](image_url)

**Figure 1.** (a) Antiferromagnetic moments as a function of hybridization at $U_{cf} = 0.5$. (b) Order parameters of the AF and CDW phases as a function of intraorbital interaction at $V = 0.1$. (c) and (d) Sketches of the AF and CDW phase respectively.

For further understanding of this system in the strong $c$-$f$ region, we observe the local spin correlation of each orbital ($S^2_\alpha$, $\alpha = c, f$) and $c$-$f$ spin correlation. These quantities reflect the CDW instability. Let us consider the hybridization dependence, from which we can find some interesting phenomena in local spin correlations. The results for $U_{cf} = 1$, and 2 are plotted in Fig. 2. For $U_{cf}=2$, the CDW phase is stabilized in $V < 0.105$. In this case, we can see a rapid change in $\langle S_c \cdot S_f \rangle$ due to CDW instability. Namely, in $V < 0.105$, $\langle S_c \cdot S_f \rangle$ is rapidly decreased with decreasing $V$. In the $U_{cf} = 1$ case, the $c$-$f$ spin correlation exhibits qualitatively the same $V$ dependence as in the $U_{cf} = 1$ case except for the influence of CDW transition.

On the other hand, we can see that the behaviors of the other quantities for the $U_{cf} = 2$ case are qualitatively different from the $U_{cf} = 1$ case, even if the system is in a paramagnetic phase. In Fig. 2(b), we can find that in the $U_{cf} = 2$ case, local spin correlation of $c$-electrons increases with increasing $V$, while in the $U_{cf} = 1$ case, the local spin correlation decreases around $V = 0.3$ with decreasing $V$. Local spin correlation of $f$-electrons ($\langle S^2_f \rangle$) also exhibits similar $V$ dependence. These qualitatively different behaviors for $U_{cf} = 1$ and 2 are attributed to the difference of charge configuration between the ground states at $V = 0$. Namely, in the case of $U_{cf} = 2$, the system has CDW order at $V = 0$ (sketch of this state is shown in Fig. 1(d)). In the case of $U_{cf} = 1$, the ground state at $V = 0$ is a paramagnetic state whose charge configuration is drawn in Fig. 1(c). Therefore, if $U_{cf} = 2$ and $V$ is small, the occupancy of an $f$-orbital is nearly two at $c$-electron rich sites. Increasing $V$, the $f$-electrons become easy to hop to $c$-orbital. On the other hand, in the $U_{cf} = 1$ case, one electron occupies each site, and the increase in $V$ leads to the increase in $f$-electron double occupancy.

In the analysis of how the system behaves with increasing $V$, we have observed that the $f$-electron double occupancy exhibits qualitatively different behaviors for $U_{cf} = 1$ and 2. These
interesting behaviors are attributed to the difference of charge configuration between the ground states at $V = 0$. The CDW phase studied in this paper emerges as a result of competition of the hybridization, the $f$-$f$ interaction and the $c$-$f$ interaction. Thus, for further understanding of the CDW phase, a more systematic study is necessary, which is currently in progress.

4. Summary
In this paper, we have studied AF and CDW instabilities in the extended periodic Anderson model with $c$-$f$ correlations. The $c$-$f$ spin correlation and the local spin correlation for each orbital have been calculated as a function of hybridization. From the behavior of local spin correlation, it has been found that the system exhibits qualitatively different behaviors depending on $c$-$f$ correlation even if the system is in the paramagnetic phase. We have also elucidated how the AF phase, emerging in the ordinary periodic Anderson model, changes into the CDW phase in the presence of strong $c$-$f$ correlation.

To conclude this paper, a brief comment on a VT is in order. It should be naturally expected that the interorbital correlation can induce a VT. In our study, however, the VT has not been found. This is due to our choice of parameters. Namely, we have restricted ourselves to the particle-hole symmetric case, where the deep $f$-electron level suppresses the valence fluctuations and thus the condition for the VT is not satisfied. We will extend our analysis to the valence fluctuation regime to incorporate the possibility of VT in our treatment.

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