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Rattling-Induced Heavy Fermion State in the Anharmonic Holstein Model

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We investigate the heavy fermion states in the half-filled anharmonic Holstein model by using the dynamical mean-field theory combined with the exact diagonalization method at low temperatures down to $1/10^4$ of the conduction bandwidth. For the weak anharmonic cases with single-well or shallow double-well potentials, the bipolaronic first order phase transition takes place at a critical value of the electron-phonon coupling below a critical temperature as recently observed in the harmonic Holstein model. On the other hand, for the strong anharmonic case with deep double-well potential, the bipolaronic transition is suppressed and changes to a crossover where the heavy fermion state with a large effective mass is realized due to the effect of largely anharmonic local oscillations called rattling.

KEYWORDS: polarons, bipolarons, bipolaronic transition, Holstein model, rattling, anharmonic potential, heavy fermion

Recently, an interesting phenomenon is found in the filled skutterudite compound $SmOs_4Sb_{12}$ where the heavy fermion behavior is robust against external magnetic fields.[1)] Since a heavy fermion state is generally formed by a spin-dependent mechanism, this phenomenon implies an unconventional mechanism for the heavy fermion system, and has attracted much attention. To explain the phenomenon, several theoretical studies have been done previously.[2–4)] One of the ideas is suggested that the multipole made from the local f-electrons of Sm plays an important role.[5)] Since higher-rank multipoles do not directly couple with the magnetic field generally, the multipole Kondo effect is not easily suppressed by the magnetic field. Then, considering the multipole Kondo effect, the magnetically robust heavy fermion state can be explained compatibly.

Here, we want to point out another way to understand the phenomenon that the rattling, large amplitude anharmonic local vibrations of an ion in a cage structure, leads to the heavy fermion state. The electron-phonon interaction and the anharmonicity of a potential are important effects for the discussion about rattling, and these effects have been studied as a possible mechanism of heavy fermion state for a long time. The theory of electron-phonon interaction has been developed through the standard model suggested by Anderson,[6,7)] which becomes equivalent to the two level system (TLS) problem in a strong electron-phonon coupling region,[8)] since the effective potential of phonons becomes double-well anharmonic type. Furthermore, especially at low temperature, it is known that the TLS can be treated the same as the Kondo model with spin $S = 1/2$, in which heavy fermion states are suggested.[9)]

The TLS and the TLS like problems are extensively studied, and many results of the possibilities of heavy fermion state are shown in there.[3,10)] However, a few discussions have been given for the heavy fermion state in the periodic model in which we can treat the electron-phonon coupling and the anharmonicity of a potential, such as the Holstein model. In the present work, in order to discuss the possibility of a heavy fermion state induced by the rattling, we study the anharmonic Holstein model, which contains the effects of both the electron-phonon coupling and the anharmonicity of a potential, at low temperatures down to $1/10^4$ of the conduction bandwidth.

The anharmonic Holstein model is given by the following Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + g \sum_i \sqrt{2M\omega_0} Q_i \left(\sum_\sigma n_{i\sigma} - 1 \right) + \sum_i \frac{{P_i}^2}{2M} + \frac{1}{2} M {\omega_0}^2 \sum_i \left(\alpha {Q_i}^2 + \beta {Q_i}^4 \right), \quad (1)$$

where $c^\dagger_{\mathbf{k}\sigma}$ ($c^\dagger_{i\sigma}$) is a creation operator for a conduction electron with wave vector $\mathbf{k}$ (site i) and spin σ, and $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. $b^\dagger_i$ is a creation operator for a phonon at site i, where the lattice displacement operator is given by $Q_i = (b^\dagger_i + b_i)/\sqrt{2M\omega_0}$. $\epsilon_{\mathbf{k}}$, M, ω_0, g, α and β are the energy for a conduction electron, the mass of oscillating ions, the frequency of the local bare Einstein phonons, the electron-phonon coupling strength, the coefficients of the second and fourth order terms for the potential of oscillating ions, respectively. The 4th term of the Hamiltonian describes anharmonic potential of bare phonon, in which we can treat several types of potential characterized by parameters α and β.

To solve the model eq.(1), we use the dynamical mean field theory (DMFT)[11)] in which the model is mapped onto an effective impurity anharmonic Anderson-Holstein model.[12)] The semielliptic density of state for the bare conduction band with the bandwidth $W = 1$ is given as $\rho(\epsilon) = 4\sqrt{1 - 4\epsilon^2}/\pi$. Then, the local electron Green's function $G(i\omega_n)$ satisfies the following self-consistency condition, $\mathcal{G}_0(i\omega_n)^{-1} = i\omega_n - \mu - (W/4)^2 G(i\omega_n)$, where μ is the chemical potential and

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$\mathcal{G}_0(i\omega_n)$ is the bare local electron Green's function for the effective impurity Anderson model with $g = 0$ in an effective medium which will be determined self-consistently. The effective impurity Anderson model with finite g is solved by using the exact diagonalization method for a finite-size cluster to obtain $G(i\omega_n)$ at finite temperature $T > 0$. In the present paper, we use the 5-site cluster and the cutoff of phonon number is set to be 12. We note that the numerical results for the 6-site cluster are almost the same as those for the 5-site cluster, and that the 15 phonons lead to almost the same results as the 12 phonons. We concentrate our attention on the particle-hole symmetric case at half-filling with $\langle n_i\rangle = \langle\sum_\sigma n_{i\sigma}\rangle = 1$, and we set $\omega_0 = 0.1$. Likewise we restrict ourselves to the case with the normal state without any symmetry breaking.

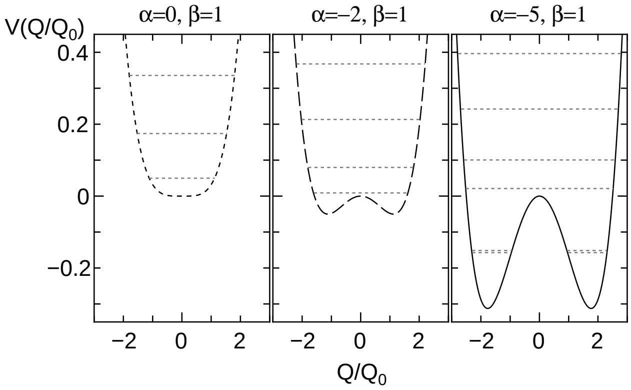

Fig. 1. The bare phonon potential $V(Q/Q_0)$ for $\alpha = 0, -2, -5$ and $\beta = 1$ fixed. The dotted lines in the potential well indicate the bare phonon energy levels.

In this paper, we show the results for three bare phonon potentials $\alpha = 0,\ -2,\ -5$ with a fixed $\beta = 1$. In the case of $\alpha = 0, -2$ and -5, the bare phonon potential $V(Q/Q_0)$ given in the last term of the r.h.s. in eq.(1) is a flat-well type, a shallow double-well type, and a deep double-well type, respectively, as shown in Fig.1, where ${Q_0}^2 = \langle Q^2\rangle_0 = 1/2\omega_0$ is the value for the zero-point oscillation with $\alpha = 1$ and $\beta = g = 0$. Thus, we can consider α as an anharmonicity parameter. Here, for the following discussion, we want to emphasize that a quasi-degenerate ground state is formed due to the double-well type potential for $\alpha = -5$.

In Fig.2 (a), we show the g dependence of the square root of the normalized local lattice fluctuation $\sqrt{\langle Q^2\rangle/\langle Q^2\rangle_0}$ for several α and $T = 0.0025$. For $\alpha = 0$ and -2, when g increases, $\langle Q^2\rangle$ increases gradually for small g, while it does steeply at $g = g_{\rm cr} \sim 0.425$ for $\alpha = 0$ and at $g_{\rm cr} \sim 0.275$ for $\alpha = 2$. In these cases $\langle Q^2\rangle$ finally shows a linear increase for large g. At $g \sim g_{\rm cr}$, the solutions for the small and large lattice fluctuation coexist. In this coexistence region, the system shows a first order bipolaronic phase transition as recently observed in the harmonic case with $\alpha = 1$, $\beta = 0$.[13)] On the other hand, for $\alpha = -5$, we can see that the bipolaronic transition is suppressed and changes to a crossover. It is also found

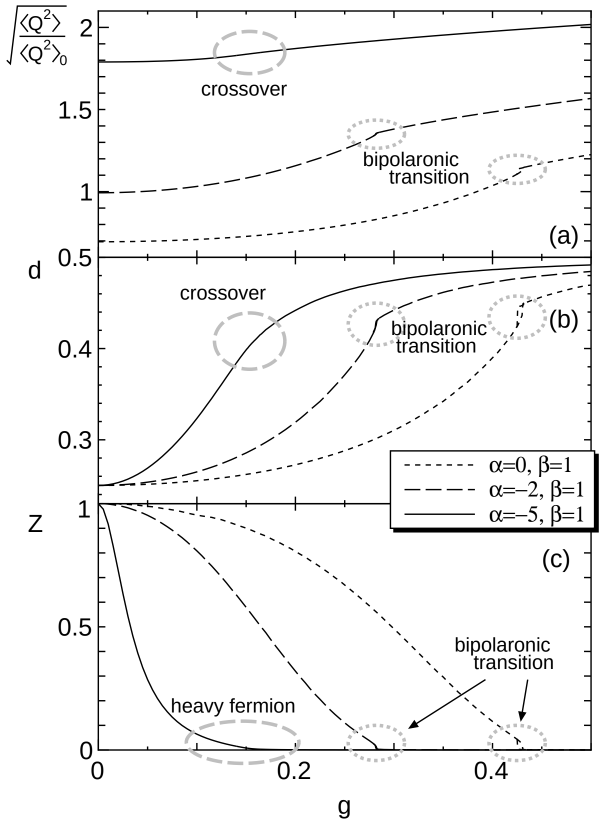

Fig. 2. The square root of the normalized local lattice fluctuation $\sqrt{\langle Q^2\rangle/\langle Q^2\rangle_0}$ (a), the double occupancy d (b), and the renormalization factor Z (c) as functions of the electron-phonon coupling g for $\alpha = 0, -2$ and -5, $\beta = 1$, $T = 0.0025$.

that the first order bipolaronic phase transition point $g_{\rm cr}$ (or the crossover point) decreases as α gets more negative value, namely as the anharmonicity is enhanced.

In Fig.2 (b), we plot another typical physical quantity, the double occupancy $d = \langle n_\uparrow n_\downarrow\rangle$ as a function of g for several α and $T = 0.0025$. Here, we can see the behaviors similar to those shown in Fig.2 (a), such as the first order bipolaronic phase transition for the weak anharmonicity cases $\alpha = 0, -2$ and the crossover for the strong anharominicity case $\alpha = -5$.

In Fig.2 (c), the renormalization factor $Z = (1 - d\Sigma(\omega)/d\omega|_{\omega=0})$ is plotted as a function of g for several α and $T = 0.0025$, where $\Sigma(\omega)$ is the self-energy calculated from the Green's function. For the weak anharmonicity cases $\alpha = 0$ and -2, Z decreases gradually with increasing g, and then becomes to zero at $g_{\rm cr}$, at which the bipolaronic transition occurs. On the other hand, for the strong anharmonicity case $\alpha = -5$, a steep decrement of Z is shown with increasing g, while it changes to a gradually decrement showing a tail like behavior in the area around the crossover.

Here, we focus on the behavior of Z as an aspect of a heavy fermion state. Z means a renormalization effect of a conduction electron in general. It corresponds to the effective mass as $m^*/m = Z^{-1}$ at zero temperature, that is, small Z indicates the heavy electron mass. For the weak anharmonicity cases, small Z leading to a heavy fermion state is seen only near the transition point in the weak coupling side $g < g_{\rm cr}$, while $Z = 0$ resulting in the disappearance of the quasi-particles is observed in the strong coupling side $g > g_{\rm cr}$. A similar behavior of Z has also been observed in the Hubbard model,[11] where small Z is observed in a narrow parameter region in the vicinity of the Mott metal-insulator transition as similar to the cases with the harmonic[13] and weak-anharmonic Holstein models where small Z is observed in a narrow parameter region in the vicinity of the bipolaronic transition. In contrast, the Holstein model with the strong anharmonic phonons shows small Z in a wide parameter region around the crossover as shown in Fig.2 (c), where the heavy fermion state is remarkably stabilized.

Previously, a similar heavy fermion behavior due to the electron-phonon interaction was reported in the periodic Anderson-Holstein model,[14] in which the local f electrons couple to the (harmonic) local phonons and hybridize with the conduction electrons. In this model, the large entropy due to the local charge (valence) degrees of freedom of f electrons is responsible for the large effective mass in the heavy fermions state realized in a wide parameter region for the strong electron-phonon coupling. This is a striking contrast to the case with the usual periodic Anderson model where the large entropy due to the local spin degrees of freedom of f electrons is responsible for the large effective mass in the heavy fermion state realized for the strong Coulomb interaction between f electrons.

When the bare phonon potential is double-well type as shown in Fig.1 with $\alpha = -5$, the bare phonon energy levels show quasi-degenerate groundstates which correspond to the left-well and the right-well states. Then, the large entropy due to the local phonon degrees of freedom with the double-well potential is responsible for the large effective mass in the heavy fermions state realized in a wide parameter region for the intermediate electron-phonon coupling regime in the strong-anharmonic Holstein model as shown in Fig.2 (c). As for the the cases with the harmonic[13] and weak-anharmonic Holstein models, the effective phonon potential which is renormalized due to the effect of the electron-phonon coupling becomes double-well type in the strong coupling regime. In these cases, the system shows the bipolaronic transition in stead of the heavy fermion state as the conduction electrons are strongly coupled to the effective double-well potential resulting in the infinite quasi-particle mass $m^*/m = Z^{-1} = \infty$ with $Z = 0$. On the contrary, in the strong-anharmonic Holstein model, the double-well potential is preformed for the non-interacting case and the intermediate electron-phonon coupling yields the heavy-fermion state where Z is small but finite. Therefore, the anharmonicity is crucial to obtain the heavy-fermion state in a wide parameter region in the Holstein model.

In summary, we investigate the half-filled anharmonic Holstein model by using the dynamical mean field theory combined with the exact diagonalization method. We found that, for the weak anharmonic cases, the bipolaronic first order phase transition takes place at a critical value of the electron-phonon coupling g where the physical quantities show discontinuities. While for the strong anharmonic case, the bipolaronic transition is suppressed and changes to a crossover where the heavy fermion state with a large effective mass $m^*/m = 1/Z$ is realized due to the effect of the rattling. A more detailed discussion will be given in a subsequent paper. The calculation for the ordered states, such as a charge density wave state, is now under the way.

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