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2003 J. Phys.: Condens. Matter 15 S2215

(http://iopscience.iop.org/0953-8984/15/28/354)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) S2215–S2218 PII: S0953-8984(03)62799-2

Effects of degenerate orbitals on the Anderson lattice model

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Received 12 November 2002
Published 4 July 2003
Online at stacks.iop.org/JPhysCM/15/S2215

Abstract

We investigate the effects of degenerate orbitals on the periodic Anderson model by means of the dynamical mean field theory. A new formulation is proposed for the effective impurity problem where the corresponding action is represented by two distinct formulae. This enables us to perform the self-consistent calculation efficiently. Upon introducing the inter-orbital interaction among conduction electrons, the charge gap in the Kondo insulator is increased once and then decreased. Eventually, the Kondo insulator is driven to an ordinary Mott–Hubbard insulator.

Most of interesting phenomena in rare-earth heavy-fermion compounds may be described by the simple periodic Anderson lattice model, which is given by itinerant conduction electrons and localized f electrons. However, it was pointed out that in some uranium-based compounds, the multi-orbital effects may be important for explaining anomalous magnetic response data [1]. Also, it was recently suggested that the multi-orbital conduction electrons with a localized array of moments may be relevant for heavy-fermion behaviour in the transition metal compound LiV_2O_4 [2, 3]. Therefore, it is desirable to investigate the effects of multi-orbitals on the Anderson lattice model for such heavy-fermion systems.

We consider a correlated electron system coupled to the localized f electrons, which is described by the two-orbital Anderson lattice model:

$$H = \sum_{(ij),\alpha,\sigma} t_{ij} c^{\dagger}_{i\alpha\sigma} c_{j\alpha\sigma} + U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + U' \sum_{i,\sigma,\sigma'} n_{i1\sigma} n_{i2\sigma'} + \sum_{i,\sigma} E_F f^{\dagger}_{i\sigma} f_{i\sigma} + \sum_{i,\alpha,\sigma} V (c^{\dagger}_{i\alpha\sigma} f_{i\sigma} + f^{\dagger}_{i\sigma} c_{i\alpha\sigma}) + U'' \sum_{i} n_{fi\uparrow} n_{fi\downarrow}, \quad (1)$$

where $c_{i\alpha\sigma}$ ($f_{i,\sigma}$) annihilates an electron with spin σ and orbital α (f electron with spin σ) at the ith site. Conduction electrons are assumed to have the intra-orbital (inter-orbital) interaction U (U'), and hybridize with localized f electrons having the f–f interaction U''.

To discuss the effects of degenerate orbitals on the Anderson lattice model, we make use of the dynamical mean field theory (DMFT) [4, 5]. In this theory, the lattice model is mapped

onto an effective impurity model, where local electron correlations can be taken into account precisely. We propose here a new formulation of the impurity problem, based on the fact that the interactions in the Hamiltonian equation (1) are divided into two parts for conduction electrons and f electrons. This observation allows us to embed the original model into the effective impurity model in two distinct ways. That is, we represent the effective action S_{eff} by two formulae:

$$S_{eff}[i] = -\sum_{\sigma}\int_0^\beta d\tau \int_0^\beta d\tau' \, c^\dagger_{i\alpha\sigma}[G_0^{(c)}]^{-1}_{\alpha\beta}c_{i\beta\sigma} + \int_0^\beta d\tau \left[U\sum_{\alpha} n_{i\alpha\uparrow}n_{i\alpha\downarrow} + U'\sum_{\sigma,\sigma'} n_{i1\sigma}n_{i2\sigma'}\right]$$
$$= -\sum_{\sigma}\int_0^\beta d\tau \int_0^\beta d\tau' \, f^\dagger_{i\sigma}[G_0^{(f)}]^{-1}f_{i\sigma} + \int_0^\beta d\tau \, U'' n_{fi\uparrow}n_{fi\downarrow}, \tag{2}$$

where $G_0^{(c)}$ and $G_0^{(f)}$ are the bare Green functions in the reduced impurity problem. These actions can be described by standard Anderson models:

$$H^c_{imp} = \sum_{k,\alpha,\sigma}\epsilon_k^{(c)}a^\dagger_{k\alpha\sigma}a_{k\alpha\sigma} + \sum_{\alpha,\sigma}E_c c^\dagger_{\alpha\sigma}c_{\alpha\sigma} + \sum_{k,\alpha,\sigma}v_k^{(c)}(a^\dagger_{k\alpha\sigma}c_{\alpha\sigma} + c^\dagger_{\alpha\sigma}a_{k\alpha\sigma})$$
$$+ U\sum_{\alpha} n^c_{\alpha\uparrow}n^c_{\alpha\downarrow} + U'\sum_{\sigma,\sigma'} n^c_{1\sigma}n^c_{2\sigma'}, \tag{3}$$

$$H^f_{imp} = \sum_{k,\sigma}\epsilon_k^{(f)}b^\dagger_{k\sigma}b_{k\sigma} + \sum_{\sigma}E_f f^\dagger_\sigma f_\sigma + \sum_{k,\sigma}v_k^{(f)}(b^\dagger_{k\sigma}f_\sigma + f^\dagger_\sigma b_{k\sigma}) + U'' n^f_\uparrow n^f_\downarrow, \tag{4}$$

where $a_{k\alpha\sigma}$ and $b_{k\sigma}$ are the newly introduced annihilation operators for host electrons, and $\{\epsilon_k, v_k\}$ is the set of the energy levels and hybridizations to be determined self-consistently. The lattice Green function is given in terms of the self-energies Σ_c, Σ_c', and Σ_f due to U, U', and U'' as

$$G(k,z)^{-1} = \begin{pmatrix} z+\mu-\epsilon_k-\Sigma_c & -\Sigma_c' & -V \\ -\Sigma_c' & z+\mu-\epsilon_k-\Sigma_c & -V \\ -V & -V & z-E_F-\Sigma_f \end{pmatrix}. \tag{5}$$

By performing the summation over the wavenumber k, we obtain the full Green functions $G^{(f)}_{loc}$ and $G^{(c)}_{loc}$, where the semicircular density of states

$$\rho(x) = \frac{1}{N}\sum_k \delta(x-\epsilon_k) = \frac{2}{\pi D}\sqrt{1-\left(\frac{x}{D}\right)^2}$$

is used. Imposing the self-consistent conditions, $G^{(c)}_{loc} = G^{(c)}_{imp}$ and $G^{(f)}_{loc} = G^{(f)}_{imp}$, completes our DMFT formulation.

It is remarkable that the method proposed here has the advantage of treating the ground state properties of the system efficiently. In fact, when the impurity problem is solved, we can perform the exact diagonalization calculation for a much larger cluster size compared with that of the ordinary DMFT.

In this paper, we make use of the exact diagonalization method together with the cost function method proposed by Caffarel and Krauth [6]. We focus here on the symmetric model, and investigate the charge excitation gap Δ, which may reveal some essential effects due to the interactions. The results for the charge gap are shown in figure 1. In the following, we take the bandwidth D as the unit of energy. The charge gap is written approximately, in terms of the renormalization factors Z_c and Z_f, as

$$\Delta = \sqrt{Z_c^2 + 8Z_cZ_fV^2} - Z_c, \tag{6}$$

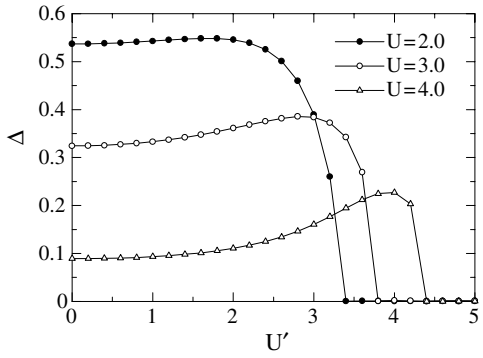

Figure 1. The charge gap as a function of the inter-band Coulomb interaction. We set $U = U''$ for simplicity.

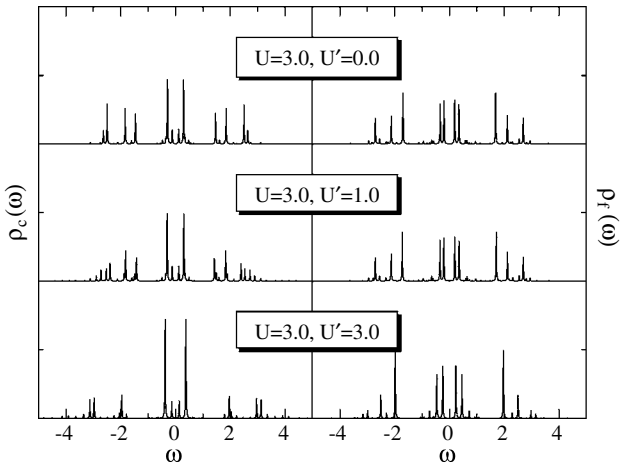

Figure 2. Densities of states ρ_c and ρ_f for $V = 0.5$ obtained by exact diagonalization with the clusters $N_c = 6 \times 2$ and $N_f = 10$, respectively.

where $Z_a^{-1} = 1 - \mathrm{d}\,\mathrm{Re}\,\Sigma_a/\mathrm{d}\omega$ (subscript $a = c$ or f). In the case where $U' = 0$, the system belongs to the Kondo insulating phase with the reduced charge gap in the presence of the f–f interaction U''. This kind of renormalization is also caused by the Hubbard-type interaction U for conduction electrons, as seen in figure 1. On the other hand, the inter-band interaction U' for conduction electrons causes somewhat different effects: the charge gap is increased up to $U' \sim U$, and then decreased. The slight increment in the charge gap may be due to charge fluctuations induced by U'. As discussed below, $\Delta = 0$ means that the sharp peak in the density of states of the Kondo insulator disappears, and the system is driven to another insulating phase of Mott–Hubbard type.

Some of the above properties are indeed seen in the densities of states for conduction electrons (ρ_c) and f electrons (ρ_f) computed by exact diagonalization, as shown in figure 2. As U' increases from zero, the density of states is enhanced around the Fermi surface. This suggests that orbital fluctuations induced by U' among conduction electrons reduce the correlation effects caused by U, making the Kondo-type renormalization somewhat weaker. Beyond $U' \sim U$, however, the charge gap is decreased rapidly, as already mentioned in figure 1. Eventually, the charge gap of the Kondo insulator vanishes at a certain critical value, inducing

a transition from the Kondo insulator to the Mott–Hubbard insulator. In this region ($U' > U$), the Mott–Hubbard gap solely characterizes the nature of the insulating phase.

In summary, we have investigated the effects of degenerate orbitals on the Anderson lattice model. We have proposed a new formulation of the effective impurity problem in the DMFT, for which the effective action is represented by two distinct formulae. This makes the self-consistent calculation much more efficient. It has been clarified that the inter-band interaction among conduction electrons causes a non-monotonic renormalization effect on the charge gap, which eventually drives the Kondo insulator to a Mott–Hubbard insulator. The results are consistent with those discussed in the degenerate Hubbard model, where the inter-band Hubbard interaction gives rise to non-monotonic behaviour of the renormalized mass in the Fermi liquid phase [7, 8]. Dynamical properties and finite-temperature properties in the Anderson lattice with degenerate orbitals are interesting in connection with multi-channel Kondo effects; this is now under consideration.

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