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Heavy fermions and superconductivity in the periodic Anderson-Holstein model

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Recent discovery of rattling motions in the filled skutterdites such as $PrOs_4Sb_{12}$ [1] and the clathrates such as $Ce_3Pa_{20}Ge_6$ [2] has stimulated much interest in the strong coupling of Einstein phonons to electrons in heavy-fermion systems. The simplest realization of such systems is the periodic Anderson-Holstein model where the Einstein phonons at each site couple to the local (f-) electrons which hybridize with the conduction electrons. We study this model on the basis of the dynamical mean-field theory in which the effective impurity Anderson-Holstein model is solved by using the exact diagonalization method [3]. Our Hamiltonian is given by

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

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, g and ω_0 are the atomic f-level, the c-f mixing, the on-site Coulomb interaction, the electron-phonon coupling strength and the phonon frequency, respectively. We assume a semielliptic DOS for the bare conduction band with the half-bandwidth $W = 1$.

As shown in Fig.1(a), for the strong electron-phonon coupling $g \gtrsim g_c$, the system shows an anomalous heavy-fermion behaviour which is accompanied by a large lattice fluctuation and an extreme phonon softening. We also calculate an effective potential for the ions and find that a simple harmonic potential for $g \lesssim g_c$ changes into a double-well potential for $g \gtrsim g_c$ (Fig.1(b)). The effective pairing interaction between the conduction electrons Γ_c has a maximum at $g \approx g_c$ where the superconducting transition temperature is expected to show a peak (Fig.1(c)).

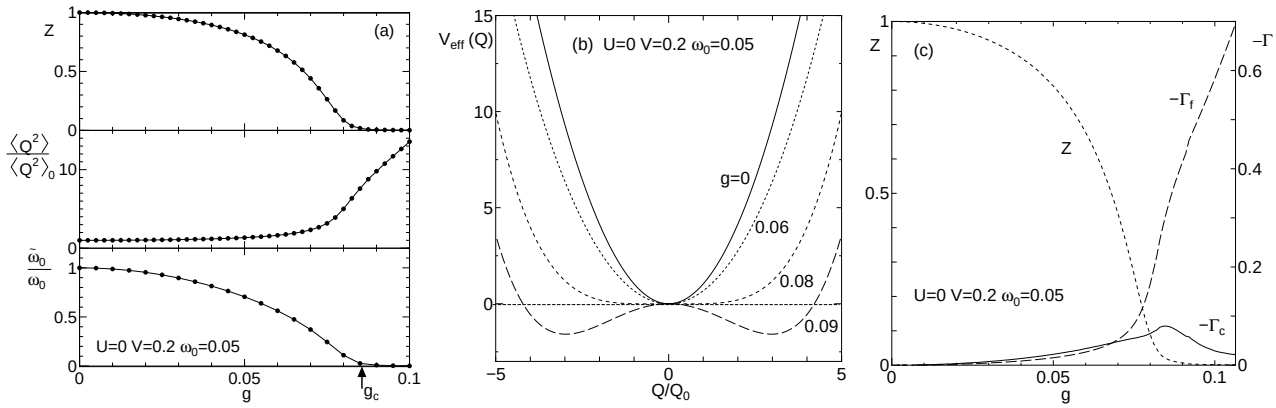

Figure 1: (a) The quasiparticle weight Z ($= m/m^*$), the lattice fluctuation $\langle Q^2 \rangle$ and the lowest excited energy of the phonons $\tilde{\omega}_0$. (b) The effective potential for the ions $V_{\rm eff}(Q)$ for several values of g. (c) The vertex function for f-electrons Γ_f and that for c-electrons Γ_c.

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[2] Y. Nemoto, T. Yamaguchi, T. Horino, M. Akatsu, *et al.*, Phys. Rev. B**68** (2003) 184109.
[3] W. Koller, D. Meyer, Y. Ōno and A. C. Hewson, Europhys. Lett. **66** (2004) 559.