Heavy Ferminos and Rattling Motions in the Periodic Anderson-Holstein Model

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Abstract

We investigate a heavy fermion behaviour and a deformation of an effective potential fo the ions due to electron-phonon interaction for the the periodic Anderson-Holstein model by using the dynamical mean-field theory combined with the exact diagonalization method. For the strong electron-phonon coupling, the system shows an anomalous heavy fermion behaviour with a large lattice fluctuation and an extreme phonon softening, and then an effective potential for the ions changes from a simple harmonic potential for the non-interacting case to a double-well potential for the strong electron-phonon coupling.

Key words: heavy fermion, electron-phonon interaction, rattling
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The A15 compounds such as V_3Si have long been attracted much interest as they show high T_c and high H_{c2} superconductivity as well as anomalously large resistivity and Debye-Waller factor. Yu and Anderson[1] originally proposed a local electron-phonon model where the strong electron-phonon coupling causes an effective double-well potential for the ion. As a strong coupling fixed point, the two-level Kondo systems were investigated to describe a heavy-fermion [2]. More recently, the local electron-phonon model have been extensively studied by using the NRG approach[3,4], but periodic (lattice) models were not discussed there.

Recently, another interesting class of materials has been observed in the filled skutterdites such as $PrOs_4Sb_{12}$[5] and the clathrates such as $Ce_3Pa_{20}Ge_6$[6], where the rare-earth ion shows a rattling motion under a potential with several off-center minima. With the new findings, theoretical studies on a periodic Anderson model coupled with local phonons, *i.e.*, the periodic Anderson-Holstein model are highly desirable. The purpose of this paper is to present the results of the dynamical mean-filed theory (DMFT) for the periodic Anderson-Holstein model to elucidate the effect of the strong electron-phonon coupling on the heavy-fermion behaviour and the effective potential for the ions.

Our Hamiltonian is given by

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

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, V, U and g, are 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

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phonons whose frequency is ω_0.

To solve this model eq.(1), we use the DMFT in combination with the exact diagonalization (ED) method[7]. In the DMFT, the model eq.(1) is mapped onto an effective single impurity Anderson-Holstein model[8,9], because the self-energy $\Sigma(\mathrm{i}\omega_n)$ becomes purely site-diagonal in infinite dimensions. Then we use the ED method for a finite-size cluster[9,10] to solve the impurity Anderson-Holstein model. All calculations are performed at $T = 0$, and we replace the Matsubara frequencies by a fine grid of imaginary frequencies $\omega_n = (2n+1)\pi/\tilde{\beta}$ with a fictitious inverse temperature $\tilde{\beta}$ which determines the energy resolution. The calculations are performed for 8-site and $\tilde{\beta} = 4000$ at half-filling, and we define the cutoff of phonon number is 30 [11]. In the following numerical results, we set $\omega_0 = 0.05$ and $U = 0$.

The quasiparticle weight, $Z = (1 - \frac{\mathrm{d}\Sigma(\omega)}{\mathrm{d}\omega}|_{\omega=0})^{-1}$, is plotted as a function of g for $V = 0.2$ and 0.15 in Fig.1(a). Z decreases with increasing g and becomes extremely small but finite for the strong coupling where the mass enhancement factor $m^*/m = Z^{-1}$ becomes more than one hundred. Thus we can conclude that the periodic Anderson-Holstein model eq.(1) shows heavy-fermion behaviour due to the strong electron-phonon coupling in the wide parameter range. This is a striking contrast to the Holstein-Hubbard model [8,9].

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. In the heavy fermion regime, we can see the extreme enhancement of the lattice fluctuation accompanied by the enhancement of the local charge fluctuation. We calculate the phonon spectral function and find that the multi-phonon state appears and the lowest excited energy, $\tilde{\omega}_0$, shifts to low energy with increasing g. A remarkable soft phonon mode with $\tilde{\omega}_0 \approx 0$ is observed in the heavy fermion regime as shown in the Fig.1(c).

The large lattice fluctuation and the extreme phonon softening can be explained by thinking in terms of an effective potential for the ions. Therefore we introduce a variational wave function for the ions[4], $|\Psi_v(Q)|^2 = A\exp[-(Bq^2 + Cq^4 + Dq^6 + Eq^8)]$, with $q \equiv Q/Q_0$. The coefficients A, B, C, D and E are the variational parameters which will be determined to make $\langle Q^{2n}\rangle = \int Q^{2n}|\Psi_v(Q)|^2\mathrm{d}Q$ $(n = 0, 1, 2, 3, 4)$ as close to $\langle Q^{2n}\rangle$ from the DMFT as possible. Then we define the effective potential for the ions, $V_{\mathrm{eff}}(Q) = \log[|\Psi_v(0)|^2/|\Psi_v(Q)|^2]$.

An effective potential for the ions has simple harmonicity in the non-interacting case but deforms to double-well in the heavy fermion regime as shown in Fig.2. This behaviour has already been observed in the previous theories [1,3,4] where the local electron-phonon model was discussed in contrast to the present theory where the periodic (lattice) model is discussed.

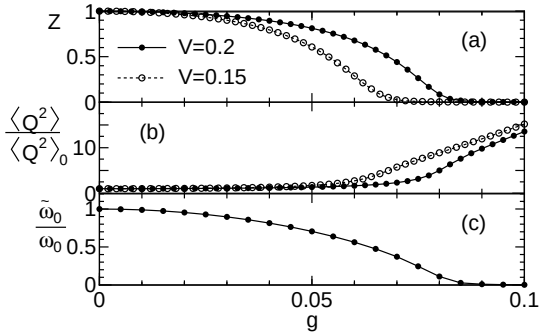

Fig. 1. The quasipaticle weight Z, the lattice fluctuation $\frac{\langle Q^2\rangle}{\langle Q^2\rangle_0}$ and the lowest excited energy of the phonon spectral function $\tilde{\omega}_0$ as functions of the electron-phonon coupling g for $V = 0.2$ (filled circles) and $V = 0.15$ (open circles). $\langle Q^2\rangle_0$ and ω_0 are the corresponding value for $g = 0$

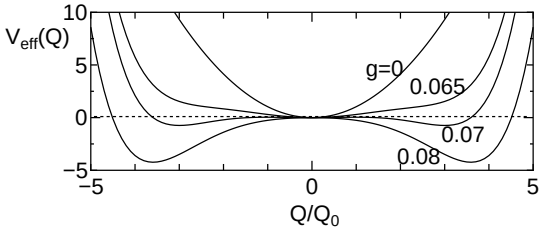

Fig. 2. The effective potential for the ions $V_{\mathrm{eff}}(Q)$ for several values of g at $V = 0.15$.

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