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Heavy Fermion State in the Periodic Anderson-Holstein Model away from Half Filling

K. Mitsumoto [a,*], Y. Ōno [a,b]

[a] Department of Physics, Niigata University, Ikarashi, Niigata 950-2181, Japan
[b] Center for Transdisciplinary Research, Niigata University, Ikarashi, Niigata 950-2181, Japan

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Abstract

We investigate the electronic state of the periodic Anderson-Holstein model, which includes both the electron-electron Coulomb interaction and the electron-phonon coupling, away from half filing. The model is solved by using the dynamical mean-field theory combined with the exact diagonalization method. The heavy fermion state with large effective mass due to the electron-phonon coupling is realized in the wide range of the f-electron number n_f, while that due to the Coulomb interaction is realized in the narrow range of $n_f \sim 1$.

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The filled skutterudite $PrOs_4Sb_{12}$ has received much attention as it is the first example of a Pr-based heavy fermion superconductor and shows a large specific heat coefficient $\gamma = 750\mathrm{mJ/K^2mol}$ together with a large jump in the specific heat $\Delta C/T_c \sim 500\mathrm{mJ/K^2mol}$ at $T_c = 1.85\mathrm{K}$ [1]. In this compound, the crystal-field ground state of the Pr^{3+} ($4f^2$) ion is known to be singlet [2], in contrast to the usual Ce-based heavy fermion compounds where the multiplet ground states of the Ce^{3+} ($4f^1$) ion play crucial roles for the heavy fermion behavior. Recently, Goto *et al.* [3] have found that the elastic constant exhibits a remarkable Debye-type dispersion around 30 K together with an anomalous softening down to T_c; which reveals an off-center rattling motion of the Pr ion in the Sb cage. Then, several authors have discussed a possible mechanism of the heavy fermion behavior due to the strong coupling between the rattling motion and electrons [4–7].

To elucidate the strong coupling effects on the heavy fermion behavior, we investigate the periodic Anderson-Holstein model, where both the coupling of the local phonons to f-electrons and the Coulomb interaction between f-electrons are considered. In the previous work [6,7], we studied this model in the case of half filling with the particle-hole symmetry by using the dynamical mean-field theory (DMFT) [8]. What we have found are: (1) In the strong electron-phonon coupling regime $g \gtrsim g_c$, the system shows an anomalous heavy fermion behavior which is accompanied by a large lattice fluctuation and an extreme phonon softening. (2) A simple harmonic potential for ions for $g \lesssim g_c$ changes into an effective double-well potential for $g \gtrsim g_c$. (3) The pairing interaction between the conduction electrons has a maximum at $g \approx g_c$. In the present study, as an extension to the previous work, we discuss the electronic state in the model away from half filling.

Our model Hamiltonian is given by

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \epsilon_f \sum_{i\sigma} f^\dagger_{i\sigma} f_{i\sigma} + V \sum_{i\sigma} (f^\dagger_{i\sigma} c_{i\sigma} + h.c.) + U \sum_i n_{fi\uparrow} n_{fi\downarrow} + \omega_0 \sum_i b^\dagger_i b_i + g \sum_i (b^\dagger_i + b_i)(\sum_\sigma n_{fi\sigma} - 1), \quad (1)$$

where $c^\dagger_{i\sigma}$, $f^\dagger_{i\sigma}$ and $b^\dagger_i$ are creation operators for a conduction (c)-electron with spin σ at site i, for a f-electron and for a phonon, respectively, and $n_{fi\sigma} = f^\dagger_{i\sigma} f_{i\sigma}$. The quantities, ϵ_f, V, U and g, are the atomic f-level, the mixing between the c- and f-electrons, the on-site Coulomb interaction and the electron-phonon coupling strength. The density of f-electrons couples with the Einstein phonons

* Corresponding author.
Email address: mitsumoto@phys.sc.niigata-u.ac.jp (K. Mitsumoto).

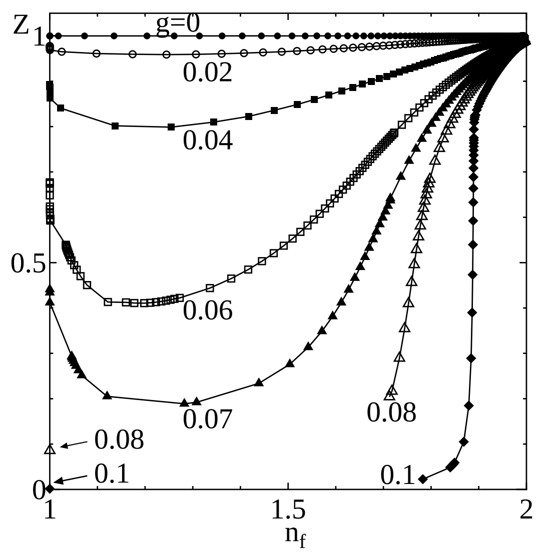

Fig. 1. The quasiparticle weight Z as a function of f-electron number n_f for several values of the electron-phonon coupling g in the case with $U = 0$.

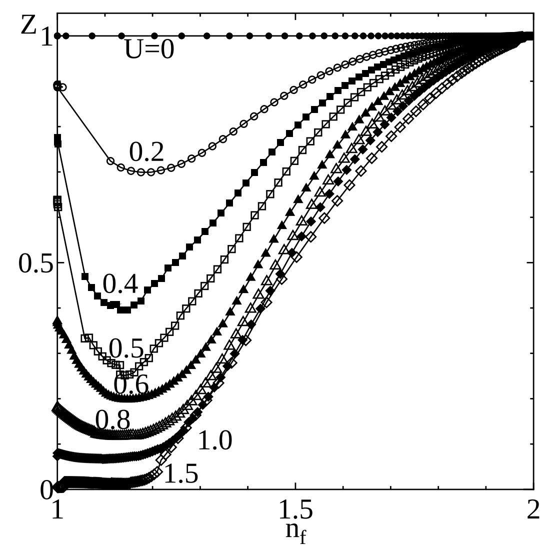

Fig. 2. The quasiparticle weight Z as a function of f-electron number n_f for several values of the Coulomb interaction U in the case with $g = 0$.

whose frequency is ω_0.

To solve this model eq.(1), we use the DMFT in which the model is mapped onto an effective single impurity Anderson-Holstein model [6,7]. The local Green's function $G_f(\mathrm{i}\omega_n)$ and the local self-energy $\Sigma(\mathrm{i}\omega_n)$ for f-electrons satisfy the following self-consistency condition:

$$G_f(\mathrm{i}\omega_n) = \int d\epsilon \frac{\rho(\epsilon)}{\mathrm{i}\omega_n - \epsilon_f - \Sigma(\mathrm{i}\omega_n) - \frac{V^2}{\mathrm{i}\omega_n - \epsilon}} = [\tilde{G}(\mathrm{i}\omega_n)^{-1} - \Sigma(\mathrm{i}\omega_n)]^{-1}, \quad (2)$$

where $\rho(\epsilon)$ is the density of states (DOS) for c-electrons. In the above equation, $\tilde{G}(\mathrm{i}\omega_n)$ is the Green's function for the effective impurity Anderson-Holstein model with $U = g = 0$ and is determined self-consistently. The effective impurity Anderson-Holstein model is solved by using the exact diagonalization method for a finite-size cluster [9,10]. In the present study, we use 8 site cluster and the cutoff of phonon number is set to be 30 [6,7]. We assume a semielliptic DOS with the bandwidth $W = 1$, $\rho(\epsilon) = \frac{2}{\pi}\sqrt{1-\epsilon^2}$, and we set $\omega_0 = 0.05$, $V = 0.2$ and $\epsilon_f = -\frac{U}{2}$.

In Fig. 1, the quasiparticle weight, $Z = (1 - \frac{\partial \Sigma(\omega)}{\partial \omega}|_{\omega=0})^{-1}$, is plotted as a function of the f-electron number n_f for several values of the electron-phonon coupling g in the absence of the Coulomb interaction U. Z decreases with increasing g for all n_f and the heavy fermion behavior with a large mass enhancement factor $m^*/m = Z^{-1}$ is observed in a wide range of n_f in the strong coupling regime $g \gtrsim 0.1$. We note that the stable solutions for $1 < n_f \lesssim 1.7$ with $g > 0.08$ have not been obtained yet, but the calculations are under way.

Fig. 2 shows the n_f dependence of Z for several values of U in the case with $g = 0$. When n_f is close to unity, $|n_f - 1| \lesssim 0.2$, Z monotonically decreases with increasing U and finally becomes $Z \sim 0$ in the strong correlation regime $U \gtrsim 1.5$. On the other hand, when n_f is away from unity, $|n_f - 1| \gtrsim 0.2$, Z tends to be a finite value even in the strong correlation regime. Then, the heavy fermion state due to the Coulomb interaction is realized only in the narrow range of $n_f \sim 1$, where the local spin fluctuation, which is responsible for the heavy fermion behavior, is enhanced due to the strong correlation effect. It is a striking contrast to the heavy fermion state in the strong electron-phonon coupling regime, where the local charge fluctuation is responsible for the heavy fermion behavior and is enhanced in a wide range of n_f.

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