Periodic Anderson model with d-f interaction

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We investigate an extended version of the periodic Anderson model where an interaction is switched on between the doubly occupied d- and f-sites. We perform variational calculations using the Gutzwiller trial wave function. We calculate the f-level occupancy as a function of the f-level energy with different interaction strengths. It is shown that the region of valence transition is sharpened due to the new interaction.

I. INTRODUCTION

The heavy-fermion phenomenon, which is observable in many rare-earth materials is still an active field of researched area. The simplest model, which can account for these phenomena is the periodic Anderson model. For a review on this topic see [1–3]. The model in its simplest form describes a hybridization (v) between a wide conduction band and correlated f-electrons localized at lattice sites. Despite its simple form there is no general solution to this problem, exact solutions have been obtained only in some special cases [4]. Nonperturbative approaches like variational methods [5–9] are applicable even if the Coulomb interaction (U_f) between the f-electrons is large, though we have to use some uncontrolled approximation when calculating the expectation values. In a recent paper [10] it was shown that the repulsion between the d- and f-electrons plays an important role in valence transition. It has been argued that the sudden change of valence of Ce can account for the presence of a sharp peak in the transition temperature of some superconducting Ce based compounds. The effects of this new interaction have been examined with dynamical mean field theory [11–13], slave-boson method [10, 14], variational Monte Carlo technique [15] and projector-based renormalization approach [16]. It has been found in these papers that intermediate valent region narrows in the presence of d-f coupling.

In this paper we examine the ground state properties of this extended model using the Gutzwiller method. However, the conventional d-f interaction

$$U_{df} \sum_{j,\sigma,\sigma'} \hat{n}^f_{j\sigma} \hat{n}^d_{j\sigma'} \tag{1}$$

is too difficult to handle within the framework of this method, so we consider a modified d-f interaction

$$\widetilde{U}_{df} \sum_{j} \hat{n}^f_{j\uparrow} \hat{n}^f_{j\downarrow} \hat{n}^d_{j\uparrow} \hat{n}^d_{j\downarrow}, \tag{2}$$

where electrons repel each other only when site j is fully occupied. The reason for this modification is that it can be treated easier, since much less electron configurations need to be taken into account.

II. VARIATIONAL CALCULATION

We summarize the main steps of the performed variational calculation following Ref. [17]. For simplicity in the present work we restrict ourselves to a nonmagnetic half-filled band, although the variational procedure can be carried out without these assumptions. Assuming that there are $N_\uparrow = N_\downarrow$ up- and down-spin electrons in an arbitrary dimensional lattice with L lattice sites, we consider the following Hamiltonian:

$$\mathcal{H} = \sum_{\boldsymbol{k},\sigma} \varepsilon_d(\boldsymbol{k}) \hat{d}^\dagger_{\boldsymbol{k},\sigma} \hat{d}_{\boldsymbol{k},\sigma} - v \sum_{\boldsymbol{j},\sigma} \left(\hat{f}^\dagger_{\boldsymbol{j},\sigma} \hat{d}_{\boldsymbol{j},\sigma} + \hat{d}^\dagger_{\boldsymbol{j},\sigma} \hat{f}_{\boldsymbol{j},\sigma} \right)$$
$$+ \epsilon_f \sum_{\boldsymbol{j},\sigma} \hat{n}^f_{\boldsymbol{j},\sigma} + U_f \sum_{\boldsymbol{j}} \hat{n}^f_{\boldsymbol{j}\uparrow} \hat{n}^f_{\boldsymbol{j}\downarrow} + \widetilde{U}_{df} \sum_{\boldsymbol{j}} \hat{n}^f_{\boldsymbol{j}\uparrow} \hat{n}^f_{\boldsymbol{j}\downarrow} \hat{n}^d_{\boldsymbol{j}\uparrow} \hat{n}^d_{\boldsymbol{j}\downarrow}, \tag{3}$$

where $\hat{n}^f_{\boldsymbol{j},\sigma} = \hat{f}^\dagger_{\boldsymbol{j},\sigma} \hat{f}_{\boldsymbol{j},\sigma}$, and $\hat{n}^d_{\boldsymbol{j},\sigma} = \hat{d}^\dagger_{\boldsymbol{j},\sigma} \hat{d}_{\boldsymbol{j},\sigma}$. The symbol $\boldsymbol{k}$ denotes the wave vector, and $\boldsymbol{j}$ the site index. The width of the d-band is W. The trial wave function of Gutzwiller-type is expressed as

$$|\Psi\rangle = \hat{P}^{df}_{\mathrm{G}} \hat{P}^f_{\mathrm{G}} \prod_{\boldsymbol{k}} \prod_{\sigma} [u_{\boldsymbol{k}} \hat{f}^\dagger_{\boldsymbol{k},\sigma} + v_{\boldsymbol{k}} \hat{d}^\dagger_{\boldsymbol{k},\sigma}] |0\rangle, \tag{4}$$

where the mixing amplitudes $u_{\boldsymbol{k}}/v_{\boldsymbol{k}}$ are also variational parameters, and $\hat{P}^{df}_{\mathrm{G}}$ and $\hat{P}^f_G$ are the Gutzwiller projectors, which are written down as follows:

$$\hat{P}^{df}_{\mathrm{G}} = \prod_{\boldsymbol{j}} [1 - (1 - \eta_{df}) \hat{n}^f_{\boldsymbol{j}\uparrow} \hat{n}^f_{\boldsymbol{j}\downarrow} \hat{n}^d_{\boldsymbol{j}\uparrow} \hat{n}^d_{\boldsymbol{j}\downarrow}], \tag{5}$$

$$\hat{P}^f_{\mathrm{G}} = \prod_{\boldsymbol{j}} [1 - (1 - \eta_f) \hat{n}^f_{\boldsymbol{j}\uparrow} \hat{n}^f_{\boldsymbol{j}\downarrow}], \tag{6}$$

where the variational parameters η_{df} and η_f are controlled by $\widetilde{U}_{df}$ and U_f, respectively. We use the so-called Gutzwiller approximation to evaluate the expectation values of the Hamiltonian. Optimizing the ground

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state energy density with respect to the mixing amplitudes, we obtain the following expression for that:

$$\mathcal{E} = \frac{1}{L} \sum_{\boldsymbol{k} \in \text{FS}} \left[q_d \epsilon_d(\boldsymbol{k}) + \tilde{\epsilon}_f - \sqrt{(q_d \epsilon_d(\boldsymbol{k}) - \tilde{\epsilon}_f)^2 + 4\tilde{v}^2} \right]$$
$$+ (\epsilon_f - \tilde{\epsilon}_f) n_f + \widetilde{U}_{df} \nu_{df} + U_f \nu_f, \tag{7}$$

where n_f is the average number of f–electrons per site, i.e.

$$n_f = \frac{1}{L} \left\langle \sum_{\sigma} \hat{n}^f_{\boldsymbol{j},\sigma} \right\rangle, \tag{8}$$

ν_f denotes the density of the doubly occupied f-sites and ν_{df} is the density of such sites when both the f- and d-

sites are doubly occupied, $\tilde{\epsilon}_f$ is the quasiparticle energy level of the f-electron (the effective f-level, its precise form is not presented here due to its lengthy form), $\tilde{v}$ denotes the renormalized hybridized amplitude, $\tilde{v} = \sqrt{q_d q_f} v$, and the summation is carried out over all wave numbers, $\boldsymbol{k}$, of electrons in the Fermi sea (FS). The q_d and q_f are the kinetic energy renormalization factors for the d-electrons and f-electrons respectively and are functions of n (the total numbers of electrons per site), n_f, ν_d (the density of the doubly occupied d-sites), ν_f, and ν_{df}. The determination of these quantities is the main task of the Gutzwiller method. Their forms in the present model are much more complicated than in those models which do not contain the interaction $\widetilde{U}_{df}$. The results are written in the following complete square (Gutzwiller-like) form:

$$q_f = \frac{1}{\frac{n_f}{2}\left(1 - \frac{n_f}{2}\right)} \left(\sqrt{\left(\frac{n_f}{2} - \nu_f\right)(1 - n_f + \nu_f)} + \sqrt{\frac{\left(\frac{n_f}{2} - \nu_f\right)(\nu_f - \nu_{df})(1 - \nu_f - \nu_d)}{1 - \nu_f}} + \sqrt{\frac{\nu_d \nu_{df} \left(\frac{n_f}{2} - \nu_f\right)}{1 - \nu_f}} \right)^2, \tag{9}$$

$$q_d = \frac{1}{\frac{n - n_f}{2}\left(1 - \frac{n - n_f}{2}\right)} \left(\sqrt{\left(\frac{n - n_f}{2} - \nu_{df} - \nu_d\right)(1 - n + n_f + \nu_d + \nu_{df})} + \sqrt{\frac{\nu_d \left(\frac{n - n_f}{2} - \nu_d - \nu_{df}\right)(1 - \nu_d - \nu_f)}{1 - \nu_d - \nu_{df}}} \right.$$
$$\left. + \sqrt{\frac{\nu_{df}(\nu_f - \nu_{df})\left(\frac{n - n_f}{2} - \nu_d - \nu_{df}\right)}{1 - \nu_d - \nu_{df}}} \right)^2, \tag{10}$$

where n is the total number of electrons per site, i.e. $n = \frac{1}{L} \left\langle \sum_{\boldsymbol{j},\sigma} \hat{n}^f_{\boldsymbol{j},\sigma} + \sum_{\boldsymbol{j},\sigma} \hat{n}^d_{\boldsymbol{j},\sigma} \right\rangle$. It is worth mentioning that without $\widetilde{U}_{df}$, q_f depends only on n_f and ν_f [17]. Since there is no direct hopping between the different f-sites, q_f appears only in the renormalized hybridized amplitude $\tilde{v} = \sqrt{q_d q_f} v$. It should be emphasized that q_d is not unity, i.e. the width of the d-band is narrowed, though there is no Coulomb repulsion between the d-electrons. It is also remarkable that the renormalization amplitude of the hybridization still can be written as the square root of the product of q_f and q_d in spite of this new interaction. These are the main results of this paper.

III. RESULTS

For further calculations we assume that the density of states of the d-band is constant, $\rho(\epsilon) = 1/W$, when ϵ is in the interval $[-W/2, W/2]$. Using this assumption the summation over the wave vectors in Eq. (7) can still be performed analytically. The ground state energy density thus obtained should be optimized with respect to ν_d, ν_f, ν_{df} and n_f. After this procedure we arrive at a non-

linear system of equations for these unknown quantities. We solve the obtained equations numerically. Typical results are shown in Fig. 1. One can see that switching
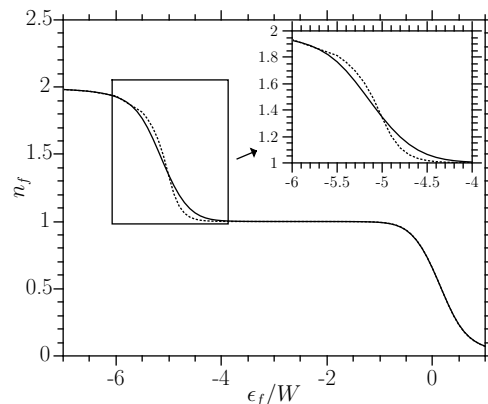

FIG. 1: The f-level occupancy as a function of the energy ϵ_f of the f-level at half-filling, $v/W = 0.1875$ and $U_f/W = 5$. The continuous and dotted curves belong to $\widetilde{U}_{df}/W = 0$ and 10, respectively. The inset shows the enlarged view of the framed region.

on $\widetilde{U}_{df}$ also results in the narrowing of the intermediate valent regime of $2> n_f >1$ as the conventional d-f interaction (see Eq.(1)) [10, 16], while no narrowing occurs in the region of $1> n_f >0$, since the d-f interaction we used is effective only when there are many doubly occupied f- and d-sites. The conventional d-f interaction significantly narrows the intermediate valent regime of $1> n_f >0$, too.

It is interesting to investigate the q_f renormalization factor, since it is related to the effective mass ($m^* \sim q_f^{-1}$). The results are shown in Fig. 2. The same effect can be seen here too, furthermore the heavy-fermion regime extends to smaller f-level energies.

In Fig. 3 the renormalization factor for the d-band is plotted. As it was outlined in Eq. (10) the d-electrons become correlated in the presence of $\widetilde{U}_{df}$, despite the fact that there is no direct d-d Coulomb interaction present in the model.
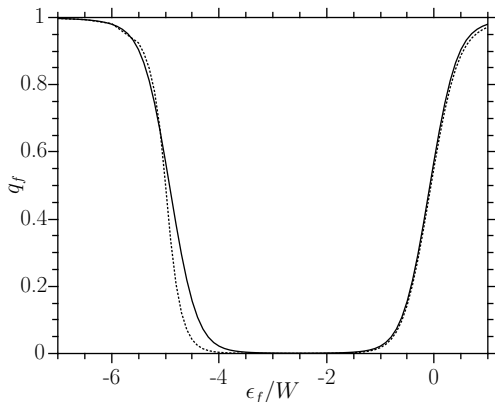

FIG. 2: The f-level renormalization factor as a function of the energy ϵ_f of the f-level at half-filling, $v/W = 0.1875$ and $U_f/W = 5$. The continuous and dotted curves belong to $\widetilde{U}_{df}/W = 0$ and 10, respectively.
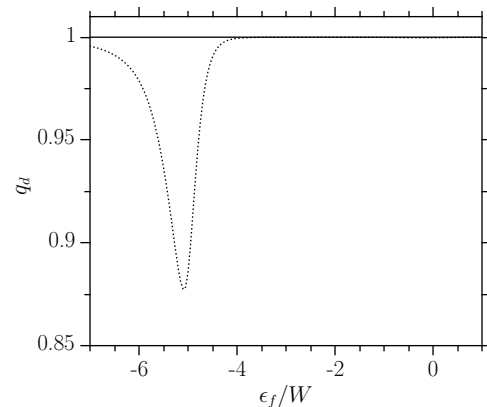

FIG. 3: The d-band renormalization factor as a function of the energy ϵ_f of the f-level at half-filling, $v/W = 0.1875$ and $U_f/W = 5$. The continuous and dotted curves belong to $\widetilde{U}_{df}/W = 0$ and 10, respectively.

IV. CONCLUSIONS

We have investigated an extended version of the usual periodic Anderson model, where an additional repulsive interaction among the d and f electrons was taken into account. We have shown analytically that the conduction band is narrowed owing to the new interaction. We have demonstrated that a finite $\widetilde{U}_{df}$ expands the regime of heavy-fermion character to a lower value of ϵ_f and narrows the intermediate valent regime at the same time. It is expected that the full d-f interaction (Eq. (1)) has an even sharper effect. The calculation is in progress.

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