Dynamical mean-field study of the heavy-fermion state in the multi-orbital Anderson lattice model coupled with Jahn-Teller phonons

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Abstract

We investigate electronic states and phononic states in the 2-orbital Anderson lattice model, where orbital fluctuation of f-electrons couples with the Jahn-Teller phonons, in the quarter-filling using the dynamical mean-field theory in conjunction with the exact diagonalization method. We find that a heavy fermion state is enhances due to cooperation between the electron-electron interaction and the electron-phonon interaction, besides the large lattice fluctuation and the anormalous softening are enhanced due to the Coulomb interaction.

Key words: electron-phonon interaction; heavy-fermion state; multi-orbital Anderson lattice model; Dynamical mean-field theory
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The filled skutterudite compounds RX_4X_{12} (R is a rare earth, T is a transition metal, and X is a pnictogen) have been attracted much attention because of their various physical properties. Especially, $PrOs_4Sb_{12}$ is the first example of a Pr-based heavy fermion superconductor and show a large specific heat coefficient $\gamma = 750\mathrm{mJ/K^2mol}$ together with a large jump in the specific heat $\Delta C/T_\mathrm{C} \gtrsim 500\mathrm{mJ/K^2mol}$ at $T_\mathrm{c} = 1.85\mathrm{K}$ [1]. ROs_4Sb_{12} (R=La, Pr, Sm, and Nd, except for Ce) exhabits ultrasonic frequency dependence of the elastic constant in low temperature region [2,3], and is proposed an off-center rattling motion of the rare earth ion in the pnictogen cage [2]. Besides, ROs_4Sb_{12} (R=Ce, Pr, Sm, and Nd, except for La) shows an anormally softening down to T_c due to fluctuation of f-electrons in levels splitted due to the crystalline electric field (CEF). A degenerated ground state of 4f-electrons plays a clucial role in the softening, in particular, the ground state determined by the CEF effect is Γ_7 doublet, $\Gamma_8^{(2)}$ quartet, and Γ_7 doublet or Γ_8 quartet in R=Ce, Nd, and Sm, respectively [4–6]. $PrOs_4Sb_{12}$ shows a weaker softening than former compounds due to the quadrupolar fluctuation between Γ_1 singlet ground state and the $\Gamma_4^{(2)}$ first exited state with a small gap energy $\Delta = 7.9\mathrm{K}$ [7].

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In our previous work, to investigate simply a strong coupling effect on heavy fermion behavior, we studied the periodic Anderson-Holstein model that charge fluctuation of f-electron couple with the breathing mode of local phonons in the half-filling [8,9] and in away from the half-filling [10] by using the dynamical mean-field theory (DMFT) [11]. And we found that the system shows a heavy fermion state behavior which is accompanied by a large lattice fluctuation and an anormalous softening. But, the model competes between the electron-electron interaction and the electron-phonon interaction because both interactions act in the single band. Recently, the dynamical Jahn-Teller effect is discussed in the multi-impurity Anderson model [12]. We need to study a model which cooperated between the interactions to discuss an effect of orbital fluctuation of f-electrons realistically. In the present study, we discuss electronic states and phononic states in the 2-orbital Anderson lattice model coupled with local phonons.

Our model Hamiltonian is given by,

$$
\begin{aligned}
H = & \sum_{\mathbf{k}l\sigma} \epsilon_{\mathbf{k}l} c^\dagger_{\mathbf{k}l\sigma} c_{\mathbf{k}l\sigma} + \sum_{il\sigma} \epsilon_{fl} f^\dagger_{il\sigma} f_{il\sigma} \\
& + \omega_0 \sum_i b^\dagger_i b_i + V \sum_{il\sigma} (f^\dagger_{il\sigma} c_{il\sigma} + h.c.) \\
& + U \sum_{il} n_{fil\uparrow} n_{fil\downarrow} + U' \sum_{i\sigma\sigma'} n_{fi1\sigma} n_{fi2\sigma'}
\end{aligned}
$$

$$+g\sum_i (b_i^\dagger + b_i)\sum_\sigma (f_{i1\sigma}^\dagger f_{i1\sigma} - f_{i2\sigma}^\dagger f_{i2\sigma}), \qquad (1)$$

where $c_{il\sigma}^\dagger$, $f_{il\sigma}^\dagger$ and $b_i^\dagger$ are creation operators for a conduction (c)-electron with orbital $l(=1,2)$ and spin σ at site i, for a f-electron and for a phonon, respectively, and $n_{fil\sigma} = f_{il\sigma}^\dagger f_{il\sigma}$. Parameters $\epsilon_{\mathbf{k}l}$ and ϵ_{fl}, V, and ω_0 are dispersion of c-electron and f-electron, c-f hybridization, and local phonon frequency, respectively. The electron-electron interaction term is expressed using the intra-orbital Coulomb interaction U, and the inter-orbital Coulomb interaction U', which satisfy the rotational invariant, $U' = U$. In the electron-phonon interaction, we assume orbital fluctuation of f-electron with E_g symmetry couples with $(3z^2 - r^2)$-type Jahn-Teller phonon with same symmetry [12], where g is the electron-phonon coupling constant.

To solve this model eq.(1), we use the DMFT in which the model is mapped onto an extended effective multi-impurity Anderson model coupled with the local phonons [13,14]. 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:

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

where $\rho(\epsilon)$ is the density of states (DOS) for c-electrons. In the above equation, $\tilde{G}(\mathrm{i}\omega_n)$ is the bare Green's function for an extended effective multi-impurity Anderson model and is determined self-consistently. The extended effective multi-impurity Anderson model is solved by using the exact diagonalization method for a finite-size cluster [15,16]. In the present study, we use 4 site cluster and the cutoff of phonon number is set to be 10. We assume a semielliptic DOS with the bandwidth $W = 1$, $\rho(\epsilon) = \frac{2}{\pi}\sqrt{1-\epsilon^2}$, and set $\epsilon_f = -\mu$ (μ is the chemical potential), $V = 0.1$, and $\omega_0 = 0.01$. We concentrate our attention on the quarter-filling, *i. e.*, we consider the Γ_7 doublet ground state.

In Fig. 1(a), the quasiparticle weight Z is plotted as a function of g for several values of the Coulomb interaction U. In the strong coupling regime, Z is enhanced due to the electron-electron interaction. The lattice fluctuation is defined by $\langle Q^2\rangle = \langle \hat{Q}_i^2 - \langle \hat{Q}_i\rangle^2\rangle$ with the lattice displacement operator, $\hat{Q}_i = \frac{1}{\sqrt{2\omega_0}}(b_i + b_i^\dagger)$. Fig. 1(b), shows the normalized lattice fluctuation, $\langle Q^2\rangle/\langle Q^2\rangle_0$, where $\langle Q^2\rangle_0 = \frac{1}{2\omega_0}$ is the lattice fluctuation for $g = 0$, *i.e.*, the zero-point oscillation. The lattice fluctuation is enhanced due to the Coulomb interaction in the strong couplong regime, besides, an enhancement of an anormalous softening is shown same behavior as the lattice fluctuation too. Their behavior are striking contrasts to those in the periodic Anderson-Holstein model in which an effective mass of electrons become small due to the Coulomb interaction in the strong coupling regime [8].

In summary, however, electronic states and phononic states in the model eq.(1) without the electron-electron interaction are smilar to those in the periodic Anderson-Holstein model without the Coulomb interaction, behavior in the model eq.(1) with the electron-electron interaction are contrast to that in the periodic Anderson-Holstein model with the Coulomb interaction.

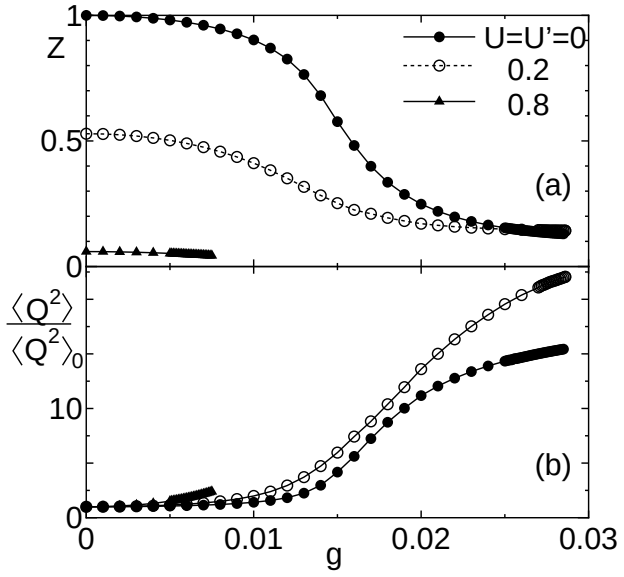

Fig. 1. The quasiparticle weight Z, and the lattice fuluctuation $\langle Q^2\rangle/\langle Q^2\rangle_0$ as a function of electron-phonon coupling constant g for several values of the intra-Coulomb interaction U. $\langle Q^2\rangle_0$ is the value for $g = 0$.

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