Eur. Phys. J. B **52**, 345–353 (2006)
DOI: 10.1140/epjb/e2006-00303-x

THE EUROPEAN PHYSICAL JOURNAL B

Valence transition in the periodic Anderson model

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Received 14 November 2005 / Received in final form 12 July 2006
Published online 1st August 2006 –

Abstract. A very rich phase diagram has recently been found in $CeCu_2Si_2$ from high pressure experiments where, in particular, a transition between an intermediate valence configuration and an integral valent heavy fermion state has been observed. We show that such a valence transition can be understood in the framework of the periodic Anderson model. In particular, our results show a breakdown of a mixed-valence state which is accompanied by a drastic change in the f occupation in agreement with experiment. This valence transition can possibly be interpreted as a collapse of the large Fermi surface of the heavy fermion state which incorporates not only the conduction electrons but also the localized f electrons. The theoretical approach used in this paper is based on the novel projector-based renormalization method (PRM). With respect to the periodic Anderson model, the method was before only employed in combination with the basic approximations of the well-known slave-boson mean-field theory. In this paper, the PRM treatment is performed in a more sophisticated manner where both mixed as well as integral valent solutions have been obtained. Furthermore, we argue that the presented PRM approach might be a promising starting point to study the competing interactions in $CeCu_2Si_2$ and related compounds.

PACS. 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 71.27.+a Strongly correlated electron systems; heavy fermions – 75.30.Mb Valence fluctuation, Kondo lattice, and heavy-fermion phenomena

1 Introduction

Since the discovery [1] of a superconducting state formed by heavy quasi-particles in $CeCu_2Si_2$ this and related compounds have attracted a lot of scientific interest. Despite its long history only recently a whole variety of new physical phases has been observed which was possible by the intriguing development of experimental techniques. By substituting Si by Ge in the parent compound $CeCu_2Si_2$ a continuous change from a heavy fermion (HF) superconducting phase to an antiferromagentic state was observed [2]. An even more complex phase diagram has been found in pure $CeCu_2Si_2$ by applying high pressure [3,4]: there two superconducting phases with different pairing mechanisms have been found besides an antiferromagnetic and a HF phase. Furthermore, a transition between intermediate and integral valence states has been observed. (For a recent review on superconductivity in Ce based HF materials see Ref. [5].)

From the theoretical point of view the periodic Anderson model (PAM) is considered to be the basic microscopic model for the investigation of HF systems [6]. The PAM describes the interaction between localized, strongly correlated f and itinerant conduction electrons. In the limit of infinitely large Coulomb repulsion on f sites the PAM can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \tag{1}$$

$$\mathcal{H}_0 = \varepsilon_f \sum_{i,m} \hat{f}^\dagger_{im} \hat{f}_{im} + \sum_{\mathbf{k},m} \varepsilon_{\mathbf{k}}\; c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m},$$

$$\mathcal{H}_1 = \frac{1}{\sqrt{N}} \sum_{\mathbf{k},i,m} V_{\mathbf{k}} \left(\hat{f}^\dagger_{im} c_{\mathbf{k}m}\, e^{\mathrm{i}\mathbf{k}\mathbf{R}_i} + \mathrm{h.c.} \right).$$

Here, ε_f and $\varepsilon_{\mathbf{k}}$, both measured from the chemical potential, are the excitation energies of localized f and itinerant conduction electrons. As a simplification, often both types of electrons are assumed to have the same angular momentum index m with ν_f values, $m = 1...\nu_f$. The infinitely large local Coulomb repulsion is taken into account by Hubbard operators

$$\hat{f}^\dagger_{im} = f^\dagger_{im} \prod_{\tilde{m}(\neq m)} (1 - f^\dagger_{i\tilde{m}} f_{i\tilde{m}})$$

which enable either empty or singly occupied f sites.

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Due to the complexity of the PAM, most theoretical studies only focus on certain aspects of the rich phase diagrams of rare earth materials. Slave-boson mean-field (SB) methods, large-N expansions, and the dynamical mean-field theory [7] have been applied to discuss the interplay between RKKY and Kondo interactions. Thereby, a transition between an antiferromagnetic phase and a paramagnetic state was discussed. On the other hand, to describe the valence transition and HF superconductivity in $CeCu_2Si_2$ an extended PAM was studied. This model includes an additional Coulomb interaction between f and conduction electrons and was discussed within a slave-boson fluctuation approximation [4,8].

In this paper we apply a novel projector-based renormalization method (PRM) [9] to the PAM with the aim to address the question whether a valence transition, as experimentally observed in $CeCu_2Si_2$ [3,4], can occur in the plain model. For that purpose we extend in this paper our previous work on the PAM [10], which was restricted to the HF phase. The PRM provides a natural way to discuss the interplay of competing interactions which naturally emerge from the renormalization treatment of the PAM. Therefore, we believe that the PRM represents a suited approach for a deeper understanding of the rich phase diagram of $CeCu_2Si_2$ or of related compounds. However, in this paper we concentrate on the valence transition, nevertheless, we are able to sketch how superconducting phases and RKKY interactions could also be included in our approach.

This paper is organized as follows. In the next section we briefly describe the novel PRM approach [9] that is applied to the PAM in Section 3. Here, the Hubbard operators, introduced to take into account the infinitely large Coulomb repulsion on f sites, cause the main problems of any theoretical approach. It will turn out that the well-known SB theory [11,12] as well as our recent analytical approach based on the PRM [10] do not sufficiently prevent from unphysical states with doubly occupied f sites. In contrast, the modified PRM treatment of Section 3 strictly suppresses doubly occupied f sites by taking into account electronic correlations by means of the Hubbard operators. Results are presented in Section 4 where mixed valent as well as integral valent states are found, and a valence transition is observed. Furthermore, we compare our results with the solutions of the SB theory and our PRM approach of reference [10]. Finally, we summarize in Section 5.

2 Methodology

The PRM approach [9] starts from a decomposition of a given many-particle Hamiltonian, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where the perturbation $\mathcal{H}_1$ should not contain any terms that commute with the unperturbed part $\mathcal{H}_0$. Thus, $\mathcal{H}_1$ represents transitions between eigenstates of $\mathcal{H}_0$ with *different* eigenenergies. In the following, we assume that the eigenvalue problem of $\mathcal{H}_0$ is solved,

$$\mathcal{H}_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle.$$

A crucial idea of the PRM is the definition of projection operators by

$$\mathbf{P}_\lambda \mathcal{A} = \sum_{m,n} |n^{(0)}\rangle\langle m^{(0)}|\langle n^{(0)}|\mathcal{A}|m^{(0)}\rangle \times \Theta(\lambda - |E_n^{(0)} - E_m^{(0)}|). \quad (2)$$

Note that $\mathbf{P}_\lambda$ and $\mathbf{Q}_\lambda = \mathbf{1} - \mathbf{P}_\lambda$ are super-operators acting on ordinary operators $\mathcal{A}$ of the unitary space. $\mathbf{P}_\lambda$ projects on those parts of $\mathcal{A}$ which are formed by transition operators $|n^{(0)}\rangle\langle m^{(0)}|$ with energy differences $|E_n^{(0)} - E_m^{(0)}|$ less than a given cutoff λ. (λ is smaller than the cutoff Λ of the original model.) On the other hand, $\mathbf{Q}_\lambda$ projects on the high-energy transitions of an operator. Note, in particular, that in equation (2) neither $|n^{(0)}\rangle$ nor $|m^{(0)}\rangle$ have to be low-energy eigenstates of $\mathcal{H}_0$.

Next, an effective Hamiltonian $\mathcal{H}_\lambda$ is derived from the original Hamiltonian $\mathcal{H}$ by an unitary transformation

$$\mathcal{H}_\lambda = e^{X_\lambda}\, \mathcal{H}\, e^{-X_\lambda}\,, \quad (3)$$

where the anti-Hermitian generator of the transformation, $X_\lambda = -X_\lambda^\dagger$, shall be chosen in such a way that only transition operators (between eigenstates of $\mathcal{H}_0$) with transition energies less than the given cutoff λ contribute to $\mathcal{H}_\lambda$. Thus, the condition

$$\mathbf{Q}_\lambda \mathcal{H}_\lambda = 0 \quad (4)$$

must be fulfilled and will be used below to determine X_λ. Note that it is straightforward to evaluate equations (3) and (4) in perturbation theory [9]. However, using an appropriate ansatz for the generator X_λ, the effective Hamiltonian $\mathcal{H}_\lambda$ can also be calculated in non-perturbative manner.

A renormalization scheme can be derived if the elimination procedure for the interaction $\mathcal{H}_1$ is not performed in one step but rather a sequence of unitary transformations of the form

$$\mathcal{H}_{(\lambda-\Delta\lambda)} = e^{X_{\lambda,\Delta\lambda}}\, \mathcal{H}_\lambda\, e^{-X_{\lambda,\Delta\lambda}} \quad (5)$$

is applied to the original Hamiltonian $\mathcal{H}$. Thus, transitions between eigenstates of $\mathcal{H}_0$ caused by the interaction $\mathcal{H}_1$ are eliminated in steps where the respective transition energies are used as renormalization parameter λ. Furthermore,

$$\mathbf{Q}_{(\lambda-\Delta\lambda)} \mathcal{H}_{(\lambda-\Delta\lambda)} = 0 \quad (6)$$

is used to specify the generator $X_{\lambda,\Delta\lambda}$ of the unitary transformation. Note that equations (5) and (6) describe a renormalization step that decreases the cutoff of the Hamiltonian from λ to $(\lambda - \Delta\lambda)$, as one can see from a comparison with equations (3) and (4). Therefore, difference equations for the λ dependence of the Hamiltonian can be derived from (5) and (6), and we call the resulting equations for the parameters of the Hamiltonian renormalization equations. Note, that the solutions of these renormalization equations strongly depend on the parameters

of the original Hamiltonian $\mathcal{H}$, and that the limit $\lambda \to 0$ provides the desired effective Hamiltonian without any interactions.

The stepwise elimination procedure for the interaction $\mathcal{H}_1$ as described above resembles Wegner's flow equation method [13] and the similarity renormalization [14] in some aspects. However, there are also substantial differences between these methods: both flow equation method [13] and similarity renormalization [14] start from continuous unitary transformations in differential form. In contrast, the PRM is based on a sequence of discrete transformations. Therefore, as shown in reference [9], there is a direct connection between the PRM and usual perturbation theory.

3 Renormalization of the PAM

In the following, we want to apply the framework of the PRM as discussed above to the PAM. It is well known that much of the physics of the PAM (1) can be understood in terms of an uncorrelated model, that is for vanishing Coulomb repulsion on f sites where the Hubbard operators $\hat{f}^\dagger_{im}$ are replaced by usual fermionic operators $f^\dagger_{im}$. This model can be solved exactly. However, the parameters have to be renormalized appropriately. Various theoretical methods have been developed to generate renormalized Hamiltonians. Most popular is the one derived from slave-boson mean-field (SB) theory [11,12]. Note however that only HF type solutions can be obtained in this way. In particular, the SB solution breaks down if the original f level is located too far below the Fermi level [15] or, equivalently, if the hybridization strength between f and conduction electrons becomes too weak.

In the Hamiltonian (1) the Hubbard operators $\hat{f}^\dagger_{im}$ take care of the infinitely large local Coulomb repulsion on f sites so that multiple occupied f sites are strictly forbidden. Consequently, any effective model has to satisfy this requirement as well. However, SB mean-field theory as well as our recent PRM treatment of the PAM [10] map the Hamiltonian of equation (1) onto an effectively free system consisting of two non-interacting fermionic quasiparticles,

$$\mathcal{H}_{\text{eff}} = \sum_{\mathbf{k},m} \omega^c_{\mathbf{k}}\ c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \sum_{\mathbf{k},m} \omega^f_{\mathbf{k}}\ f^\dagger_{\mathbf{k}m} f_{\mathbf{k}m} + E_{\text{shift}}, \quad (7)$$

with renormalized parameters $\omega^c_{\mathbf{k}}$, $\omega^f_{\mathbf{k}}$, E_{shift}. It is important to notice that due to construction the effective Hamiltonian $\mathcal{H}_{\text{eff}}$ of equation (7) *does not prevent* from multiple occupation of f sites. This follows from the occurrence of the fermionic operators $f_{\mathbf{k}m}$ and $f^\dagger_{\mathbf{k}m}$ in equation (7) instead of the Hubbard operators $\hat{f}_{\mathbf{k}m}$ and $\hat{f}^\dagger_{\mathbf{k}m}$. However, an approximation that involves a replacement of the Hubbard operators $\hat{f}_{\mathbf{k}m}$ and $\hat{f}^\dagger_{\mathbf{k}m}$ by usual fermionic operators $f_{\mathbf{k}m}$ and $f^\dagger_{\mathbf{k}m}$ might lead to useful results as long as only very few f type states are below the Fermi level. Thus, only HF-like solutions with a renormalized f level above the Fermi level can be obtained based on effective Hamiltonians of type (7), and SB mean-field theory as well as our recent PRM treatment of the PAM [10] can not describe integral valent states.

3.1 Renormalization ansatz

In this paper we want to describe the transition of the PAM between mixed valent and integral valent states. Thus, a theoretical treatment is needed that reliably prevents from unphysical multiple occupation of f sites. For that purpose, we again apply the framework of the PRM to the PAM, but, in contrast to our recent work [10], we now keep the Hubbard operators during the whole renormalization procedure. Thus, the renormalization ansatz reads

$$\begin{aligned}
\mathcal{H}_\lambda &= \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda} \quad (8)\\
\mathcal{H}_{0,\lambda} &= \mu_{f,\lambda} \sum_{\mathbf{k},m} \hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} + \sum_{\mathbf{k},m} \Delta_{\mathbf{k},\lambda} \left(\hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \right)_{\text{NL}} \\
&\quad + \sum_{\mathbf{k},m} \varepsilon_{\mathbf{k},\lambda}\ c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + E_\lambda \\
\mathcal{H}_{1,\lambda} &= \mathbf{P}_\lambda \mathcal{H}_1 = \sum_{\mathbf{k},m} V_{\mathbf{k}}\ \mathbf{P}_\lambda \left(\hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \text{h.c.} \right)
\end{aligned}$$

after all excitations with energies larger than the cut-off λ have been eliminated. Due to the renormalization process all parameters depend on λ, and an additional energy shift E_λ and a hopping between different f sites,

$$\left(\hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \right)_{\text{NL}} = \frac{1}{N} \sum_{i,j(\neq i)} \hat{f}^\dagger_{im} \hat{f}_{jm} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)},$$

have been generated. Here, we have introduced Fourier transformed f operators,

$$\hat{f}^\dagger_{\mathbf{k}m} = \frac{1}{\sqrt{N}} \sum_i \hat{f}^\dagger_{im} e^{i\mathbf{k}\cdot\mathbf{R}_i}.$$

The initial parameter values of the original model (at cut-off $\lambda = \Lambda$) are

$$\mu_{f,\Lambda} = \varepsilon_f,\ \Delta_{\mathbf{k},\Lambda} = 0,\ \varepsilon_{\mathbf{k},\Lambda} = \varepsilon_{\mathbf{k}},\ E_\Lambda = 0. \quad (9)$$

To perform the PRM scheme we also need the commutator of the unperturbed Hamiltonian with the hybridization. For convenience, we introduce the unperturbed Liouville operator $\mathbf{L}_{0,\lambda}$ which is defined by $\mathbf{L}_{0,\lambda}\mathcal{A} = [\mathcal{H}_{0,\lambda}, \mathcal{A}]$ for any operator variable $\mathcal{A}$, and to simplify the calculations, the one-particle operators $\hat{f}^\dagger_{\mathbf{k}m}$ and $c^\dagger_{\mathbf{k}m}$ are considered as approximate eigenoperators of $\mathbf{L}_{0,\lambda}$,

$$\mathbf{L}_{0,\lambda}\ \hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} \approx (\varepsilon_{f,\lambda} + D\Delta_{\mathbf{k},\lambda} - \varepsilon_{\mathbf{k},\lambda})\, \hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m}. \quad (10)$$

Here, we introduced the local f energy,

$$\varepsilon_{f,\lambda} = \mu_{f,\lambda} - D\bar{\Delta}_\lambda, \quad (11)$$

and defined $D = 1 - \langle \hat{n}_i^f \rangle + \langle \hat{n}_i^f \rangle / \nu_f$ and $\bar{\Delta}_\lambda = \frac{1}{N} \sum_{\mathbf{k}} \Delta_{\mathbf{k},\lambda}$. The factors D in equations (9) and (10) are caused by the Hubbard operators in the renormalization ansatz (8). Similar expressions without factors D have also been found in reference [10] where a renormalization ansatz consisting of fermionic quasi-particles has been used.

As one can see from equation (10), the operator product $\hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m}$ can also be interpreted as an approximate eigenoperator of the Liouville operator $\mathbf{L}_{0,\lambda}$. The corresponding eigenvalues are excitation energies and can be used to rewrite $\mathcal{H}_{1,\lambda}$,

$$\mathcal{H}_{1,\lambda} = \sum_{\mathbf{k},m} \Theta_{\mathbf{k},\lambda} \; V_{\mathbf{k}} \left(\hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \text{h.c.} \right),$$

where the Θ functions

$$\Theta_{\mathbf{k},\lambda} = \Theta \left(\lambda - |\varepsilon_{f,\lambda} + D\Delta_{\mathbf{k},\lambda} - \varepsilon_{\mathbf{k},\lambda}| \right)$$

restrict the particle-hole excitations to transition energies smaller than λ.

3.2 Renormalization equations

Next we want to follow the discussion of reference [10] to derive renormalization equations for the parameters of the renormalized Hamiltonian $\mathcal{H}_\lambda$. It turns out that the actual calculations are only slightly modified by the new renormalization ansatz (8) which now includes correlated Hubbard operators.

To evaluate the new Hamiltonian $\mathcal{H}_{(\lambda - \Delta\lambda)}$ according to equation (5), an unitary transformation has to be performed to eliminate excitations within the energy shell between $(\lambda - \Delta\lambda)$ and λ. As in reference [10], we use the following operator ansatz for the generator $X_{\lambda,\Delta\lambda}$ of the unitary transformation,

$$X_{\lambda,\Delta\lambda} = \sum_{\mathbf{k},m} \Theta_{\mathbf{k}}(\lambda, \Delta\lambda) \, A_{\mathbf{k}}(\lambda, \Delta\lambda) \, (\hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} - c^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m})$$

where the $\Theta_{\mathbf{k}}(\lambda, \Delta\lambda)$ are products of two Θ functions,

$$\Theta_{\mathbf{k}}(\lambda, \Delta\lambda) = \Theta_{\mathbf{k},\lambda} \left[1 - \Theta_{\mathbf{k},(\lambda - \Delta\lambda)} \right].$$

Note that the $\Theta_{\mathbf{k}}(\lambda, \Delta\lambda)$ confine the excitations which have to be eliminated by the renormalization step from λ to $(\lambda - \Delta\lambda)$. The unknown parameters $A_{\mathbf{k}}(\lambda, \Delta\lambda)$ have to be fixed in such a way so that only transition with energies smaller than the new cut-off $(\lambda - \Delta\lambda)$ contribute to $\mathcal{H}_{(\lambda - \Delta\lambda)}$.

As described in reference [10], equations for the parameters $A_{\mathbf{k}}(\lambda, \Delta\lambda)$ of the generator of the unitary transformation as well as for the parameters of the renormalized Hamiltonian $\mathcal{H}_\lambda$ can be found by comparing the coefficients of the operators in the renormalization ansatz (8) at cutoff $(\lambda - \Delta\lambda)$ and in the explicitly evaluated unitary transformation (5).

Thus, we obtain the following equations:

$$A_{\mathbf{k}}(\lambda, \Delta\lambda) = \frac{\Theta_{\mathbf{k}}(\lambda, \Delta\lambda)}{2\sqrt{D}} \arctan \left[\frac{2\sqrt{D} V_{\mathbf{k}}}{\mu_{f,\lambda} + D \left(\Delta_{\mathbf{k},\lambda} - \bar{\Delta}_\lambda \right) - \varepsilon_{\mathbf{k},\lambda}} \right] \quad (12)$$

$$\begin{aligned} \varepsilon_{\mathbf{k},(\lambda - \Delta\lambda)} - \varepsilon_{\mathbf{k},\lambda} = & \\ & - \frac{1}{2} \left[\mu_{f,\lambda} + D \left(\Delta_{\mathbf{k},\lambda} - \bar{\Delta}_\lambda \right) - \varepsilon_{\mathbf{k},\lambda} \right] \\ & \quad \times \left\{ \cos \left[2\sqrt{D} A_{\mathbf{k}}(\lambda, \Delta\lambda) \right] - 1 \right\} \\ & - \sqrt{D} V_{\mathbf{k}} \sin \left[2\sqrt{D} A_{\mathbf{k}}(\lambda, \Delta\lambda) \right], \end{aligned} \quad (13)$$

$$\Delta_{\mathbf{k},(\lambda - \Delta\lambda)} - \Delta_{\mathbf{k},\lambda} = - \frac{1}{D} \left[\varepsilon_{\mathbf{k},(\lambda - \Delta\lambda)} - \varepsilon_{\mathbf{k},\lambda} \right] \quad (14)$$

$$\begin{aligned} \mu_{f,(\lambda - \Delta\lambda)} - \mu_{f,\lambda} = & \\ & - \frac{1}{D} \frac{1}{N} \sum_{\mathbf{k}} \left[\varepsilon_{\mathbf{k},(\lambda - \Delta\lambda)} - \varepsilon_{\mathbf{k},\lambda} \right] \\ & \quad \times \left[1 + (\nu_f - 1) \left\langle c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} \right\rangle \right] \\ & + \frac{\nu_f - 1}{4D^{3/2}} \frac{1}{N} \sum_{\mathbf{k}} \left\{ \left[\mu_{f,\lambda} + D \left(\Delta_{\mathbf{k},\lambda} - \bar{\Delta}_\lambda \right) - \varepsilon_{\mathbf{k},\lambda} \right] \right. \\ & \quad \times \sin \left[2\sqrt{D} A_{\mathbf{k}}(\lambda, \Delta\lambda) \right] \\ & \quad \left. - \; 2\sqrt{D} V_{\mathbf{k}} \left\{ \cos \left[2\sqrt{D} A_{\mathbf{k}}(\lambda, \Delta\lambda) \right] - 1 \right\} \right\} \\ & \quad \times \left\langle \hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \text{h.c.} \right\rangle \\ & - \frac{\nu_f - 1}{2D} \frac{1}{N} \sum_{\mathbf{k}} \left[\mu_{f,\lambda} - D \left(\Delta_{\mathbf{k},\lambda} - \bar{\Delta}_\lambda \right) - \varepsilon_{\mathbf{k},\lambda} \right] \\ & \quad \times A_{\mathbf{k}}(\lambda, \Delta\lambda) \left\langle \hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \text{h.c.} \right\rangle \end{aligned} \quad (15)$$

$$\begin{aligned} E_{(\lambda - \Delta\lambda)} - E_\lambda = & \\ & - N \langle \hat{n}_i^f \rangle \left[\mu_{f,(\lambda - \Delta\lambda)} - \mu_{f,\lambda} \right] \\ & \quad - \frac{\langle \hat{n}_i^f \rangle}{D} \sum_{\mathbf{k}} \left[\varepsilon_{\mathbf{k},(\lambda - \Delta\lambda)} - \varepsilon_{\mathbf{k},\lambda} \right]. \end{aligned} \quad (16)$$

Note that besides the factor $1/D$ in equation (14) these renormalization equations exactly agree with those derived in reference [10]. However, the underlying Hamiltonians differ significantly because now the renormalization ansatz (8) contains correlation effects by means of the Hubbard operators. It will turn out that the Hubbard operators not only complicate the further evaluation of the renormalization equations but also successfully prevent the system from unphysical multiple occupation of the f sites.

In deriving the renormalization equations (12–16) a factorization approximation has been employed so that

the obtained equations still depend on expectation values which have to be determined simultaneously (see Ref. [10] for details). Furthermore, an expansion in $1/\nu_f$ has been avoided (and spin fluctuations have been neglected) so that the derived renormalization equations are valid for large as well as small degeneracies ν_f. The limit $\lambda \to 0$ provides the parameters $\tilde{\varepsilon}_{\mathbf{k}}$, $\tilde{\mu}_f$, $\tilde{\Delta}_{\mathbf{k}}$, and $\tilde{E}$ of the effective Hamiltonian $\tilde{\mathcal{H}} = \mathcal{H}_{\lambda\to 0} = \mathcal{H}_{0,\lambda\to 0}$,

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k},m} \tilde{\varepsilon}_{\mathbf{k}}\; c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \tilde{\mu}_f \sum_{\mathbf{k},m} \hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} + \sum_{\mathbf{k},m} \tilde{\Delta}_{\mathbf{k}} \left(\hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \right)_{\mathrm{NL}} + \tilde{E}\,, \quad (17)$$

we are interested in. Here, it is important to notice that the renormalized Hamiltonian $\tilde{\mathcal{H}}$ no longer contains the hybridization between conduction and localized electrons. However, $\tilde{\mathcal{H}}$ is *not* a non-interacting fermionic system because $\tilde{\mathcal{H}}$ still takes into account electronic correlations by means of the Hubbard operators $\hat{f}^\dagger_{\mathbf{k}m}$. Note that these correlations turn out to be crucial for a description of integral valent states. On the other hand, the Hubbard operators $\hat{f}^\dagger_{\mathbf{k}m}$ also cause challenging difficulties in the further theoretical treatment because they do *not* obey the usual fermionic anticommutator relations.

The PRM as applied here to the PAM is a non-perturbative method which in most cases generates new interactions in every renormalization step. In order to obtain a closed set of renormalization equations (which is crucial for further evaluation) one needs to trace back complicated operator objects to simpler ones included in the renormalization ansatz. In this work, this aim is achieved by means of a factorization approximation. In order to estimate the effect of the neglected fluctuations one would need to add operator terms to the renormalization ansatz which are automatically generated during the renormalization procedure. Such an extension of the renormalization scheme might also allow the explanation of for instance magnetic and superconducting phases which is beyond the scope of this paper.

3.3 Approximate solutions

In the following we want to develop a strategy to solve the renormalization equations (12–16) approximately. Here, similar approximations as in reference [10] shall be used to decouple the renormalization of the different $\mathbf{k}$ values. In this way, all relevant quantities can be expressed as functions of a renormalized f energy $\tilde{\varepsilon}_f$ which is determined by numerical minimization of the free energy.

As in reference [10], we use the following approximations for further evaluation of the renormalization equations (12–16):

(i) All expectation values (which occur due to the exploited factorization approximation) are assumed to be independent from the renormalization parameter λ and are calculated using the full Hamiltonian $\mathcal{H}$.

(ii) To decouple the renormalization of the different $\mathbf{k}$ values, the λ dependence of the renormalized f level is neglected, $\mu_{f,\lambda} - D\bar{\Delta}_\lambda \approx \tilde{\varepsilon}_f$. The spirit of this approximation is similar to that assumed in the SB theory where a renormalized f energy is also used from the very beginning. Note that $\tilde{\varepsilon}_f$ has to be interpreted as local f energy of the renormalized model (17).

At this point it is important to notice, that our old analytical solution of reference [10] can be easily obtained if the Hubbard operators in the final Hamiltonian (17) are replaced by usual fermionic operators. Formally, one employs

(iii) $\sum_{\mathbf{k},m} \hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \approx \sum_{\mathbf{k},m} f^\dagger_{\mathbf{k}m} f_{\mathbf{k}m}$ and $(\hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m})_{\mathrm{NL}} \approx D\; (f^\dagger_{\mathbf{k}m} f_{\mathbf{k}m})_{\mathrm{NL}}$

to ensure that, on a mean-field level, the renormalized Hamiltonian does not generate unphysical states. However, as already discussed above, the obtained effective model does not prevent anymore from multiple occupation of f sites if (iii) has been employed. We have already argued that such an approximation can only lead to useful results as long as only very view f type states below the Fermi level are occupied. Thus, only HF-like solutions can be observed in this way. To obtain the analytical solution of reference [10], one also has to employ.

(iv) $\frac{1}{N} \sum_{\mathbf{k}} \Delta_{\mathbf{k},\lambda} \approx \tilde{\Delta} \approx 0$

for further simplification.

In the following we only want to employ approximations (i) and (ii). In particular, we keep the Hubbard operators in the final Hamiltonian (17) so that both mixed valent and integral valent states can be described.

Equations (14) and (16) can be easily integrated between the lower cutoff $\lambda \to 0$ and the cutoff of the original model Λ,

$$\tilde{\Delta}_{\mathbf{k}} = -\frac{1}{D}\left[\tilde{\varepsilon}_{\mathbf{k}} - \varepsilon_{\mathbf{k}}\right], \quad (18)$$

$$\tilde{E} = -N\langle \hat{n}^f_i \rangle \left[\tilde{\varepsilon}_f - \varepsilon_f\right] + \frac{D-1}{D} \langle \hat{n}^f_i \rangle \sum_{\mathbf{k}} \left[\tilde{\varepsilon}_{\mathbf{k}} - \varepsilon_{\mathbf{k}}\right]. \quad (19)$$

As already mentioned above, the approximations (i), (ii) decouple the different $\mathbf{k}$ values from each other so that equation (12) and (13) are completely similar to those obtained for the Fano-Anderson model (compare Ref. [10]). Thus, two quasi-particle branches are obtained,

$$\tilde{\varepsilon}_{\mathbf{k}} = \frac{\tilde{\varepsilon}_f + \varepsilon_{\mathbf{k}}}{2} - \frac{\mathrm{sgn}(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}})}{2} W_{\mathbf{k}}, \quad (20)$$

$$\tilde{\omega}_{\mathbf{k}} := \tilde{\varepsilon}_f + D\tilde{\Delta}_{\mathbf{k}} = \frac{\tilde{\varepsilon}_f + \varepsilon_{\mathbf{k}}}{2} + \frac{\mathrm{sgn}(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}})}{2} W_{\mathbf{k}}, \quad (21)$$

where

$$W_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f)^2 + 4D|V_{\mathbf{k}}|^2}.$$

Note that the one-particle energies (20) and (21) still depend on two unknown quantities: the renormalized f level

$\tilde{\varepsilon}_f$ and the f occupation number $\langle \hat{n}_i^f \rangle$ (that determines D as defined above).

In reference [10] all expectation values as well as the renormalized f level $\tilde{\varepsilon}_f$ have been determined by functional derivative of the free energy. However, here, this approach can not easily be applied because the Hubbard operators contained in the renormalized Hamiltonian (17) do not fulfill the usual fermionic anti-commutator relations. Furthermore, the derivation of the free energy would also lead to problematic δ functions that are caused by the abrupt change of the statistic of the quasi-particle excitations at $\tilde{\varepsilon}_f$. (In Ref. [10] these contributions do not appear because both c-like and f-like excitations are caused by fermionic quasi-particles.) Therefore, a different approach has to be developed to determine the renormalized f level $\tilde{\varepsilon}_f$ and the expectation values.

In the following, the expectation values of the original Hamiltonian $\mathcal{H}$ will be calculated using the renormalized one-particle operators as derived in reference [10],

$$c^\dagger_{\mathbf{k}m}(\lambda \to 0) = \tilde{u}_{\mathbf{k}} c^\dagger_{\mathbf{k}m} + \tilde{v}_{\mathbf{k}} \hat{f}^\dagger_{\mathbf{k}m}, \tag{22}$$

$$\hat{f}^\dagger_{\mathbf{k}m}(\lambda \to 0) = -D\, \tilde{v}_{\mathbf{k}} c^\dagger_{\mathbf{k}m} + \tilde{u}_{\mathbf{k}} \hat{f}^\dagger_{\mathbf{k}m}, \tag{23}$$

where we defined

$$|\tilde{u}_{\mathbf{k}}|^2 = \frac{1}{2}\left\{1 - \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}} \mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right)\right\}, \tag{24}$$

$$|\tilde{v}_{\mathbf{k}}|^2 = \frac{1}{2D}\left\{1 + \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}} \mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right)\right\}. \tag{25}$$

Thus, the required expectation values of the *full* Hamiltonian $\mathcal{H}$ can be traced back to those calculated with respect to the *renormalized* Hamiltonian $\tilde{\mathcal{H}}$ because $\langle A \rangle = \lim_{\lambda \to 0} \langle A(\lambda) \rangle_{\mathcal{H}_\lambda}$ holds,

$$\left\langle c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} \right\rangle = \frac{1}{2}\left[1 - \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}} \mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right)\right] f(\tilde{\varepsilon}_{\mathbf{k}}) + \frac{1}{2}\left[1 + \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}} \mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right)\right] \bar{f}(\tilde{\omega}_{\mathbf{k}}), \tag{26}$$

$$\left\langle \hat{f}^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \mathrm{h.c.} \right\rangle = -\,2\,\mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right) \frac{D|V_{\mathbf{k}}|}{W_{\mathbf{k}}} \left[f(\tilde{\varepsilon}_{\mathbf{k}}) - \bar{f}(\tilde{\omega}_{\mathbf{k}})\right]. \tag{27}$$

Here, we introduced the Fermi function

$$f(\tilde{\varepsilon}_{\mathbf{k}}) := \langle c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} \rangle_{\tilde{\mathcal{H}}} = \frac{1}{1 + e^{\beta \tilde{\varepsilon}_{\mathbf{k}}}},$$

and defined

$$\bar{f}(\tilde{\omega}_{\mathbf{k}}) := \frac{1}{D} \langle \hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \rangle_{\tilde{\mathcal{H}}}. \tag{28}$$

Note that the factor D in equation (28) has been introduced to underline the similarities of equation (26) and (27) with the corresponding results of the analytical treatment of reference [10].

In principle, the f occupation number $\langle \hat{n}_i^f \rangle$ could also be calculated using the renormalized one-particle operators. However, here we alternatively employ the particle conservation under unitary transformations. Thus, we obtain

$$\langle \hat{n}_i^f \rangle = \frac{1}{2}\frac{\nu_f}{N} \sum_{\mathbf{k}} \left[1 + \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}} \mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right)\right] f(\tilde{\varepsilon}_{\mathbf{k}}) + \frac{1}{2}\frac{\nu_f}{N} \sum_{\mathbf{k}} \left[2D - 1 - \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}} \mathrm{sgn}\left(\tilde{\varepsilon}_f - \varepsilon_{\mathbf{k}}\right)\right] \bar{f}(\tilde{\omega}_{\mathbf{k}}). \tag{29}$$

For actual calculations one needs to evaluate equation (28) in order to determine the expectation values of the full Hamiltonian as given in equations (26, 27), and (29). Because of the unusual properties of the Hubbard operators, there is no straightforward way to evaluate equation (28) and further approximations are necessary. As long as the renormalized f level is situated *above* the chemical potential a mean-field treatment of the electronic correlations contained in $\mathcal{H}$ might be sufficient, and we would find $\bar{f}(\tilde{\omega}_{\mathbf{k}}) \approx f(\tilde{\omega}_{\mathbf{k}})$ as directly obtained by employing approximation (iii) mentioned above. On the other hand, here we are also interested in solutions of the PAM with a renormalized f level *below* the Fermi level which require a theoretical treatment of the electronic correlations in $\mathcal{H}$ *beyond* a mean-field approximation. Therefore, equation (28) is evaluated as follows

$$\langle \hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \rangle_{\tilde{\mathcal{H}}} = \frac{1}{\mathrm{Tr}\, e^{-\beta\tilde{\mathcal{H}}}} \mathrm{Tr}\left(e^{\beta\tilde{\mathcal{H}}} \hat{f}_{\mathbf{k}m} e^{-\beta\tilde{\mathcal{H}}} \hat{f}^\dagger_{\mathbf{k}m} e^{-\beta\tilde{\mathcal{H}}}\right) \approx f(\tilde{\omega}_{\mathbf{k}}) \left\langle \left\{\hat{f}^\dagger_{\mathbf{k}m}, \hat{f}_{\mathbf{k}m}\right\}_+ \right\rangle_{\tilde{\mathcal{H}}}$$

where the approximated f excitation energy as derived in equation (10) has been used. Thus, (28) can be rewritten as

$$\bar{f}(\tilde{\omega}_{\mathbf{k}}) := \frac{\frac{1}{D} f(\tilde{\omega}_{\mathbf{k}})}{1 + \frac{\nu_f - 1}{N} \sum_{\mathbf{k}'} f(\tilde{\omega}_{\mathbf{k}'})}. \tag{30}$$

Unfortunately, approximation (30) does not offer a direct link to the mean-field result, $\bar{f}(\tilde{\omega}_{\mathbf{k}}) \approx f(\tilde{\omega}_{\mathbf{k}})$, for renormalized f energies above the Fermi level. Thus, differences between the presented treatment and the analytical solution of reference [10] will appear.

At this point all physical quantities can be calculated as function of the renormalized f energy $\tilde{\varepsilon}_f$. Because we have employed approximation (ii) it is not possible anymore to use the renormalization equation (15) for $\mu_{f,\lambda}$ to determine $\tilde{\varepsilon}_f$. Therefore, the local f energy $\tilde{\varepsilon}_f$ is considered as a free parameter and is determined by minimization of the free energy. Because of the unusual anticommutator relations of the Hubbard operators $\hat{f}^\dagger_{\mathbf{k}m}$, the free

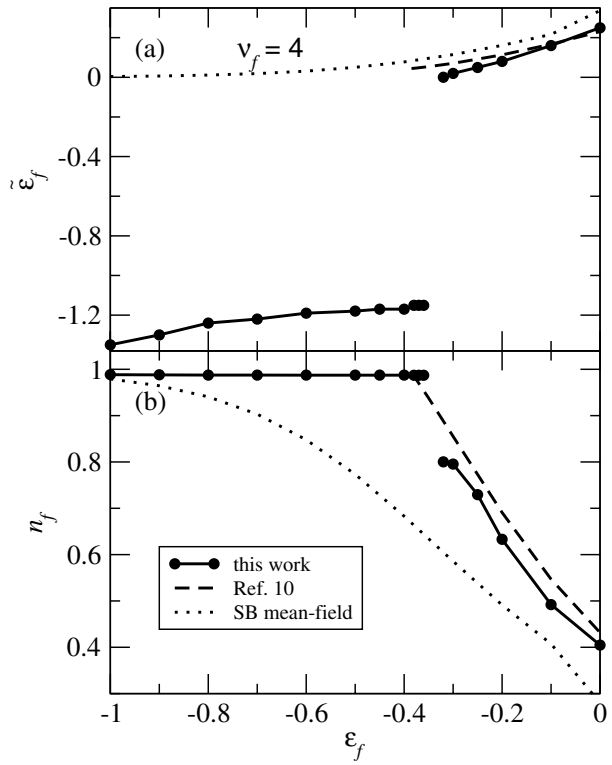

Fig. 1. Renormalized f level $\tilde{\varepsilon}_f$ [panel (a)] and averaged f occupation number $n_f = \langle \hat{n}_i^f \rangle$ [panel (b)] as function of the unrenormalized f energy ε_f where an one-dimensional PAM ($N = 10\,000$, $\nu_f = 4$, $\nu_f V^2 = 0.36$, $\mu = 0$, $T = 0.00001$) with a linear dispersion relation for the conduction band in the energy range between -1 and 1 has been considered. (All energies are given in units of the half bandwidth.) For comparison, the results of the PRM approach of reference [10] and of the SB mean-field theory are drawn with dashed and dotted lines.

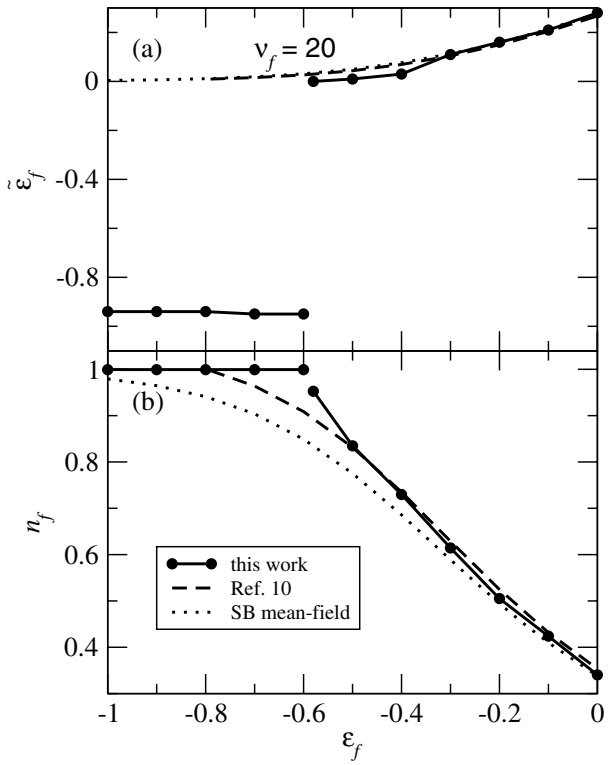

Fig. 2. Renormalized f level $\tilde{\varepsilon}_f$ [panel (a)] and averaged f occupation number $n_f = \langle \hat{n}_i^f \rangle$ [panel (b)] as function of the unrenormalized f energy ε_f for an one-dimensional PAM with $\nu_f = 20$. Other parameters are chosen as in Figure 1.

energy can not be directly determined. Instead,

$$\frac{\mathrm{d}F}{\mathrm{d}\tilde{\varepsilon}_f} = \sum_{\mathbf{k},m} \frac{\mathrm{d}\tilde{\varepsilon}_{\mathbf{k}}}{\mathrm{d}\tilde{\varepsilon}_f} \left\langle c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} \right\rangle_{\tilde{\mathcal{H}}} + \frac{\mathrm{d}\tilde{\mu}_f}{\mathrm{d}\tilde{\varepsilon}_f} \sum_{\mathbf{k},m} \left\langle \hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \right\rangle_{\tilde{\mathcal{H}}} + \sum_{\mathbf{k},m} \frac{\mathrm{d}\tilde{\Delta}_{\mathbf{k}}}{\mathrm{d}\tilde{\varepsilon}_f} \left\langle \left(\hat{f}^\dagger_{\mathbf{k}m} \hat{f}_{\mathbf{k}m} \right)_{\mathrm{NL}} \right\rangle_{\tilde{\mathcal{H}}} + \frac{\mathrm{d}\tilde{E}}{\mathrm{d}\tilde{\varepsilon}_f} \tag{31}$$

is numerically integrated in order to calculate the free energy F as function of the renormalized f energy $\tilde{\varepsilon}_f$. Note that equation (31) has been obtained from the renormalized Hamiltonian (17). Actual results are discussed in the next section.

4 Results

It is believed that the one-particle energy ε_f of the localized f electrons is smoothly changed in $CeCu_2Si_2$ due to pressure [4]. Therefore, we want to discuss the physical properties of the PAM as a function of ε_f.

At first let us consider an one-dimensional PAM with a linear dispersion relation $\varepsilon_{\mathbf{k}}$ for the conduction electrons in the energy range between -1 and 1, and a $\mathbf{k}$ independent hybridization $V_{\mathbf{k}} = V$. The other parameters are chosen as follows $\nu_f V^2 = 0.36$, chemical potential $\mu = 0$, and $T = 0.00001$ where all energies are given in units of the half bandwidth.

As one can see from Figures 1 and 2, we obtain two different types of solutions depending on the value of the unrenormalized f level ε_f. First of all, we obtain the usual SB type solutions with intermediate valence states $n_f < 1$ where the renormalized energy $\tilde{\varepsilon}_f$ is energetically located above the Fermi energy. If the unrenormalized energy ε_f is lowered the renormalization contributions are no longer sufficient to push $\tilde{\varepsilon}_f$ above the Fermi level, and the renormalized f energy $\tilde{\varepsilon}_f$ is located far below the Fermi energy. In this case, the averaged f occupation n_f is almost exactly 1 and an integral valence state is obtained.

Figures 1 and 2 also reveal the very good agreement between the HF type solutions of the presented PRM approach and the analytical results of reference [10]. In this way it is proven that the Hubbard operators can be replaced by usual fermionic operators (compare approximation (iii) in Sect. 3.3) because in this case only very few f type states below the Fermi level are occupied as discussed above. In this regard one needs to keep in mind an important difference between the SB theory and our PRM approach: the quasi-particles of the SB theory change their character as function of $\mathbf{k}$ between more f-like and more c-like behavior. In the PRM excitations do not change their

character as function of **k**, and the quasi-particle energies show jumps in their **k** dependence if $\tilde{\varepsilon}_f$ is energetically located within the conduction band. Note, however, that the various parts of the quasiparticle bands fit perfectly together, as one can see from equations (20) and (21).

For comparison, the results of the analytical solution of reference [10] and of the SB theory are shown as well in Figures 1 and 2. As one can see, no solution with renormalized f level $\tilde{\varepsilon}_f < 0$ could be found for these analytical approaches because both do not explicitly ensure that f sites can only be either empty or singly occupied as already discussed above.

The well-defined transition between the two different solution types is of particular interest. As expected, for the HF-like solution the f-charge is always smaller than 1 due to hybridization processes between f and c-electrons. Simultaneously heavy quasiparticle bands are formed at the Fermi surface. To describe the HF behavior the full Anderson model has to be considered. As the bare f-level moves to smaller energies a transition to an integral valence charge of $n_f = 1$ is observed (similar to the Anderson impurity model [16]). In this case only the c electrons should form the Fermi surface. Thus, the observed valence transition can also be interpreted as a collapse of the large Fermi surface of the HF state which is formed by conduction as well as by localized f electrons. Note, however, that the question whether localized electrons contribute to the Fermi sea volume or not is still controversially discussed in the literature [17].

As one can see from Figures 1 and 2, the obtained valence transition is much more pronounced for small degeneracies ν_f, and a smooth transition can be expected in the limit $\nu_f \to \infty$ of the SB theory. Therefore, a sharp valence change in generalized SB theories can only be obtained if a rather large additional Coulomb repulsion between f and conduction electrons is present in the system [4,8]. However, here we have shown that such a valence transition can also be obtained in the plain PAM if corrections for small degeneracies ν_f are properly taken into account.

One of the advantages of the analytical PRM is the opportunity to consider much larger systems than accessible by numerical methods. Therefore, we are also able to study two- and three-dimensional systems of reasonable sizes. In this way we can easily show that the observed valence transition is not an unique phenomenon of the one-dimensional PAM. The valence transition also occurs in two- and three-dimensional systems as can been seen in Figure 3. Therefore, the observed behavior has to be considered as a general feature of the PAM, and our results should also be of relevance for actual physical HF systems like $CeCu_2Si_2$ or related compounds.

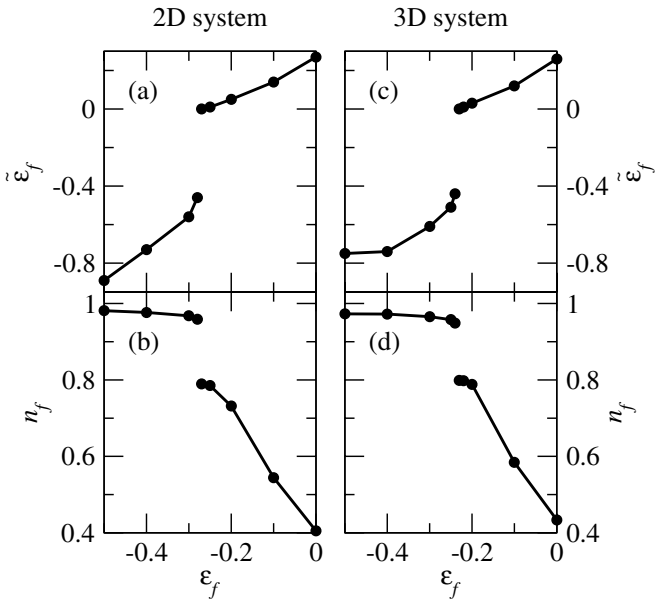

Fig. 3. Panel (a) and (b) [(c) and (d)] show the results for the renormalized f level $\tilde{\varepsilon}_f$ and the f occupation number $n_f = \langle \hat{n}_i^f \rangle$ for a two-dimensional [three-dimensional] system with 100×100 [$26 \times 26 \times 26$] lattice sites. As in Figures 1 and 2, a linear dispersion relation $\varepsilon_{\mathbf{k}} = \varepsilon(|\mathbf{k}|)$ has been chosen, and the electronic band covers an energy range between –1.5 and 0.5 [–1.8 and 0.2] where $\mu = 0$, $\nu_f = 4$, $\nu_f V^2 = 0.36$, and $T = 0.00001$. (Energies are given in units of the half bandwidth.) Note that the conduction band has been energetically shifted in in order to ensure a filling comparable to the one-dimensional case of Figure 1 because a smaller filling of the conduction band reduces the change in the f occupation n_f at the transition point.

5 Discussion and summary

The occurrence of a valence transition in the plain PAM is the main finding of this paper. In contrast, a rather large additional Coulomb repulsion has been claimed to be necessary for the valence transition in an extended PAM [4,8]. The studies of references [4,8] were based on a slave-boson fluctuation approximation that extends the well-known slave-boson mean-field theory [11,12] but still employs the limit of large degeneracy $\nu_f \to \infty$. Our results show (compare Figures 1 and 2) that the observed valence transition becomes smooth in this limit. Therefore, it is reasonable that an additional interaction was found to be necessary in order to obtain a valence transition in an approach employing $\nu_f \to \infty$.

Our work also shows the importance of taking care of a physical f occupation in theoretical approaches. In particular, it turns out that a completely uncorrelated model is not able to prevent from unphysical multiple occupation of f sites, and no integral valence states can be found in this way. In contrast, the presented PRM approach to the PAM explicitly suppresses unphysical multiple f occupation which is, in particular, crucial for integral valence states.

We obtain two solution types: a mixed valence state with a renormalized f level $\tilde{\varepsilon}_f$ above the Fermi energy and an integral valence state with $\tilde{\varepsilon}_f$ below the Fermi level. Furthermore, parameter regimes exist where the transition between the two solution types is accompanied by a drastic change in the f occupation. Such a sharp valence transition occurs in one-dimensional as well as in two- and three-dimensional systems so that this behavior has to be

considered as a general feature of the PAM. Note that a similar valence transition has been experimentally found in $CeCu_2Si_2$ from high pressure experiments [3,4].

In the case of an integral valence state one would expect that the system can be described by a Kondo Hamiltonian which is gained from the PAM by the Schrieffer-Wolff transformation [18] for $V/|\varepsilon_f| \ll 1$. Note, however, that in the present approach spin fluctuations have been neglected altogether but Kondo-like and RKKY-like interactions as well as higher charge fluctuation terms are automatically generated during the renormalization procedure. These contributions will have to be considered in the future. One might expect that additional spin and charge fluctuations might possibly give rise to magnetic and superconducting phases both for the intermediate valence and for the integer valence regime. Also, one may speculate that the magnitude of the magnetic moment will be different for these cases due to additional screening processes.

The PRM approach presented in this paper only addresses the question for the valence transition in the plain PAM. However, as mentioned above, the PRM scheme offers great opportunities to include additional interactions which are automatically generated during the renormalization procedure. Therefore, extensions of the PRM treatment might be promising starting points to study the competing interactions in $CeCu_2Si_2$ and related compounds in more detail.

We would like to acknowledge stimulating and enlightening discussions with T. Bryant and V. Zlatić. This work was supported by the DFG through the research program SFB 463. A.H. is grateful for the support of the DFG through Grant No. HU 993/1-1, and of the US Department of Energy, Division of Materials Research, Office of Basic Energy Science.

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