GROUND-STATE PROPERTIES OF THE MODIFIED PERIODIC ANDERSON MODEL IN INFINITE DIMENSIONS *

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Ground-state properties of the periodic Anderson model with a dispersion of f-electrons are investigated at half-filling in infinite dimensions. We determine the magnetic phase diagram by using dynamical mean field theory combined with a perturbative treatment of the f-f Coulomb interaction. Nonmonotonic behavior is found in the phase boundary when a dispersion of f-electrons is changed, the origin of which is discussed in the light of formation of renormalized quasi-particles.

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1. Introduction

There has been much interest in heavy fermion systems, which exhibit a variety of remarkable phenomena [1]. The periodic Anderson model is a simplified model, which may describe essential physics of heavy fermions. This model has been intensively studied by various analytical and numerical methods. Among others, dynamical mean field theory (DMFT) [2], which is justified in infinite dimensions [3, 4], allows systematical studies of thermodynamic as well as dynamical properties [5–7].

In this paper, we investigate a modified version of the periodic Anderson model with a f-electron dispersion. By combining DMFT with a perturbation method, we determine the magnetic phase diagram at half-filling. In particular, we discuss how a dispersion of f-electrons affects a magnetic phase transition by calculating the density of states (DOS) for f-electrons.

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2. Model and method

The Hamiltonian we study here is a modified version of the periodic Anderson model,

$$\begin{aligned} H &= \sum_{k,\sigma} \epsilon^c_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,\sigma} \epsilon^f_k f^\dagger_{k\sigma} f_{k\sigma} + V \sum_{k,\sigma} (c^\dagger_{k\sigma} f_{k\sigma} + \text{H.c.}) \\ &+ \frac{U}{N} \sum_{k,k',q} f^\dagger_{k+q\uparrow} f_{k\uparrow} f^\dagger_{k'-q\downarrow} f_{k'\downarrow} , \end{aligned} \tag{1}$$

where $c_{k\sigma}$ ($f_{k\sigma}$) is the annihilation operator of a conduction- (f)-electron with momentum k and spin $\sigma(\uparrow,\downarrow)$. Here, V is the hybridization between two bands, U the f–f Coulomb interaction, and N the number of total lattice sites. We focus on the effects of a f-electron dispersion,

$$\epsilon^f_k = \alpha \epsilon^c_k , \tag{2}$$

by changing the ratio α continuously.

In DMFT [2], electron correlations are treated by mapping the lattice system to an effective impurity one, which is further supplemented by self-consistent procedures to reproduce the original lattice system. We combine DMFT with an iterated perturbation theory [2], in which the f–f interaction U is treated via a self-consistent second-order perturbation. Furthermore, in order to deal with a commensurate magnetic order, we consider an antiferromagnetic state with the two-sublattice structure [2, 7, 8]. For simplicity, we employ the semielliptic DOS for conduction electrons, $D(\epsilon) = 2\sqrt{D^2 - \epsilon^2}/\pi D^2$ with the bandwidth D.

3. Numerical results

We numerically iterate the self-consistent procedure in DMFT until the calculated quantities converge within desired accuracy. In the following discussions, the bandwidth D is taken to be unity and we shall deal with the commensurate magnetization at half-filling and absolute zero temperature.

In Fig. 1, we show the magnetic phase diagram obtained. Note that our results for $\alpha = 0$ are consistent with those of Rosenberg [7]. Let us now observe what happens for a quantum phase transition, when α is changed. In the small U region, a paramagnetic insulator (PI) is realized for $\alpha = 0$. As increasing α, the hybridization gap disappears, and consequently a paramagnetic metal (PM) emerges. Note that the phase boundary between PI and PM hardly depends on the strength of U. On the other hand, as U increases, an antiferromagnetic insulator (AFI) is stabilized. In all the results shown in the inset, the phase boundary exhibits nonmonotonic behavior as a function of α: as α increases, the phase boundary goes down and then increases again. For sufficiently large α, the system favors PM state, which is caused by an itinerant character of f-electrons. To see the origin

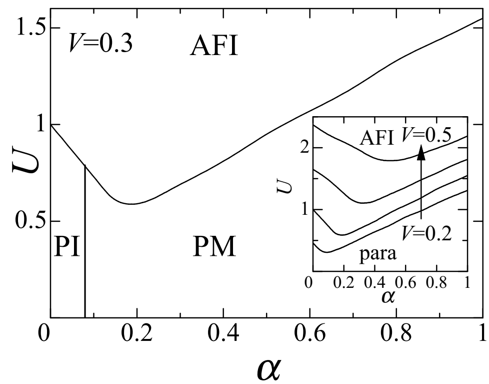

Fig. 1. $\alpha - U$ phase diagram for $V = 0.3$. The inset shows phase diagram for several choices of V. The phase boundary between the paramagnetic phase (para) and AFI exhibits nonmonotonic behavior. In order to refrain from complexity, we do not show the phase boundary between PI and PM in the inset.

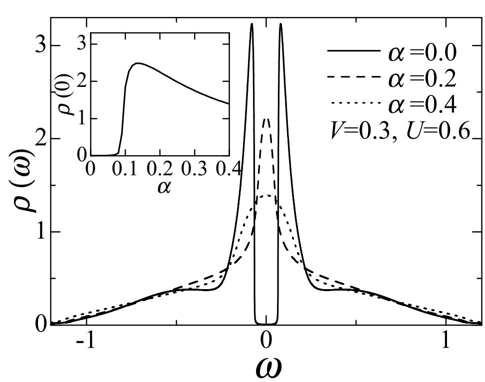

Fig. 2. DOS for f-electrons in the paramagnetic regime for $V = 0.3$ and $U = 0.6$. The inset shows the DOS at the Fermi level ($\omega = 0$) as a function of α.

of this nonmonotonic behavior clearly, we show the DOS for f-electrons in Fig. 2. Note that a paramagnetic solution is stable regardless of α in these parameters. For $\alpha = 0$, where the Kondo insulator is realized, the spectrum has a renormalized hybridization gap around the Fermi level ($\omega = 0$). As

α increases, the hybridization gap disappears and then heavy quasiparticles appear. The inset in Fig. 2 shows the DOS at the Fermi level, where its maximum is located around $\alpha \sim 0.15$. This value roughly corresponds to an inflection point of the phase boundary for $V = 0.3$ (Fig. 1). We can thus say that the introduction of a f-electron dispersion drives the system from the insulator to a metallic phase with the enhanced DOS at the Fermi level, and therefore the system becomes somewhat unstable against an antiferromagnetic order. However, further increase in α decreases the DOS at the Fermi level, making the system more stable against such a magnetic instability. This gives rise to the nonmonotonic behavior observed in the phase boundary. Therefore, the dispersion of f-electrons is expected to play a role for the magnetism when the f-electron dispersion is comparable to the gap in the spectral function.

4. Summary

We have investigated the periodic Anderson model with a dispersion of f-electrons. By using dynamical mean field theory combined with a self-consistent perturbation method, we have discussed how the phase diagram is affected by the itineracy of f-electrons. It has been shown that when the dispersion of f-electrons is introduced, the paramagnetic phase becomes once unstable, but further increase in α again favors a paramagnetic phase. This nonmonotonic behavior has been shown to be related to formation of renormalized quasi-particles.

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