Renormalization of the periodic Anderson model: an alternative analytical approach to heavy Fermion behavior

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In this paper a recently developed projector-based renormalization method (PRM) for many-particle Hamiltonians is applied to the periodic Anderson model (PAM) with the aim to describe heavy Fermion behavior. In this method high-energetic excitation operators instead of high energetic states are eliminated. We arrive at an effective Hamiltonian for a quasi-free system which consists of two non-interacting heavy-quasiparticle bands. The resulting renormalization equations for the parameters of the Hamiltonian are valid for large as well as small degeneracy $\nu_f$ of the angular momentum. An expansion in $1/\nu_f$ is avoided. Within an additional approximation which adapts the idea of a fixed renormalized $f$ level $\tilde{\varepsilon}_f$, we obtain coupled equations for $\tilde{\varepsilon}_f$ and the averaged $f$ occupation $\langle n_f \rangle$. These equations resemble to a certain extent those of the usual slave boson mean-field (SB) treatment. In particular, for large $\nu_f$ the results for the PRM and the SB approach agree perfectly whereas considerable differences are found for small $\nu_f$.

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I. INTRODUCTION

In comparison to ordinary metals metallic heavy fermion systems have remarkable low-temperature properties\textsuperscript{[1]}: both the conduction electron specific heat and the magnetic susceptibility can be two or more orders of magnitude larger than in normal metals though the ratio of both quantities is similar to that of usual metals. Usually, in metals an increasing resistivity $\rho(T)$ with increasing temperature is observed. In contrast, a much richer behavior is found in heavy fermion systems: At higher temperatures $\rho(T)$ only changes slightly and might even increase with decreasing temperature. Below a characteristic coherence temperature a strong decrease of the resistivity with decreasing temperatures is observed. At very low temperatures, a $T^2$ dependence of the temperature is found. Another important finding is that a correspondence between the low-energy excitations of heavy fermion systems and those of a free electron gas with properly renormalized parameters can be established. Therefore, the high density of states at the Fermi surface observed in heavy fermion systems implies an effective mass of the (heavy) quas_particles which is some hundred times larger than the free electron mass.

Prototype heavy fermion systems like CeAl\textsubscript{3} and UPt\textsubscript{3} contain rare-earth or actinide elements. Thus, the basic microscopic model for the investigation of such materials is believed to be the periodic Anderson model (PAM) which describes the interaction between nearly localized, strongly correlated $f$ electrons and conduction electrons\textsuperscript{[2]}. Within a simplified version the Hamiltonian of the PAM can be written as

\begin{equation}
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1,
\end{equation}

\begin{align}
\mathcal{H}_0 &= \varepsilon_f \sum_{i,m} \hat{f}_i^\dagger \hat{f}_i + \sum_{k,m} \varepsilon_k c_k^\dagger c_k,
\mathcal{H}_1 &= \frac{1}{\sqrt{N}} \sum_{k,i,m} V_k \left( \hat{f}_i^\dagger c_k e^{i k R_i} + h.c. \right).
\end{align}

Here, $i$ is the $4f$ or $5f$ site index, $k$ is the conduction electron wave vector, and $V_k$ is the hybridization matrix element between conduction and localized electrons. $\varepsilon_f$ and $\varepsilon_k$, both measured from the chemical potential $\mu$, are the excitation energies for $f$ and conduction electrons, respectively. As a simplification, both types of electrons are assumed to have the same angular momentum index $m$ with $\nu_f$ values, $m = 1...\nu_f$. Finally, the local Coulomb repulsion $U_f$ at $f$ sites has been assumed to be infinitely large so that localized sites can either be empty or singly occupied, i.e., the Hubbard operators $\hat{f}_i^\dagger$ are defined by

\begin{equation}
\hat{f}_i^\dagger = f_i^\dagger \prod_{\tilde{m}(\neq m)} (1 - n_{i\tilde{m}}^f).
\end{equation}
where $n^f_{im} = f^\dagger_{im} f_{im}$. The unexpected and exciting properties of the PAM (1) are mainly due to the presence of the strong correlations at $f$ sites. In turn the strong correlations also cause the great difficulties in any theoretical treatment of the model. In the present approach the correlations are taken care of by the Hubbard operators (2) which do not obey the usual fermionic anticommutator relations. Instead one has

$$[\hat{f}^\dagger_{im}, \hat{f}_{im}]_+ = D_{im}$$

(3)

where

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

(4)

The quantity $D_{im}$ can be interpreted as a local projection operator at $f$ site $i$ on $f$ states which are either empty or singly occupied with one electron with index $m$. Also it is helpful to introduce separately the projection operator $P^0(i)$ on the empty $f$ state at site $i$ and the projection operator $\hat{n}^f_{im}$ on the singly occupied $f$ state when one electron with index $m$ is present. $D_{im}$ can be rewritten as

$$D_{im} = P^0(i) + \hat{n}^f_{im} = 1 - \sum_{\tilde{m}(\neq m)} \hat{n}^f_{i\tilde{m}}$$

(5)

where we have defined

$$P^0(i) = \prod_{\tilde{m}} (1 - f^\dagger_{i\tilde{m}} f_{i\tilde{m}}),$$

(6)

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

(7)

The second equation in (4) is the completeness relation for $f$ electrons at site $i$.

For the case of vanishing Coulomb repulsion $U_f$ the PAM (1) is equivalent to the Fano-Anderson model [3, 4] which can be easily solved (see, for example, appendix A). However, much of the physics of the correlated model can also be understood in terms of a renormalization of the parameters of the uncorrelated Fano-Anderson model. Various theoretical methods have been developed in the past to generate such renormalized Hamiltonians, for instance the Gutzwiller projection [5] or the slave-boson mean-field (SB) theory [6, 7]. Here we use a recently developed projector-based renormalization method (PRM) to map the PAM to a free system consisting of two bands of uncorrelated quasi-particles. Furthermore, we avoid an expansion with respect to the degeneracy $\nu_f$ of the angular momentum and take all $1/\nu_f$ corrections into account.

The PRM has already been applied before to the PAM in Ref. [8]. However, in the present approach the treatment from Ref. [8] will be improved in various points: (i) The PRM is performed in a completely non-perturbative manner. (ii) All $1/\nu_f$ corrections are taken into account. (iii) The dispersion of both quasiparticle bands is considered.

Furthermore, we shall compare the results of the PRM with those of the SB treatment in much more detail.

The paper is organized as follows. First, in Sec. II we briefly repeat the recently developed PRM [8]. In Sec. III the PRM is applied to the PAM whereby the renormalization equations for the model parameters are derived non-perturbatively. An analytical solution of the renormalization equations is found in Sec. IV using a constant renormalized $f$ level $\tilde{\varepsilon}_f$. Furthermore, we compare our results with the solutions of the SB theory. Finally, our conclusions are presented in Sec. V.

II. PROJECTOR-BASED RENORMALIZATION METHOD (PRM)

The PRM [8] starts from a decomposition of a given many-particle Hamiltonian $\mathcal{H}$ into an unperturbed part $\mathcal{H}_0$ and into a perturbation $\mathcal{H}_1$,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1.$$  

(7)

We assume that the eigenvalue problem of $\mathcal{H}_0$ is known

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

(8)
$H_I$ is the interaction. Its presence usually prevents the exact solution of the eigenvalue problem of the full Hamiltonian. Let us define a projection operator $P_\lambda$ by

$$P_\lambda A = \sum_{m,n} |n\rangle \langle m| A|m\rangle.$$  

Note that $P_\lambda$ is a super-operator acting on usual operators $A$ of the unitary space. It projects on those parts of $A$ which are formed by all dyads $|n\rangle \langle m|$ with energy differences $|E_n^{(0)} - E_m^{(0)}|$ less or equal to a given cutoff $\lambda$, where $\lambda$ is smaller than the cutoff $\Lambda$ of the original model. Note that in (9) neither $|n\rangle$ nor $|m\rangle$ have to be low-energy eigenstates of $H_0$. However, their energy difference has to be restricted to values $\leq \lambda$. Furthermore, it is useful to define the projection operator

$$Q_\lambda = 1 - P_\lambda \quad (10)$$

which is orthogonal to $P_\lambda$. $Q_\lambda$ projects on high energy transitions larger than the cutoff $\lambda$.

The goal of the present method is to transform the initial Hamiltonian $H$ (with a large energy cutoff $\Lambda$) into an effective Hamiltonian $H_\lambda$ which has no matrix elements belonging to transitions larger than $\lambda$. This is achieved by a unitary transformation so that the effective Hamiltonian will have the same eigenspectrum as the original Hamiltonian $H$. However, as it will turn out, the method is especially suitable to describe low-energy excitations of the system. $H_\lambda$ is defined by

$$H_\lambda = e^{X_\lambda} H e^{-X_\lambda}. \quad (11)$$

The generator $X_\lambda$ of the transformation has to be anti-Hermitian, $X_\lambda^\dagger = -X_\lambda$, so that $H_\lambda$ is Hermitian for any $\lambda$. We look for an appropriate generator $X_\lambda$ so that $H_\lambda$ has no matrix elements belonging to transitions larger than $\lambda$. This means that the following condition

$$Q_\lambda H_\lambda = 0 \quad (12)$$

has to be fulfilled. Eq. (12) will be used below to specify $X_\lambda$. In contrast to Ref. [8], where $H_\lambda$ was evaluated perturbatively, the transformation (11) will be treated non-perturbatively.

Next we discuss the elimination procedure for the interaction $H_I$. Instead of transforming the Hamiltonian in one step as in Eq. (11) the transformation will be done successively. Or more formally spoken, instead of applying the elimination of high-energy excitations in one step a sequence of stepwise transformations is used in order to obtain an effectively diagonal model. This procedure resembles Wegner’s flow equation method [3] and the similarity renormalization [10] in some aspects. In the PRM approach difference equations for the $\lambda$ dependence of the parameters of the Hamiltonian are derived. They will be called renormalization equations. To find these equations we start from the renormalized Hamiltonian

$$H_\lambda = H_{0,\lambda} + H_{1,\lambda} \quad (13)$$

after all excitations with energy differences larger than $\lambda$ have been eliminated. Next we consider an additional renormalization of $H_\lambda$ by eliminating all excitations inside an energy shell between $\lambda$ and a smaller energy cutoff $(\Delta \lambda)$ where $\Delta \lambda > 0$. The new Hamiltonian $H_{(\lambda - \Delta \lambda)}$ is obtained by an unitary transformation similar to that of Eq. (11)

$$H_{(\lambda - \Delta \lambda)} = e^{X_{\lambda,\Delta \lambda}} H_\lambda e^{-X_{\lambda,\Delta \lambda}} \quad (14)$$

where $X_{\lambda,\Delta \lambda}$ is determined by

$$Q_{(\lambda - \Delta \lambda)} H_{(\lambda - \Delta \lambda)} = 0. \quad (15)$$

Note that there are two strategies to exploit Eq. (15) in order to determine the generator $X_{\lambda,\Delta \lambda}$ of the unitary transformation (14). The most straightforward route is to analyze Eqs. (14) and (15) in perturbation theory as it was done in Refs. [8] and [11]. Here, we want to perform the renormalization step from $\lambda$ to $(\lambda - \Delta \lambda)$ in a non-perturbative way.

Eqs. (14) and (15) describe the renormalization of the Hamiltonian by decreasing the cutoff from $\lambda$ to $(\lambda - \Delta \lambda)$ and can be used to derive difference equations for the $\lambda$-dependence of the Hamiltonian. The resulting equations for the parameters of the Hamiltonian will be called renormalization equations. Their solution depends on the initial values of the parameters of the Hamiltonian and fixes the final Hamiltonian in the limit $\lambda \to 0$. Note that for $\lambda \to 0$ the resulting Hamiltonian only consists of the unperturbed part $H_{0,(\lambda \to 0)}$. The interaction $H_{1,(\lambda \to 0)}$ vanishes since it is completely used up in the renormalization procedure. Thus, an effectively diagonal Hamiltonian is obtained.
III. RENORMALIZATION OF THE PERIODIC ANDERSON MODEL (PAM)

The PRM described above will be applied in this section to the PAM \( \mathcal{H} \). As an illustration of the method the Fano-Anderson model is discussed as a further application of the PRM in appendix B. This model can be considered as a PAM without electronic correlations. It turns out that the renormalization of the full PAM \( \mathcal{H} \) is somewhat similar to that of the uncorrelated model. However, in the Anderson-Fano model the elimination of excitations with energies larger than \( \lambda \) can be done in one step. For the PAM \( \mathcal{H} \) the \( f \) electron one-particle energy \( \varepsilon_f \) will also be renormalized. This is due to the presence of strong local correlations at \( f \) sites in the PAM \( \mathcal{H} \). Therefore, the elimination procedure has to be done stepwise by repeatedly integrating over small energy steps of width \( \Delta \lambda \). In this way one is led to renormalization equations for the parameters of the model in terms of difference equations which have to be solved.

A. Renormalization ansatz

Let us start by formally writing down the effective Hamiltonian \( \mathcal{H}_\lambda = e^{X_\lambda} \mathcal{H} e^{-X_\lambda} = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda} \) for the periodic Anderson model after all excitations with energy differences larger than \( \lambda \) have been eliminated. By comparing with the starting model \( \mathcal{H} \) one might be in favor of choosing an unperturbed part \( \mathcal{H}_{0,\lambda} \) which contains correlated \( f \)-electrons \( f^\dagger_{im}, f_{im} \) as in Eq. (1). However, because the eigenvalue problem of such an Hamiltonian would not exactly be solvable, we prefer to start from an uncorrelated Hamiltonian where only usual Fermi operators \( \hat{c}^\dagger_{k}, \hat{c}_{k} \) enter but keep the correlations in the renormalized interaction \( \mathcal{H}_{1,\lambda} \), i.e.

\[
\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda}
\]

where

\[
\mathcal{H}_{0,\lambda} = \varepsilon_{f,\lambda} \sum_{k,m} f^\dagger_{km} f_{km} + \sum_{k,m} \Delta_{k,\lambda} \left( f^\dagger_{km} f_{km} \right)_{NL} + \sum_{k,m} \varepsilon_{k,\lambda} \hat{c}^\dagger_{km} \hat{c}_{km} + E_\lambda, \tag{16}
\]

\[
\mathcal{H}_{1,\lambda} = \mathbf{P}_\lambda \mathcal{H}_1 = \sum_{k,m} V_k \mathbf{P}_\lambda \left( \hat{f}^\dagger_{km} \hat{c}_{km} + \text{h.c.} \right). \tag{17}
\]

Here \( f^\dagger_{km}, f_{km} \) are Fourier transformed \( f \) operators,

\[
f^\dagger_{km} = \frac{1}{\sqrt{N}} \sum_i f^\dagger_{im} e^{ikR_i}, \quad f_{km} = \frac{1}{\sqrt{N}} \sum_i f_{im} e^{ikR_i}. \tag{18}
\]

Moreover, in \( \mathcal{H}_{0,\lambda} \) we have discriminated between local,

\[
(f^\dagger_{km} f_{km})_L := \frac{1}{N} \sum_k f^\dagger_{km} f_{km} = \frac{1}{N} \sum_i f^\dagger_{im} f_{im}, \tag{19}
\]

and nonlocal,

\[
(f^\dagger_{km} f_{km})_{NL} := \frac{1}{N} \sum_{i\neq j} f^\dagger_{im} f_{jm} e^{i(k R_i - R_j)} = f^\dagger_{km} f_{km} - (f^\dagger_{km} f_{km})_L, \tag{20}
\]

\( f \) particle-hole excitations in order to properly take into account the strong Coulomb interaction at local \( f \) sites. Due to renormalization processes the one-particle energies \( \varepsilon_{f,\lambda} \) and \( \varepsilon_{k,\lambda} \) in Eq. (16) depend on the cutoff energy \( \lambda \). Moreover, two new parameters enter: \( \Delta_{k,\lambda} \) describes the \( f \) dispersion due to the hybridization of \( f \) electrons at different sites \( i \neq j \), and \( E_\lambda \) is an additional energy shift. Finally, the projector \( \mathbf{P}_\lambda \) in (17) guarantees that only excitations contribute to \( \mathcal{H}_{1,\lambda} \) which have energies (with respect to \( \mathcal{H}_{0,\lambda} \)) which are smaller than \( \lambda \). The initial parameter values of the original model (at \( \lambda = \Lambda \)) are

\[
\varepsilon_{f, (\Lambda = \Lambda)} = \varepsilon_f, \quad \Delta_{k, (\Lambda = \Lambda)} = 0, \quad \varepsilon_{k, (\Lambda = \Lambda)} = \varepsilon_k, \quad E_{(\Lambda = \Lambda)} = 0. \tag{21}
\]

As it turns out, the hybridization \( V_k \) is not changed by the renormalization procedure.
As mentioned before, correlation effects have been neglected in Eq. (10). First, this means that doubly occupancies of \( f \)-sites \((f_{im} - \hat{f}_{im})\) are assumed to be negligibly small though they are not properly excluded by the choice of uncorrelated \( f \) operators in \( \mathcal{H}_{0,\lambda} \). Note that this assumption is also used for the subsidiary condition within the SB approach [7]. Doubly occupied \( f \)-sites could in principle be generated by the non-local \( f \)-part of \( \mathcal{H}_{0,\lambda} \). As it turns out, this is explicitly excluded by keeping the correlations in the interaction part \( \mathcal{H}_{1,\lambda} \).

For the following, the commutator of the unperturbed Hamiltonian \( \mathcal{H}_{0,\lambda} \) with the operator \( \hat{f}_{km}^{\dagger}c_{km} \) has to be evaluated. By introducing the unperturbed Liouville operator \( \mathbf{L}_{0,\lambda} \), which is defined by \( \mathbf{L}_{0,\lambda}A = [\mathcal{H}_{0,\lambda}, A] \) for any operator variable \( A \), one finds

\[
\mathbf{L}_{0,\lambda}\hat{f}_{km}^{\dagger}c_{km} = [\mathcal{H}_{0,\lambda}, \hat{f}_{km}^{\dagger}c_{km}] =
\]

\[
= (\varepsilon_{f,\lambda} - \varepsilon_{k,\lambda}) \hat{f}_{km}^{\dagger}c_{km} + \frac{1}{N^{3/2}} \sum_{k',i,j} (1 - \delta_{ij}) \Delta_{k',\lambda} e^{i(k-k')R_i} e^{ik'R_j} f_{im}^{\dagger} D_{jm} c_{km}
\]

\[
+ \frac{1}{N^{3/2}} \sum_{k',m'i,j} (1 - \delta_{mm'}) \Delta_{k',\lambda} e^{i(k-k')R_i} e^{ik'R_j} f_{im}^{\dagger} \hat{f}_{jm}^{\dagger} \hat{f}_{jm'} c_{km}
\]

where contributions which lead to doubly occupied \( f \) sites have been neglected. The second and the third term on the r.h.s. of Eq. (22) follow from the special form of the anticommutator relations (3). Obviously, only \( f \) electron operators belonging to different sites \( i \neq j \) enter the second term on the r.h.s. of Eq. (22). Therefore, as approximation one may replace the operator \( D_{jm} \) by its expectation value

\[
D = \langle D_{jm} \rangle = 1 - \frac{\nu_f - 1}{\nu_f} \langle \hat{n}_f^j \rangle
\]

where

\[
\langle \hat{n}_f^j \rangle = \sum_m \langle \hat{f}_{jm}^{\dagger} \hat{f}_{jm} \rangle
\]

(24)

is the averaged occupation number of \( f \) electrons at site \( j \). Note that \( D \) is independent of \( j \) and \( m \). Furthermore, \( D \hat{f}_{km}^{\dagger} \) is replaced by \( \hat{f}_{km}^{\dagger} \). Finally, we neglect the third term on the r.h.s of Eq. (22), which represents spin-flip processes, and all contributions leading to doubly occupied \( f \) sites. (Similar approximations will also be used later.) Consequently, Eq. (22) simplifies to

\[
\mathbf{L}_{0,\lambda}\hat{f}_{km}^{\dagger}c_{km} = (\varepsilon_{f,\lambda} + \Delta_{k,\lambda} - \bar{\Delta}_\lambda - \varepsilon_{k,\lambda}) \hat{f}_{km}^{\dagger}c_{km}
\]

(25)

where

\[
\bar{\Delta}_\lambda = \frac{1}{N} \sum_k \Delta_{k,\lambda}
\]

(26)

is the averaged \( f \) dispersion. Thus, \( \hat{f}_{km}^{\dagger}c_{km} \) is an approximate eigenvector of the Liouville operator \( \mathbf{L}_{0,\lambda} \). The corresponding eigenvalue is the excitation energy \( \varepsilon_{f,\lambda} + \Delta_{k,\lambda} - \bar{\Delta}_\lambda - \varepsilon_{k,\lambda} \). Furthermore, Eq. (25) can be used to evaluate the action of the projector \( \mathbf{P}_\lambda \) in (17) so that \( \mathcal{H}_{1,\lambda} \) can be rewritten as

\[
\mathcal{H}_{1,\lambda} = \mathbf{P}_\lambda \mathcal{H}_1 = \sum_{k,m} \Theta (\lambda - |\varepsilon_{f,\lambda} + \Delta_{k,\lambda} - \bar{\Delta}_\lambda - \varepsilon_{k,\lambda}|) V_k \left( \hat{f}_{km}^{\dagger}c_{km} + \text{h.c.} \right)
\]

(27)

where the \( \Theta \)-function restricts the particle-hole excitations to transition energies smaller than \( \lambda \).

**B. Generator of the unitary transformation**

In the next step let us evaluate a new effective Hamiltonian \( \mathcal{H}_{\lambda-\Delta\lambda} \) which is obtained by a further elimination of excitations within a small energy shell between \( (\lambda - \Delta\lambda) \) and \( \lambda \). According to (13) \( \mathcal{H}_{\lambda-\Delta\lambda} \) is obtained from an unitary transformation

\[
\mathcal{H}_{\lambda-\Delta\lambda} = e^{X_{\lambda,\Delta\lambda} \mathcal{H}_\lambda} e^{-X_{\lambda,\Delta\lambda} \mathcal{H}_\lambda}
\]

(28)
where $X_{\lambda, \Delta \lambda}$ is the generator of the unitary transformation. For the explicit form of $X_{\lambda, \Delta \lambda}$ let us make the following ansatz

$$X_{\lambda, \Delta \lambda} = \sum_{k,m} A_k(\lambda, \Delta \lambda) \Theta_k(\lambda, \Delta \lambda) (f_{km}^\dagger c_{km} - c_{km}^\dagger f_{km})$$  \hspace{1cm} (29)$$

where $\Theta_k(\lambda, \Delta \lambda)$ is the product of two $\Theta$-functions

$$\Theta_k(\lambda, \Delta \lambda) = \Theta(\lambda - |\varepsilon_{f, \lambda} + \Delta_k, \lambda - \Delta \lambda - \varepsilon_k, \lambda|) \times \Theta[(\varepsilon_{f, (\lambda - \Delta \lambda)} + \Delta_k, (\lambda - \Delta \lambda) - \Delta(\lambda - \Delta \lambda) - \varepsilon_k, (\lambda - \Delta \lambda)| - (\lambda - \Delta \lambda)].$$  \hspace{1cm} (30)$$

The operator form of $X_{\lambda, \Delta \lambda}$ is suggested by its first order expression which is easily obtained by expanding (14) in powers of $H_1$ and using Eq. (15) (compare Ref. 5). The yet unknown prefactors $A_k(\lambda, \Delta \lambda)$ will be specified later and depend on $\lambda$ and $\Delta \lambda$. It will turn out that $A_k(\lambda, \Delta \lambda)$ contains contributions to all powers in $V_k$. Note that the ansatz (29) also corresponds to the operator structure of the exact generator of the uncorrelated Fano-Anderson model (see appendix A). We expect the ansatz (29) to be a good approximation also for the correlated model in which conduction and localized $f$ electrons strongly couple. Finally, the $\Theta$-functions in (29) result from the restriction of $H_\lambda$ to particle-hole excitations with $|\varepsilon_{f, \lambda} + \Delta_k, \lambda - \Delta \lambda - \varepsilon_k, \lambda| < \lambda$ and from the corresponding restriction $|\varepsilon_{f, (\lambda - \Delta \lambda)} + \Delta_k, (\lambda - \Delta \lambda) - \Delta(\lambda - \Delta \lambda) - \varepsilon_k, (\lambda - \Delta \lambda)| > \lambda - \Delta \lambda$ for the renormalized model $H_{(\lambda - \Delta \lambda)}$. The two $\Theta$-functions in $\Theta_k(\lambda, \Delta \lambda)$ confine the allowed excitations.

To determine the unknown parameters $A_k(\lambda, \Delta \lambda)$ of the unitary transformation [compare (29)] we will use Eq. (15). First, we have to carry out the unitary transformation (29) explicitly

$$H_{(\lambda - \Delta \lambda)} = \varepsilon_{f, \lambda} \sum_{k,m} e^{X_{\lambda, \Delta \lambda}} f_{km}^\dagger f_{km} e^{-X_{\lambda, \Delta \lambda}} + \sum_{k,m} \Delta_k, \lambda e^{X_{\lambda, \Delta \lambda}} f_{km}^\dagger f_{km} e^{-X_{\lambda, \Delta \lambda}} \left( f_{km}^\dagger f_{km} \right)_{NL} e^{-X_{\lambda, \Delta \lambda}} \hspace{1cm} (31)$$

The transformations for the various operators are given in appendix A [see Eqs. (B23) - (B26)]. For instance, the transformation of $c_{km}^\dagger c_{km}$ reads, (32)

$$e^{X_{\lambda, \Delta \lambda}} c_{km}^\dagger c_{km} e^{-X_{\lambda, \Delta \lambda}} - c_{km}^\dagger c_{km} =$$

$$= - \frac{1}{2D} \Theta_k(\lambda, \Delta \lambda) A_k(\lambda, \Delta \lambda) \left( f_{km}^\dagger c_{km} + \text{h.c.} \right) \left[ 1 - D - \sum_{\tilde{n}(\neq m)} \left( f_{m}^\dagger f_{\tilde{m}} \right)_{L} \right]$$

$$\hspace{1cm} - \frac{1}{2D} \Theta_k(\lambda, \Delta \lambda) \left\{ \cos \left[ 2\sqrt{D} A_k(\lambda, \Delta \lambda) \right] - 1 \right\} \left\{ D \left( f_{km}^\dagger f_{km} \right)_{NL} + (f_{m}^\dagger f_{m})_{L} \right\}$$

$$\hspace{1cm} - D c_{km}^\dagger c_{km} - \left< c_{km}^\dagger c_{km} \right> \left[ 1 - D - \sum_{\tilde{n}(\neq m)} \left( f_{m}^\dagger f_{\tilde{m}} \right)_{L} \right]$$

$$\hspace{1cm} + \frac{1}{2D} \Theta_k(\lambda, \Delta \lambda) \sin \left[ 2\sqrt{D} A_k(\lambda, \Delta \lambda) \right] \left\{ \left( f_{km}^\dagger c_{km} + \text{h.c.} \right) \right\}$$

$$\hspace{1cm} + \frac{1}{2D} \left< f_{km}^\dagger c_{km} + \text{h.c.} \right> \left[ 1 - D - \sum_{\tilde{n}(\neq m)} \left( f_{m}^\dagger f_{\tilde{m}} \right)_{L} \right].$$

Similar expressions can also be found for the transformation of the remaining operators. In deriving (B23) - (B26) an additional factorization approximation was used in order to keep only operators which are bilinear in the fermionic creation and annihilation operators. Spin-flip contributions have been neglected. Moreover, it was assumed that the number of $k$ points which are integrated out by the transformation from $\lambda$ to $\lambda - \Delta \lambda$ is small compared to the total number of $k$ points.
As already mentioned in the introduction, an expansion with respect to the degeneracy $\nu_f$ is utilized in the slave-boson mean-field (SB) theory \[7\]. In contrast, here we incorporate all $1/\nu_f$ corrections which will be reflected by the expectation value $D$ as defined in Eq. \(30\). As one can see from the two terms of the anticommutator of Eq. \(3\), new renormalization contributions are included by which a localized electron at an occupied $f$ site is annihilated and instead a conduction electron is created. These processes are of order $1/\nu_f$ smaller than the usual processes included in the SB theory by which a conduction electron is annihilated and instead a localized electron is generated at a formerly empty $f$ site.

In the next step let us determine the unknown parameters $A_k(\lambda, \Delta \lambda)$. For that purpose, we insert $H_{(\lambda-\Delta \lambda)}$ from \(31\) into Eq. \(16\) and use the transformed quantities \(B^{33} - B^{36}\). Thus, one finds

$$\Theta_k(\lambda, \Delta \lambda) \tan \left[ 2\sqrt{D} A_k(\lambda, \Delta \lambda) \right] = \Theta_k(\lambda, \Delta \lambda) \frac{2\sqrt{DV_k}}{\epsilon_{f,\lambda} + D (\Delta_{k,\lambda} - \Delta \lambda) - \epsilon_{k,\lambda}}. \tag{33}$$

The condition \(33\) for $A_k(\lambda, \Delta \lambda)$ guarantees that $H_{(\lambda-\Delta \lambda)}$ does not contain matrix elements with transition energies larger than $(\lambda - \Delta \lambda)$. Obviously, there is a strong similarity between \(33\) and the corresponding result \(A^{11}\) of the Fano-Anderson model. However, the generator \(33\) of the PAM contains some deviations which reflect the influence of the strong electronic correlations at $f$ sites. It is important to note that the expression \(33\) for $A_k(\lambda, \Delta \lambda)$ is non-perturbatively in $V_k$ and is not restricted to some low order in $V_k$. Moreover note that the values of $A_k(\lambda, \Delta \lambda)$ are determined by Eq. \(32\) only for the case that the excitation energy $(\epsilon_{f,\lambda} + \Delta_{k,\lambda} - \Delta \lambda - \epsilon_{k,\lambda})$ fits in the energy shell restricted by $\Theta_k(\lambda, \Delta \lambda)$. For all other excitations $A_k(\lambda, \Delta \lambda)$ can be set equal to zero. Thus, the parameter $A_k(\lambda, \Delta \lambda)$ of the generator $X_{\lambda,\Delta \lambda}$ is given by

$$A_k(\lambda, \Delta \lambda) = \begin{cases} \frac{1}{2\sqrt{D}} \arctan \left[ \frac{2\sqrt{DV_k}}{\epsilon_{f,\lambda} + D (\Delta_{k,\lambda} - \Delta \lambda) - \epsilon_{k,\lambda}} \right] & \text{for } \Theta_k(\lambda, \Delta \lambda) = 1 \\ 0 & \text{for } \Theta_k(\lambda, \Delta \lambda) = 0 \end{cases} \tag{34}$$

**C. Renormalization equations**

In the following we derive the renormalization equations for the parameters of the Hamiltonian. For that purpose we compare two different expressions for $H_{(\lambda-\Delta \lambda)}$. The first one is obtained by rewriting the renormalization ansatz [Eqs. \(16\) and \(17\)] at cutoff $(\lambda - \Delta \lambda)$

$$H_{(\lambda-\Delta \lambda)} = \epsilon_{f,(\lambda-\Delta \lambda)} \sum_{k,m} f^\dagger_{km} f_{km} + \sum_{k,m} \Delta_{k,(\lambda-\Delta \lambda)} \left( f^\dagger_{km} f_{km} \right)_{NL} \tag{35}$$

$$+ \sum_{k,m} \epsilon_{k,(\lambda-\Delta \lambda)} c^\dagger_{km} c_{km} + E_{(\lambda-\Delta \lambda)} + \sum_{k,m} V_k P_{\lambda} \left( f^\dagger_{km} c_{km} + h.c. \right).$$

The second equation for $H_{(\lambda-\Delta \lambda)}$ is found from Eq. \(31\) by inserting \(B^{33} - B^{36}\). By comparing in both equations the coefficients of the operators $c^\dagger_{km} c_{km}$, $(f^\dagger_{km} f_{km})_{NL}$, and $(f^\dagger_{km} f_{km})_L$ we find the following relations for the parameters
at cutoff $\lambda$ and $(\lambda - \Delta \lambda)$

$$
\epsilon_{k,(\lambda - \Delta \lambda)} - \epsilon_{k,\lambda} = - \frac{1}{2} \left[ \epsilon_{f,\lambda} + D \left( \Delta_{k,\lambda} - \Delta \lambda \right) \right] \cos \left[ 2 \sqrt{D} A_k(\lambda, \Delta \lambda) \right] + 1 
$$

(36)

Thus, the second possible approximation is more difficult and consists in calculating the expectation values with respect to the full Hamiltonian $H(\lambda)$ defined with the equilibrium distribution of $\mathcal{H}_\lambda$. In principle, the expectation values are bilinear in the fermionic creation and annihilation operators. In the case of the energy shift, for instance, we can determine the expectation values

$$
\langle \mathcal{A} \rangle = \frac{\text{Tr} \left( \mathcal{A}_{e^{-\beta H}} \right)}{\text{Tr} \left( e^{-\beta H} \right)} = \frac{\text{Tr} \left( A_{\lambda} e^{-\beta H_{\lambda}} \right)}{\text{Tr} \left( e^{-\beta H_{\lambda}} \right)}
$$

(40)

which follows from unitarity (for any operator $\mathcal{A}$). By setting up additional renormalization equations for the transformed operators $A_{\lambda}$, one can determine the expectation values $\langle \mathcal{A} \rangle$. Note that in the equations for $A_{\lambda}$ the unknown expectation values enter again so that they have to be solved self-consistently. This approach is rather involved but has the advantage that expectation values in (39) no longer depend on the cutoff energy $\lambda$. Renormalization equations for transformed operators also have to be used if dynamical correlation functions are
evaluated. For example, to find the densities of states of the $f$ electrons

$$\rho_f(\omega) = \frac{1}{N} \sum_{km} \left< \left[ \hat{f}_{km}^\dagger, \delta(L+\omega) \hat{f}_{km} \right]_+ \right>$$

(41)

and of the $c$ electrons

$$\rho_c(\omega) = \frac{1}{N} \sum_{km} \left< \left[ \hat{c}_{km}^\dagger, \delta(L+\omega) \hat{c}_{km} \right]_+ \right>$$

(42)

one has to apply the renormalization transformation on $\hat{f}_{km}^\dagger$ and $\hat{c}_{km}^\dagger$. This will be done in appendix C. Note that in Eqs. (41) and (42) the Liouville operator $L$ of the full Hamiltonian was introduced which is defined by $L A = [H, A]$ for any operator variable $A$.

IV. ANALYTICAL SOLUTION

Alternatively, one can also find approximate analytical solutions for the renormalization equations (36)-(39). For this purpose three approximations have to be used:

(i) All excitation values are calculated using the full Hamiltonian $H$ (see the discussion at the end of Sec. III), i.e.

$$\langle \ldots \rangle_H \approx \langle \ldots \rangle = \langle \ldots \rangle,$$

(43)

so that they are independent from the renormalization parameter $\lambda$.

(ii) The $\lambda$ dependence of the renormalized $f$ level will be neglected,

$$\varepsilon_{f,\lambda} \approx \tilde{\varepsilon}_f.$$  

(44)

The spirit of this approximation is similar to that used in the slave-boson theory. There a renormalized $f$ level is used from the very beginning. Within the present treatment one might expect that $\varepsilon_{f,\lambda}$ increases with decreasing $\lambda$ from its initial value $\varepsilon_f$ and reaches its final value $\tilde{\varepsilon}_f$ already at finite $\lambda$.

(iii) The averaged dispersion of $f$ electrons will be neglected,

$$\bar{\Delta}_\lambda = \frac{1}{N} \sum_k \Delta_{k,\lambda} \approx 0.$$  

(45)

These approximation enable us to map the renormalization equations of the PAM to those of the exactly solvable Fano-Anderson model (see appendix A).

A. Quasi-particle energies

Eq. (37) depends on differences of the parameters of the transformed Hamiltonians at $\lambda$ and $(\lambda - \Delta \lambda)$. Therefore, this equation can easily be integrated between a lower cutoff $\lambda \to 0$ and the cutoff $\Lambda$ of the original model. One finds

$$\tilde{\Delta}_k = - [\tilde{\varepsilon}_k - \varepsilon_k].$$  

(46)

where the initial parameter values $\langle \ldots \rangle_{\lambda=0}$ were used. Furthermore, we have defined $\tilde{\Delta}_k = \Delta_{k,(\lambda \to 0)}$ and $\tilde{\varepsilon}_k = \varepsilon_{k,(\lambda \to 0)}$. Eq. (39) can also be integrated in the same way so that we find

$$\tilde{E} = - \langle \hat{n}_f^\dagger \rangle N (\tilde{\varepsilon}_f - \varepsilon_f) - \langle \hat{n}_f^\dagger \rangle \frac{D}{\bar{\Delta}} \sum_k (\tilde{\varepsilon}_k - \varepsilon_k).$$  

(47)

Here, again the initial parameter values $\langle \ldots \rangle_{\lambda=0}$ and Eq. (29) have been used. Furthermore, we have defined $\tilde{E} = E_{(\lambda \to 0)}$ and $\tilde{\varepsilon}_f = \varepsilon_{f,(\lambda \to 0)}$. The second term on the r.h.s. of (47) vanishes if we use Eq. (10) and approximation (45) so that we obtain

$$\tilde{E} = - \langle \hat{n}_f^\dagger \rangle N (\tilde{\varepsilon}_f - \varepsilon_f).$$  

(48)
It is more difficult to solve the remaining renormalization equations (36) and (38). First, the approximations lead to a decoupling of Eq. (36) for different \( k \) values. Thus, by eliminating excitations from large to small cutoff values \( \lambda \) each \( k \) state is renormalized only once. Such a step-like renormalization behavior is also obtained in the Fano-Anderson model (see appendix A). A further similarity to this simpler model is found by inserting the one-particle energy eigenmodes \( \tilde{\epsilon}_f \) and (A10). In particular, the equivalence of the one-particle energies can be seen by replacing by functional derivative \( F \).

\[
\tan \left(2\sqrt{DA_k}\right) = \frac{2\sqrt{DV_k}}{\tilde{\epsilon}_f - \tilde{\epsilon}_k},
\]

\[
\tilde{\epsilon}_k - \tilde{\epsilon}_k = \frac{1}{2} \left[ \cos \left(2\sqrt{DA_k}\right) - 1 \right] \left[ \tilde{\epsilon}_k - \tilde{\epsilon}_f \right] - \sqrt{DV_k} \sin \left(2\sqrt{DA_k}\right).
\]

Here, the step-like renormalization behavior and the initial parameter values \( \beta \) have been used. Note that in the case of a step-like renormalization the parameters \( A_k \) of the generator of the unitary transformation do not depend on \( \lambda \) and \( \Delta \lambda \). The above equations are very similar to those obtained for the Fano-Anderson model [compare with Eqs. (A11) and (A10)]. In particular, the equivalence of the one-particle energies can be seen by replacing \( \sqrt{DV_k} \) by \( V_k \). Moreover, one immediately finds from (36) and (40) the following result for the renormalized \( c \) electron one-particle energy

\[
\tilde{\epsilon}_k = \frac{\tilde{\epsilon}_f + \tilde{\epsilon}_k - \text{sgn}(\tilde{\epsilon}_f - \tilde{\epsilon}_k)W_k}{2},
\]

where

\[
W_k = \sqrt{(\tilde{\epsilon}_k - \tilde{\epsilon}_f)^2 + 4D|V_k|^2}.
\]

Obviously, Eqs. (40) and (53) also determine the \( f \) type quasi-particle excitation energy which is given by

\[
\tilde{\omega}_k := \tilde{\epsilon}_f + \tilde{\Delta}_k = \frac{\tilde{\epsilon}_f + \tilde{\epsilon}_k + \text{sgn}(\tilde{\epsilon}_f - \tilde{\epsilon}_k)W_k}{2}.
\]

where approximation (54) has been used. Thus, we have obtained two quasi-particle excitations. According to (16) and (53) the renormalized Hamiltonian reads

\[
\tilde{\mathcal{H}} := \mathcal{H}(\lambda \rightarrow 0) = \sum_{k,m} \tilde{\omega}_k f_{km}^\dagger f_{km}^{\vphantom{\dagger}} + \sum_{k,m} \tilde{\epsilon}_k c_{km}^\dagger c_{km}^{\vphantom{\dagger}} + \tilde{E}.
\]

Note that in \( \tilde{\mathcal{H}} \) the hybridization was completely used up for the renormalization of the parameters of \( \mathcal{H}_0 \). Also the eigenmodes \( f_{km} \) and \( c_{km} \) of \( \tilde{\mathcal{H}} \) do not change their character as function of the wave vector due to the presence of the sgn-functions in (51) and (54). Instead they remain \( f \)-like or \( c \)-like for all values of \( k \). Furthermore, the one-particle energies (51) and (53) still depend on two unknown quantities, namely, the renormalized \( f \) level \( \tilde{\epsilon}_f \) and the expectation value \( D \) [see Eq. (28)] which have to be determined in the following.

### B. Free energy and equations of self-consistency

First, let us calculate the averaged \( f \) electron occupation number \( \langle n_f \rangle \) from the free energy \( F \). Note that \( \mathcal{H}_\lambda \) is connected with the original Hamiltonian \( \mathcal{H} \) by an unitary transformation. Therefore, the free energy can also be evaluated from \( \mathcal{H}_\lambda \). In particular, the relation

\[
F = -\frac{1}{\beta} \ln \text{Tr} e^{-\beta \mathcal{H}} = -\frac{1}{\beta} \ln \text{Tr} e^{-\beta \tilde{\mathcal{H}}} =: \tilde{F}
\]

holds. Because of \( \tilde{\mathcal{H}} \) describes an non-interacting Fermi system the free energy \( F \) can be easily calculated

\[
F = -\frac{\nu_f}{\beta} \sum_k \ln \left[ 1 + e^{-\beta \tilde{\epsilon}_f} \right] - \frac{\nu_f}{\beta} \sum_k \ln \left[ 1 + e^{-\beta \tilde{\omega}_k} \right] + \tilde{E}.
\]

The \( f \) electron occupation number is found from \( \tilde{F} \) by functional derivative

\[
\langle n_f \rangle = \frac{1}{N} \frac{\partial \tilde{F}}{\partial \tilde{\epsilon}_f} = \frac{1}{N} \left. \frac{\partial \tilde{\mathcal{H}}}{\partial \tilde{\epsilon}_f} \right|_{\tilde{\mathcal{H}}}.
\]
which can be easily performed. We finally obtain a relation of the following structure

\[ 0 = \{ \ldots \} \left( \frac{\partial \hat{F}}{\partial \varepsilon_f} \right) + \{ \ldots \} \left( \frac{\partial (\hat{n}_f^\dagger)}{\partial \varepsilon_f} \right). \]  

(58)

We are interested in solutions of the renormalization equations which describe mixed valence and heavy Fermion behavior. For these cases the derivatives in Eq. (58) are non-zero so that solutions can be found by setting both brace expressions equal to zero. In this way the following self-consistent equations for the renormalized \( \tilde{\varepsilon}_f \) level and the averaged \( f \) electron occupation number \( \hat{n}_f^\dagger \) are found,

\[ \langle \hat{n}_f^\dagger \rangle = \frac{\nu_f}{N} \sum_k f(\tilde{\varepsilon}_k) \left\{ \frac{1}{2} + \text{sgn}(\tilde{\varepsilon}_f - \tilde{\varepsilon}_k) \frac{\tilde{\varepsilon}_k - \tilde{\varepsilon}_f}{2W_k} \right\}, \]  

(59)

\[ \tilde{\varepsilon}_f - \varepsilon_f = \frac{\nu_f - 1}{N} \sum_k \text{sgn}(\tilde{\varepsilon}_f - \varepsilon_k) f(\tilde{\varepsilon}_k) \frac{|V_k|^2}{W_k} \]  

\[ + \frac{\nu_f - 1}{N} \sum_k \text{sgn}(\varepsilon_k - \tilde{\varepsilon}_f) f(\hat{\omega}_k) \frac{|V_k|^2}{W_k}. \]  

(60)

Note that these equations are quite similar to those which are found in the slave-boson (SB) formalism. In particular, the limit \( \nu_f \to \infty \) of Eqs. (59) and (60) perfectly agrees with the SB equations.

C. Expectation values

The remaining expectation values \( \langle \hat{c}_{km}^\dagger \hat{c}_{km} + \text{h.c.} \rangle \) can also be evaluated from the free energy

\[ \langle \hat{c}_{km}^\dagger \hat{c}_{km} \rangle = \frac{1}{\nu_f} \frac{\partial \hat{F}}{\partial \varepsilon_k} = \frac{1}{\nu_f} \left\langle \frac{\partial \hat{H}}{\partial \varepsilon_k} \right\rangle_{\hat{n}}, \]  

(61)

\[ \langle \hat{c}_{km}^\dagger \hat{c}_{km} + \text{h.c.} \rangle = \frac{1}{\nu_f} \frac{\partial \hat{F}}{\partial V_k} = \frac{1}{\nu_f} \left\langle \frac{\partial \hat{H}}{\partial V_k} \right\rangle_{\hat{n}}. \]  

(62)

Both expressions can be evaluated similarly to (57). By using (59) and (60) we find

\[ \langle \hat{c}_{km}^\dagger \hat{c}_{km} \rangle = \frac{1}{2} \left[ 1 - \text{sgn}(\tilde{\varepsilon}_f - \varepsilon_k) \frac{\tilde{\varepsilon}_k - \tilde{\varepsilon}_f}{2W_k} \right] f(\tilde{\varepsilon}_k), \]  

(63)

\[ + \frac{1}{2} \left[ 1 - \text{sgn}(\varepsilon_k - \tilde{\varepsilon}_f) \frac{\varepsilon_k - \tilde{\varepsilon}_f}{2W_k} \right] f(\hat{\omega}_k), \]  

\[ \langle \hat{c}_{km}^\dagger \hat{c}_{km} + \text{h.c.} \rangle = -2 \text{sgn}(\tilde{\varepsilon}_f - \varepsilon_k) \frac{DV_k}{W_k} f(\tilde{\varepsilon}_k) - 2 \text{sgn}(\varepsilon_k - \tilde{\varepsilon}_f) \frac{DV_k}{W_k} f(\hat{\omega}_k). \]  

(64)

Note that also Eqs. (63) and (64) are very similar to the corresponding SB results.

D. One-particle operators and density of states

Next we calculate the densities of states of the \( f \) and \( c \) electrons [compare Eqs. (41) and (42)]. For that purpose, we have to integrate the renormalization equations (C9) and (C10) to determine the transformed one-particle operators. In the case of the analytical solution, (C9) and (C10) can be exactly solved if the basic approximations (44) and (45)
are used. As already discussed above, in this case the different \( k \) values are not coupled with each other and we obtain a step-like renormalization behavior. Thus, we find

\[
\tilde{u}_k = \cos \left( \sqrt{D}A_k \right) \quad \text{and} \quad \tilde{v}_k = \frac{1}{\sqrt{D}} \sin \left( \sqrt{D}A_k \right)
\]

(65)

where the initial parameter values \((C2)\) were used. Furthermore, we have defined \( \tilde{u}_k = u_k(\lambda \rightarrow 0) \) and \( \tilde{v}_k = v_k(\lambda \rightarrow 0) \). Combining the generator of the unitary transformation \((49)\), the normalization condition \((C3)\), and Eq. \((65)\) we finally obtain

\[
|\tilde{u}_k|^2 = \frac{1}{2} \left\{ 1 - \frac{\varepsilon_k - \tilde{\varepsilon}_f \text{sgn}(\tilde{\varepsilon}_f - \varepsilon_k)}{W_k} \right\}
\]

(66)

\[
|\tilde{v}_k|^2 = \frac{1}{2D} \left\{ 1 + \frac{\varepsilon_k - \tilde{\varepsilon}_f \text{sgn}(\tilde{\varepsilon}_f - \varepsilon_k)}{W_k} \right\}.
\]

(67)

Thus, the coefficients \( \tilde{u}_k \) and \( \tilde{v}_k \) can be directly calculated from the results of the self-consistent equations \((50)\) and \((60)\).

To calculate the densities of states \((11)\) and \((12)\) we use the relation \((40)\), which follows from the unitary of all operators. Thus, Eqs. \((11)\) and \((12)\) can be rewritten as

\[
\rho_f(\omega) = \frac{1}{N} \sum_{k,m} \left\langle \left[ f_{km}^\dagger(\lambda \rightarrow 0), \delta \left( \tilde{\mathcal{L}} + \omega \right) f_{km}(\lambda \rightarrow 0) \right] \right\rangle_{\tilde{\mathcal{H}}},
\]

(68)

\[
\rho_c(\omega) = \frac{1}{N} \sum_{k,m} \left\langle \left[ c_{km}^\dagger(\lambda \rightarrow 0), \delta \left( \tilde{\mathcal{L}} + \omega \right) c_{km}(\lambda \rightarrow 0) \right] \right\rangle_{\tilde{\mathcal{H}}},
\]

(69)

where \( \tilde{\mathcal{L}} \) is the Liouville operator of the final Hamiltonian \( \tilde{\mathcal{H}} \) which is defined by \( \tilde{\mathcal{L}}A = [\tilde{\mathcal{H}}, A] \) for all operator variables \( A \). Due to the structure \((71)\) of the final Hamiltonian \( \tilde{\mathcal{H}} \), Eqs. \((68)\) and \((69)\) can be easily evaluated. Using \((71)\), \((34)\), \((66)\), and \((67)\) we obtain

\[
\rho_f(\omega) = D \frac{1}{N} \sum_{k,m} \left\{ |\tilde{u}_k|^2 \delta (\omega - \tilde{\omega}_k) + D |\tilde{v}_k|^2 \delta (\omega - \tilde{\varepsilon}_k) \right\},
\]

(70)

\[
\rho_c(\omega) = D \frac{1}{N} \sum_{k,m} \left\{ |\tilde{u}_k|^2 \delta (\omega - \tilde{\varepsilon}_k) + D |\tilde{v}_k|^2 \delta (\omega - \tilde{\omega}_k) \right\}.
\]

(71)

E. Results and comparison with slave-boson mean-field theory

In this subsection we shall compare the results of our analytical solution discussed above with those of the slave-boson mean-field (SB) treatment. As already mentioned, the limit \( \nu_f \rightarrow \infty \) of the derived self-consistent equations \((50)\) and \((60)\) is completely equivalent to the SB equations. Furthermore, in this limit the expectation values of our analytical solution [see Eqs. \((68)\) and \((69)\)] and the SB treatment also perfectly agree. Therefore, we want to concentrate on the case of small degeneracy \( \nu_f \). At this point it is important to notify that we have never exploited an \( 1/\nu_f \) expansion in the derivation of the analytical solution of the PAM so that it is valid for large as well as small degeneracy \( \nu_f \).

For simplicity, let us consider an one-dimensional PAM with 50,000 lattice sites, a linear dispersion relation for the conduction electrons, and a \( k \) independent hybridization \( V_k = V \) and compare our results with those of the slave-boson mean-field (SB) theory. In particular, we are interested in the dependence of the results on the degeneracy \( \nu_f \).

At first, let us fix the degeneracy of the angular momentum to \( \nu_f = 4 \). The other parameters are chosen as follows \( \nu_f V^2 = 0.36, \varepsilon_f = -0.3, \) chemical potential \( \mu = 0, \) and \( T = 0.00001 \) where all energies are given in units of the half bandwidth. As can be seen from Fig. 1 the renormalized quasi-particle energies, i.e. \( \tilde{\varepsilon}_k \) and \( \tilde{\omega}_k \), obtained from \((31)\), \((53)\), \((59)\), and \((60)\) (full and dashed thick lines), and the quasi-particle bands of the SB theory (dotted lines) seem to be quite similar. However, the averaged \( f \) occupation \( \langle \hat{n}_f^\dagger \rangle = 0.855 \) and the renormalized \( f \) level \( \tilde{\varepsilon}_f = 0.071 \) differ significantly from the SB results \((\langle \hat{n}_f^\dagger \rangle = 0.586 \) and \( \tilde{\varepsilon}_f = 0.115 \)). These differences are mainly caused by the fact that we have taken into account all \( 1/\nu_f \) corrections which are absent in the SB treatment. Note that \( 1/\nu_f \) corrections
FIG. 1: Dispersion relations of a one-dimensional PAM ($N = 50000$, $\nu_f = 4$, $\nu_f V^2 = 0.36$, $\varepsilon_f = -0.3$, $\mu = 0$, $T=0.00001$). Here, the unrenormalized one-particle energies $\epsilon_k$ and $\epsilon_f$ are plotted with full and dashed thin lines. The renormalized quasiparticle energies $\tilde{\epsilon}_k$ and $\tilde{\omega}_k$ are shown with full and dashed thick lines. Furthermore, the quasiparticle energies of the SB approach are drawn by use of dotted lines.

FIG. 2: Density of states of the $f$ electrons (upper panel) and of the $c$ electrons (lower panel) where all parameters are chosen as in Fig. 1. A broadening of the $\delta$-functions of 0.0001 is used. The results of the analytical PRM solution (SB theory) are drawn as solid (dashed) lines.
FIG. 3: Dependence of the renormalized $f$ level $\tilde{\varepsilon}_f$ (left panel) and of the averaged $f$ occupation $\langle \hat{n}_f \rangle$ (right panel) on the degeneracy $\nu_f$ of the angular momentum where all other parameters are chosen as in Fig. 1. The results of the analytical solution (SB theory) are drawn using solid (dashed) lines.

FIG. 4: Dependence of the renormalized $f$ level $\tilde{\varepsilon}_f$ (left panel) and of the averaged $f$ occupation $\langle \hat{n}_f \rangle$ (right panel) on the original $f$ energy $\varepsilon_f$ where all other parameters are chosen as in Fig. 1. The results of the analytical solution (SB theory) are drawn using solid (dashed) lines.
allow for additional renormalization processes which lead to a lowering of the free energy for the whole parameter space.

It is well known that the quasi-particles of the SB theory change their character as function of $k$ between a more $f$-like and more $c$-like behavior. As was mentioned before, in the present treatment excitations do not change their character as function of $k$. However, the quasi-particle energies show jumps in their $k$ dependence where the renormalization contributions change their sign from positive to negative values or vice versa. Note, that the various parts of the quasiparticle bands fit perfectly together (see Fig. 1).

As compared to the dispersion relations plotted in Fig. 1, the densities of states of the $f$- and $c$-electrons in Fig. 2 show much better the differences between the results of the present analytical solution and of the SB treatment. In particular, the smaller value for the renormalized $f$ level $\tilde{\varepsilon}_f$ obtained from our PRM treatment leads to much higher density of states at the Fermi surface than the SB treatment. Note that such an enhanced density of states at the Fermi energy is a clear signature of heavy fermion behavior.

Next, we discuss the dependence on the degeneracy parameter $\nu_f$. For that purpose we vary $\nu_f$ by keeping $\nu_f V^2 = 0.36$ fixed. In contrast to the SB results for $\langle \hat{n}_f \rangle$ and $\tilde{\varepsilon}_f$, which are almost unchanged (see Fig. 3), the analytical solutions show a remarkable dependence on the degeneracy $\nu_f$. In particular, for small $\nu_f$, the $1/\nu_f$ corrections included in the PRM approach lead to serious deviations from the SB results. From these additional $1/\nu_f$ corrections follows a more pronounced heavy Fermion behavior. As already mentioned above, the limit $\nu_f \to \infty$ of our analytical solution perfectly agrees with the SB theory. To perform this limit one has to replace the expectation value $D$ by $(1 - \langle \hat{n}_f \rangle)$ so that all processes are neglected by which a localized electron at an occupied $f$ site is annihilated and instead a conduction electron is created [compare discussion below Eq. (32)].

In Fig. 4 the renormalized $f$ level $\tilde{\varepsilon}_f$ and the averaged $f$ occupation $\langle \hat{n}_f \rangle$ are plotted as functions of the original $f$ energy $\varepsilon_f$. The momentum degeneracy has been fixed at $\nu_f = 4$. As is seen, the $1/\nu_f$ corrections do not only cause a dependence of the results on the degeneracy $\nu_f$ (as shown in Fig. 3) but also lead to a reduction of the stability range of heavy Fermion type solutions.

The $1/\nu_f$ corrections also affect the thermodynamic properties of the system. In Fig. 5 the temperature dependence of the averaged $f$ occupation $\langle \hat{n}_f \rangle$ is shown where $\nu_f$ has been fixed to $\nu_f = 4$. We observe that $\langle \hat{n}_f \rangle$ goes with increasing temperature much faster to 1 than the SB results. Thus, the $1/\nu_f$ corrections lead to a lowering of the
Kondo temperature $T_K$ which may be defined as that temperature at which $\langle \hat{n}_f^i \rangle$ becomes 1.

As can be seen from Fig. 4 the analytical PRM solution breaks down when the unrenormalized $f$ level becomes smaller than some critical values. A similar behavior is also known from the SB solution. For instance, the solution for $\langle \hat{n}_f^i \rangle$ breaks down when for fixed $\varepsilon_f$ the chemical potential $\mu$ is increased beyond some critical value. The reason for this breakdown is not completely clear. May be, it is due to some rough approximation used both in the PRM treatment and the SB theory, for instance those from Sect. III.A which have their counterparts in the SB treatment. Alternative, the breakdown of the PRM and the SB solutions might be a signature of a genuine phase transition. Recently it was suggested that in certain systems like CeCu$_2$Si$_2$ there might be a transition between an intermediate valence regime with fluctuating $f$ charges and a regime with integral $f$ charge when the pressure is decreased. In the integral regime which is described by the Kondo Hamiltonian there is no longer a renormalized $f$ level at the Fermi level. This might be the reason that the self-consistent solution for $\tilde{\varepsilon}_f$ no longer exists. Note however that such a phase transition does not appear in a recent alternative discussion of the PAM on the basis of Hubbard operators in Ref. 12. This approach is based on an extended chain approximation and gives the same quasi-particle energies as in the SB theory [6, 7]. However, it leads to completely different equations for the renormalized $\tilde{\varepsilon}_f$ level and for the averaged $f$ occupation $\langle \hat{n}_f^i \rangle$. Results have been found which are very similar to the SB solutions for those parameter regimes where the SB solution exists. In contrast, the PRM solution leads to substantial deviations from the SB results in particular for small values of $\nu_f$. Note however that apart from the $1/\nu_f$ corrections we have used similar approximations as in the SB theory to derive our analytical solution.

V. CONCLUSIONS

In summary, in this paper we have applied a recently developed projector-based renormalization method (PRM) to the periodic Anderson model (PAM) in the limit of infinitely large Coulomb repulsion at $f$ sites. By using an additional factorization approximation we have derived renormalization equations for the parameters of the Hamiltonian. In this way, the PAM is mapped to a free system consisting of two uncorrelated quasiparticle bands. Similar uncorrelated Hamiltonians have been also derived before by different theoretical approaches, such as the Gutzwiller projection and the SB theory where $1/\nu_f$ expansions have been exploited. In contrast, the present approach is valid for any $\nu_f$. Due to the factorization approximation certain expectation values enter which prevent a direct numerical evaluation of the renormalization equations. In principle, the expectation values could be determined self-consistently by deriving additional renormalization equations also for the operators which enter the expectation values. This has not been done in this paper.

To obtain instead an analytical solution we have used a renormalized $f$ level which was assumed to be constant during the renormalization process. The spirit of this approximation is similar to that used in the SB theory [6, 7]. We obtain self-consistent equations for the renormalized $f$ level $\tilde{\varepsilon}_f$ and the averaged $f$ occupation $\langle \hat{n}_f^i \rangle$ which are quite similar to those of the SB theory [6]. In particular, in the limit $\nu_f \rightarrow \infty$ our solution perfectly agrees with the SB result but strongly differs from it for smaller values of $\nu_f$. To compare our results in more detail with those of the SB approach we have also considered an one-dimensional PAM with a linear dispersion relation of the conduction electrons and a $k$ independent hybridization. Note that the character of the obtained two quasi-particle bands of the two treatments differ. Whereas the quasi-particles of the SB theory change their character as function of $k$ from a more $f$-like to a more $c$-like behavior and vice versa the excitations of the PRM treatment do not change their character. Instead, the quasi-particle energies show jumps as function of $k$ where, however, the various parts of the quasi-particle bands fit perfectly together. The influence of the degeneracy $\nu_f$ has been studied by varying $\nu_f$ with fixed $\nu_f V^2$. Whereas the SB results are almost unchanged, our analytical results show a remarkable dependence on the degeneracy $\nu_f$. Especially, serious deviations are found for small values of $\nu_f$.

Finally, from a more technical point of view, note that in this paper the PRM method was applied to a physical system for the first time without using any perturbation theory.

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APPENDIX A: RENORMALIZATION OF THE EXACT SOLVABLE FANO-ANDERSON MODEL

In this appendix we illustrate the usefulness of the projector-based renormalization method (PRM) for the case of a simple model. We apply the approach of Sec. II to the exactly solvable Fano-Anderson model \[3, 4\]. This model was already discussed in the framework of the present approach in Ref. \[8\]. However, now this will be done in a consequent non-perturbative manner.

1. Model

The Fano-Anderson model consists of dispersionless \(f\) electrons which interact with conducting electrons. Thereby all correlation effects are neglected. The Hamiltonian reads

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \tag{A1}
\]

\[
\mathcal{H}_0 = \sum_{k,m} \left( \varepsilon_f f_{km}^\dagger f_{km} + \varepsilon_k c_{km}^\dagger c_{km} \right),
\]

\[
\mathcal{H}_1 = \sum_{k,m} V_k \left( f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km} \right).
\]

As in Eq. (1) the index \(i\) denotes the \(f\) sites, \(k\) is the wave vector, and \(V_k\) describes the hybridization between conduction and localized electrons. The excitation energies \(\varepsilon_k\) and \(\varepsilon_f\) for conduction and localized electrons are measured from the chemical potential \(\mu\). Both types of electrons are assumed to have the same angular momentum index \(m\) with values \(m = 1 \ldots \nu_f\). Of course, the model is easily solved and leads to two hybridized bands

\[
\mathcal{H} = \sum_{k,m} \omega_k^{(\alpha)} \alpha_{km}^\dagger \alpha_{km} + \sum_{k,m} \omega_k^{(\beta)} \beta_{km}^\dagger \beta_{km}, \tag{A2}
\]

where

\[
\omega_k^{(\alpha,\beta)} = \frac{\varepsilon_k + \varepsilon_f}{2} \pm \frac{1}{2} W_k,
\]

\[
W_k = \sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4 |V_k|^2}.
\]

The eigenmodes \(\alpha_{km}^\dagger\) and \(\beta_{km}^\dagger\) are given by linear combinations of \(c_{km}^\dagger\) and \(f_{km}^\dagger\),

\[
\alpha_{km}^\dagger = u_k f_{km}^\dagger + v_k c_{km}^\dagger, \quad \beta_{km}^\dagger = -v_k f_{km}^\dagger + u_k c_{km}^\dagger,
\]

\[
|u_k|^2 = \frac{1}{2} \left( 1 - \frac{\varepsilon_k - \varepsilon_f}{W_k} \right), \quad |v_k|^2 = \frac{1}{2} \left( 1 + \frac{\varepsilon_k - \varepsilon_f}{W_k} \right). \tag{A3}
\]

2. Renormalization ansatz

In the renormalization approach we integrate out particle-hole excitations of conduction and \(f\) electrons which enter due to the hybridization term \(\mathcal{H}_1\). We expect to finally obtain from the PRM an effectively free model. The starting point of the method is a renormalized Hamiltonian \(\mathcal{H}_\lambda\) which is obtained after all excitations with energies larger than a given cutoff \(\lambda\) have been eliminated. Due to the result of the preceding section it should have the following form

\[
\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda}, \tag{A4}
\]

\[
\mathcal{H}_{0,\lambda} = \sum_{k,m} \left( \varepsilon_f f_{km}^\dagger f_{km} + \varepsilon_k c_{km}^\dagger c_{km} \right),
\]

\[
\mathcal{H}_{1,\lambda} = \sum_{k,m} V_k \left( f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km} \right) = P_\lambda \mathcal{H}_1.
\]
As it turns out, no renormalization of the hybridization $V_k$ occurs so that $V_k$ is assumed to be $\lambda$ independent from the beginning. Like in the exact diagonalization different $k$ states do not coupled during the renormalization process. Thus, by eliminating excitations from large to low $\lambda$ values, each $k$ state is renormalized only once leading to a step like renormalization behavior. This means, for a given cutoff $\lambda$ all $k$ states with excitations $|\varepsilon_k - \varepsilon_f| > \lambda$ have already been renormalized whereas those with $|\varepsilon_k - \varepsilon_f| < \lambda$ have not. Thus, $\mathcal{H}_\lambda$ can be written as a sum of two parts $\mathcal{H}_\lambda = \mathcal{H}_\lambda^< + \mathcal{H}_\lambda^>$ where

$$
\mathcal{H}_\lambda^< = \sum_{k,m} \left[ \varepsilon_f f_{km}^\dagger f_{km} + \varepsilon_k c_{km}^\dagger c_{km} + V_k \left( f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km} \right) \right],
$$

(A5)

$$
\mathcal{H}_\lambda^> = \sum_{k,m} \left( \varepsilon_k^f f_{km}^\dagger f_{km} + \varepsilon_k^c c_{km}^\dagger c_{km} \right).
$$

(A6)

$\mathcal{H}_\lambda^<$ is the unchanged part of $\mathcal{H}_\lambda$ whereas $\mathcal{H}_\lambda^>$ is renormalized due to the elimination of excitations $|\varepsilon_k - \varepsilon_f| > \lambda$. $\varepsilon_k^f$ and $\varepsilon_k^c$ denote the renormalized energies.

3. Transformation of the Hamiltonian

For the explicit evaluation of $\mathcal{H}_\lambda^<$ let us apply the unitary transformation \( e^{X_\lambda} \) on the original Hamiltonian $\mathcal{H}$

$$
\mathcal{H}_\lambda = e^{X_\lambda} \mathcal{H} e^{-X_\lambda}.
$$

(A7)

For the generator $X_\lambda$ of the unitary transformation an exact expression can be given. By inspection of the perturbation expansion in terms of $V_k$ one finds that $X_\lambda$ must have the following operator structure

$$
X_\lambda = \sum_{k,m} A_k \left( f_{km}^\dagger c_{km} - c_{km}^\dagger f_{km} \right)
$$

(A8)

with yet unknown prefactors $A_k$. Eq. (A8) will be taken as ansatz. Then $\mathcal{H}_\lambda^>$ can be easily evaluated since only $k$ values with $|\varepsilon_k - \varepsilon_f| > \lambda$ renormalize the Hamiltonian. Due to the fermionic anticommutator relations different $k$ values are not coupled. To find $\mathcal{H}_\lambda^>$, we consider the transformation of the various operators. For instance, we obtain

$$
e^{X_\lambda} c_{km}^\dagger c_{km} e^{-X_\lambda} - c_{km}^\dagger c_{km} = \frac{1}{2} \Theta (|\varepsilon_k - \varepsilon_f| - \lambda) \left\{ \cos (2A_k) - 1 \left( c_{km}^\dagger c_{km} - f_{km}^\dagger f_{km} \right) + \sin (2A_k) \left( f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km} \right) \right\}.
$$

(A9)

Similar relations can also be found for the transformations of the operators $f_{km}^\dagger f_{km}$ and $(f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km})$. Thus, $\mathcal{H}_\lambda^>$ reads

$$
\mathcal{H}_\lambda^> = \sum_{k,m} \left\{ \left[ \varepsilon_f - 1 \frac{1}{2} \cos (2A_k) - 1 \right] (\varepsilon_k - \varepsilon_f) + V_k \sin (2A_k) \right\} f_{km}^\dagger f_{km}
$$

(A10)

$$
+ \left\{ \varepsilon_k + 1 \frac{1}{2} \cos (2A_k) - 1 \right\} (\varepsilon_k - \varepsilon_f) - V_k \sin (2A_k) \right\} c_{km}^\dagger c_{km}
$$

$$
+ \left\{ V_k + 1 \frac{1}{2} \sin (2A_k) (\varepsilon_k - \varepsilon_f) + V_k \cos (2A_k) - 1 \right\} \left( f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km} \right).\right
$$

In contrast to the expected form \( A_7 \) for $\mathcal{H}_\lambda^>$ the expression \( A10 \) still contains a hybridization part proportional to $(f_{km}^\dagger c_{km} + c_{km}^\dagger f_{km})$ with excitation energies larger than $\lambda$. The requirement $\langle Q \rangle_\lambda \mathcal{H}_\lambda = 0$, leads to the following condition for $A_k$

$$
\tan (2A_k) = \frac{2V_k}{\varepsilon_f - \varepsilon_k}.
$$

(A11)
Eq. \((A11)\) guarantees that the hybridization vanishes in \((A10)\) and \(H^>_\lambda\) becomes diagonal. Note that according to \((A11)\), the quantity \(A_k\) changes its sign when the energy difference \(\varepsilon_f - \varepsilon_k\) changes its sign. By inserting \((A11)\) into \((A10)\) one finds

\[
H^>_\lambda = \sum_{k,m} \left( \tfrac{\varepsilon^f_k}{2} f^\dagger_k f_m + \tfrac{\varepsilon^c_k}{2} c^\dagger_k c_m \right) \tag{A12}
\]

where the renormalized energies are given by

\[
\varepsilon^f_k = \frac{\varepsilon_f + \varepsilon_k}{2} + \frac{\text{sgn}(\varepsilon_f - \varepsilon_k)}{2} W_k, \tag{A13}
\]

\[
\varepsilon^c_k = \frac{\varepsilon_f + \varepsilon_k}{2} - \frac{\text{sgn}(\varepsilon_f - \varepsilon_k)}{2} W_k.
\]

For \(\lambda \to 0\) the Hamiltonian is completely renormalized. The final Hamiltonian \(\hat{H} := H(\lambda \to 0)\) reads

\[
\hat{H} = \sum_{k,m} \left( \varepsilon^f_k f^\dagger_k f_m + \varepsilon^c_k c^\dagger_k c_m \right). \tag{A14}
\]

Note that the final result \((A14)\) corresponds to the diagonal Hamiltonian of eq. \((A2)\). In particular, all expectation values completely agree between the two approaches. (To calculate expectation values by using Eq. \((A14)\) one also has to transform the operators which enter the expectation values. For more details see Ref. \([8]\).) However, in contrast to the eigenmodes \(\alpha^f_{km}\) and \(\beta^c_{km}\) of \((A2)\) the present eigenmodes \(f^\dagger_{km}\) and \(c^\dagger_{km}\) of \((A14)\) remain \(f\)-like and \(c\)-like for all values of \(k\). In return, the \(\lambda\) dependent excitation energies \(\varepsilon^f_{k,\lambda}\) and \(\varepsilon^c_{k,\lambda}\) show as function of \(\lambda\) a step-like behavior at \(\lambda = |\varepsilon_k - \varepsilon_f|\). This step-like change guarantees that deviations from the unrenormalized energies \(\varepsilon_f\) and \(\varepsilon_k\) stay relatively small for all \(k\) values.

**APPENDIX B: TRANSFORMATION OF THE OPERATORS**

In this appendix we evaluate the transformation from \(\lambda\) to \((\lambda - \Delta \lambda)\) for the various operator quantities of Eq. \((B1)\). For example

\[
e^{X_{\lambda,\Delta \lambda} c^\dagger_{km} c_{km} e^{-X_{\lambda,\Delta \lambda}} = e^{X_{\lambda,\Delta \lambda}} \left( c^\dagger_{km} c_{km} \right) = \sum_{n=0}^{\infty} \frac{1}{n!} X_{\lambda,\Delta \lambda}^n \left( c^\dagger_{km} c_{km} \right). \tag{B1}
\]

Here, a new super-operator \(X_{\lambda,\Delta \lambda}\) was introduced which is defined by the commutator of the generator \(X_{\lambda,\Delta \lambda}\) with operators \(A\) on which \(X_{\lambda,\Delta \lambda}\) is applied, \(X_{\lambda,\Delta \lambda} A = [X_{\lambda,\Delta \lambda}, A]\). Furthermore, let us define a new operator \(X_{km}\) by

\[
X_{km} = j^\dagger_{km} c_{km} - c^\dagger_{km} j_{km},
\]

which is an ingredient of the generator of the unitary transformation

\[
X_{\lambda,\Delta \lambda} = \sum_{km} A_k(\lambda, \Delta \lambda) \Theta_k(\lambda, \Delta \lambda) X_{km}. \tag{B2}
\]
We have to evaluate various commutators

\[ [X_{k',m'}, c^\dagger_{k,m} c_k] = \delta_{k',k} \delta_{m',m} \left( \hat{f}^\dagger_{k,m} c_{k,m} + \text{h.c.} \right), \]  
(B3)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_m \hat{f}_m \right)_L] = -\frac{\delta_{m',m}}{N} \left( \hat{f}^\dagger_{k',m} c_{k',m} + \text{h.c.} \right), \]  
(B4)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_m \hat{f}_m \right)_L] = [X_{k',m'}, \left( \hat{f}^\dagger_m \hat{f}_m \right)_L], \]  
(B5)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} \right)_{NL}] = -\frac{\delta_{m',m}}{N^{3/2}} \sum_{i,j(\neq i)} \left\{ e^{i k_i R_i} e^{i (k' - k)_j R_j} \hat{f}^\dagger_{im} D_{jm} c_{k',m} + \text{h.c.} \right\}, \]  
(B6)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} \right)_{NL}] = -\frac{\delta_{m',m}}{N^{3/2}} \sum_{i,j(\neq i)} \left\{ e^{i k_i R_i} e^{i (k' - k)_j R_j} \hat{f}^\dagger_{im} D_{jm} c_{k',m} + \text{h.c.} \right\}, \]  
(B7)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} + \text{h.c.} \right)_{NL}] = [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} \right)_{NL}] + [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} \right)_{NL}], \]  
(B8)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} + \text{h.c.} \right)] = \delta_{m',m} \left\{ 2\delta_{k',k} \hat{f}^\dagger_{k,m} \hat{f}_{k,m} - \left[ c^\dagger_{k,m} c_{k',m} D_m (k' - k) + \text{h.c.} \right] \right\}, \]  
(B9)

\[ [X_{k',m'}, \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} + \text{h.c.} \right)] = \delta_{m',m} \left\{ 2\delta_{k',k} \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} + \text{h.c.} \right) - \left[ c^\dagger_{k,m} c_{k',m} D_m (k' - k) + \text{h.c.} \right] \right\}, \]  
(B10)

where we neglect all spin-flip contributions. In Eqs. (B9) and (B10) Fourier transformed quantities are introduced

\[ \mathcal{D}_m(k) = \frac{1}{N} \sum_j e^{i k R_j} D_{jm}. \]  
(B11)

Furthermore, we have defined

\[ \left( \hat{f}^\dagger_m \hat{f}_m \right)_L := \frac{1}{N} \sum_k \hat{f}^\dagger_{k,m} \hat{f}_{k,m} = \frac{1}{N} \sum_i \hat{f}^\dagger_{im} \hat{f}_{im}, \]  
(B12)

\[ \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} \right)_{NL} := \frac{1}{N} \sum_{i,j(\neq i)} \hat{f}^\dagger_{im} \hat{f}_{jm} e^{i (k_i - R_i - k_j + R_j)} = \hat{f}^\dagger_{k,m} \hat{f}_{k,m} - \left( \hat{f}^\dagger_m \hat{f}_m \right)_L, \]  
(B13)

\[ \left( \hat{f}^\dagger_{k,m} \hat{f}_{k,m} + \text{h.c.} \right)_{NL} := \frac{1}{N} \sum_{i,j(\neq i)} \left[ \hat{f}^\dagger_{im} \hat{f}_{jm} e^{i (k_i - R_i - k_j + R_j)} + \text{h.c.} \right]. \]  
(B14)

We are interested in contributions which renormalize the parameters of the Hamiltonian $\mathcal{H}_\lambda$ according to Eqs. (16) and (17). Therefore, an additional factorization has to be carried out in Eqs. (B5), (B7), (B9), and (B10) and to keep only operator terms which appear also in $\mathcal{H}_\lambda$. By neglecting more complex operators, namely spin-flip terms,
Eqs. (B6), (B7), (B9), and (B10) can be replaced by

\[
\left[ X_{k'm'}, \left( \hat{f}_{km}' \hat{f}_{km} \right)_{NL} \right] = -\delta_{m,m'} \left( \delta_{k,k'} - \frac{1}{N} \right) \left\{ D \left( \hat{f}_{km}' \hat{c}_{km} + \text{h.c.} \right) \right. \\
+ \left. \left\langle \hat{f}_{km}' \hat{c}_{km} + \text{h.c.} \right\rangle \left[ 1 - D - \sum_{\hat{m} (\neq m)} \left( \hat{f}_{\hat{m}} \hat{f}_{\hat{m}} \right)_{L} \right] \right\},
\]

(B15)

\[
\left[ X_{k'm'}, \left( f_{km}' f_{km} \right)_{NL} \right] = -\delta_{m,m'} \left( \delta_{k,k'} - \frac{1}{N} \right) \left\{ D \left( \hat{f}_{km}' \hat{c}_{km} + \text{h.c.} \right) \right. \\
+ \left. \left\langle \hat{f}_{km}' \hat{c}_{km} + \text{h.c.} \right\rangle \left[ 1 - D - \sum_{\hat{m} (\neq m)} \left( \hat{f}_{\hat{m}} \hat{f}_{\hat{m}} \right)_{L} \right] \right\},
\]

(B16)

\[
\left[ X_{k'm'}, \left( \hat{f}_{km}' c_{km} + \text{h.c.} \right) \right] = 2 \delta_{m,m'} \delta_{k,k'} \left\{ \left( \hat{f}_{km}' \hat{f}_{km} \right)_{NL} + \left( \hat{f}_{km}' \hat{f}_{km} \right)_{L} - D c_{km}' c_{km} \right. \\
- \left. \left\langle \hat{c}_{km}' c_{km} \right\rangle \left[ 1 - D - \sum_{\hat{m} (\neq m)} \left( \hat{f}_{\hat{m}} \hat{f}_{\hat{m}} \right)_{L} \right] \right\},
\]

(B17)

\[
\left[ X_{k'm'}, \left( f_{km}' c_{km} + \text{h.c.} \right) \right] = 2 \delta_{m,m'} \delta_{k,k'} \left\{ \frac{1}{2} \left( \hat{f}_{km}' f_{km} + \text{h.c.} \right)_{NL} + \left( \hat{f}_{km}' \hat{f}_{km} \right)_{L} \\
- D c_{km}' c_{km} - \left\langle c_{km}' c_{km} \right\rangle \left[ 1 - D - \sum_{\hat{m} (\neq m)} \left( \hat{f}_{\hat{m}} \hat{f}_{\hat{m}} \right)_{L} \right] \right\},
\]

(B18)

where \( \left\langle \hat{f}_{km}' c_{km} + \text{h.c.} \right\rangle \approx \left\langle \hat{f}_{km}' c_{km} + \text{h.c.} \right\rangle \) has been used. Due to this factorization, certain expectation values enter Eqs. (B15)-(B18) which have to be evaluated separately (compare the discussion in subsection III C). By using Eqs. (B5) and (B15)-(B18) one finds from (B2) for the corresponding commutators formed with the generator \( X_{\lambda,\Delta \lambda} \)

\[
\left[ X_{\lambda,\Delta \lambda}, \left( \hat{f}_{km}' c_{km} + \text{h.c.} \right) \right] = \Theta_k (\lambda, \Delta \lambda) A_k (\lambda, \Delta \lambda) \left( \hat{f}_{km}' c_{km} + \text{h.c.} \right),
\]

(B19)

\[
\left[ X_{\lambda,\Delta \lambda}, \left( \hat{f}_{km}' \hat{f}_{km} \right)_{L} \right] = -\frac{1}{N} \sum_{k'} \Theta_k (\lambda, \Delta \lambda) A_k (\lambda, \Delta \lambda) \left( \hat{f}_{k'm'} c_{k'm} + \text{h.c.} \right),
\]

(B20)

\[
\left[ X_{\lambda,\Delta \lambda}, \left( f_{km}' f_{km} \right)_{L} \right] = \left[ X_{\lambda,\Delta \lambda}, \left( \hat{f}_{km}' \hat{f}_{km} \right)_{L} \right],
\]

(B21)
\[ [X_{\lambda, \Delta \lambda}, (\hat{f}_{k m}^\dagger \hat{f}_{k m})_{\text{NL}}] = - \Theta_k(\lambda, \Delta \lambda) A_k(\lambda, \Delta \lambda) \left\{ D \left( \hat{f}_{k m}^\dagger c_{k m} + \text{h.c.} \right) + \left\langle \hat{f}_{k m}^\dagger c_{k m} + \text{h.c.} \right\rangle \left[ 1 - D - \sum_{\tilde{m}(\neq m)} (\hat{f}_{\tilde{m}}^\dagger \hat{f}_{\tilde{m}})_{\text{L}} \right] \right\} \right) + \frac{1}{N} \sum_{k'} \Theta_{k'}(\lambda, \Delta \lambda) A_{k'}(\lambda, \Delta \lambda) \left\{ D \left( \hat{f}_{k'm}^\dagger c_{k'm} + \text{h.c.} \right) + \left\langle \hat{f}_{k'm}^\dagger c_{k'm} + \text{h.c.} \right\rangle \left[ 1 - D - \sum_{\tilde{m}(\neq m)} (\hat{f}_{\tilde{m}}^\dagger \hat{f}_{\tilde{m}})_{\text{L}} \right] \right\}, \]

\[ [X_{\lambda, \Delta \lambda}, (\hat{f}_{k m}^\dagger \hat{f}_{k m})_{\text{NL}}] = - \Theta_k(\lambda, \Delta \lambda) A_k(\lambda, \Delta \lambda) \left\{ D \left( \hat{f}_{k m}^\dagger c_{k m} + \text{h.c.} \right) + \left\langle \hat{f}_{k m}^\dagger c_{k m} + \text{h.c.} \right\rangle \left[ 1 - D - \sum_{\tilde{m}(\neq m)} (\hat{f}_{\tilde{m}}^\dagger \hat{f}_{\tilde{m}})_{\text{L}} \right] \right\} \]

\[ [X_{\lambda, \Delta \lambda}, (\hat{f}_{k m}^\dagger \hat{f}_{k m} + \text{h.c.})_{\text{NL}}] = [X_{\lambda, \Delta \lambda}, (\hat{f}_{k m}^\dagger \hat{f}_{k m})_{\text{NL}}] + [X_{\lambda, \Delta \lambda}, (f_{k m}^\dagger f_{k m})_{\text{NL}}] \]

\[ [X_{\lambda, \Delta \lambda}, (\hat{f}_{k m}^\dagger \hat{f}_{k m} + \text{h.c.})] = 2 \Theta_k(\lambda, \Delta \lambda) A_k(\lambda, \Delta \lambda) \left\{ \left( \hat{f}_{k m}^\dagger \hat{f}_{k m}\right)_{\text{NL}} + \left( f_{k m}^\dagger f_{k m} \right)_{\text{L}} \right\} \]

Therefore, all operators terms appearing on the r.h. sides of Eqs. (B19)-(B26) are traced back to a bilinear form. This property will enable us to evaluate higher order commutators with \( X_{\lambda, \Delta \lambda} \) and also transformations like \( \text{NL} \). Moreover, we assume that the number of \( k \) points which are integrated out by use of the unitary transformation \( \text{NL} \) is small compared to the total number of \( K \) points. This assumption is needed for the evaluation of higher order commutators. For instance, the commutators which arise from repeated application of \( X_{\lambda, \Delta \lambda} \) to \( (\hat{f}_{k m}^\dagger c_{k m} + \text{h.c.}) \) and
(\hat{f}_{km}^{\dagger} c_{km} + \text{h.c.}) \text{ read } (n = 1, 2, 3, \cdots)

\begin{equation}
\mathbf{X}^{2n}_{\lambda, \Delta \lambda} \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) =
\begin{aligned}
&= (-1)^n \Theta_k(\lambda, \Delta \lambda) \left[ 2\sqrt{D} A_k(\lambda, \Delta \lambda) \right]^{2n} \left\{ \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) \\
&\quad + \frac{1}{2D} \left\langle \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) \right\rangle \\
&\quad \left[ 1 - D - \sum_{\vec{n}(\neq \vec{m})} \left( \hat{f}_{\vec{n}}^{\dagger} \hat{f}_{\vec{n}} \right)_L \right] \right\},
\end{aligned}
\end{equation}

\begin{equation}
\mathbf{X}^{2n+1}_{\lambda, \Delta \lambda} \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) =
\begin{aligned}
&= \left( -\frac{1}{\sqrt{D}} \right)^n \Theta_k(\lambda, \Delta \lambda) \left[ 2\sqrt{D} A_k(\lambda, \Delta \lambda) \right]^{2n+1} \left\{ \left( \hat{f}_{km}^{\dagger} f_k \right)_L + \left( \hat{f}_{m}^{\dagger} f_m \right)_L \\
&\quad - D \hat{c}_{km}^{\dagger} c_{km} - \left\langle \hat{c}_{km}^{\dagger} c_{km} \right\rangle \\
&\quad - \left[ 1 - D - \sum_{\vec{n}(\neq \vec{m})} \left( \hat{f}_{\vec{n}}^{\dagger} \hat{f}_{\vec{n}} \right)_L \right] \right\},
\end{aligned}
\end{equation}

\begin{equation}
\mathbf{X}^{2n}_{\lambda, \Delta \lambda} \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) = \mathbf{X}^{2n}_{\lambda, \Delta \lambda} \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) + (-1)^n \Theta_k(\lambda, \Delta \lambda) \left[ \sqrt{D} A_k(\lambda, \Delta \lambda) \right]^{2n} \\
\times \left\{ \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) - \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) \right\}
\end{equation}

\begin{equation}
\mathbf{X}^{2n+1}_{\lambda, \Delta \lambda} \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) = \mathbf{X}^{2n+1}_{\lambda, \Delta \lambda} \left( \hat{f}_{km}^{\dagger} c_{km} + \text{h.c.} \right) + \left( -\frac{1}{\sqrt{D}} \right)^n \Theta_k(\lambda, \Delta \lambda) \left[ \sqrt{D} A_k(\lambda, \Delta \lambda) \right]^{2n+1} \\
\times \left\{ \left( \hat{f}_{km}^{\dagger} f_k \right)_L + \left( \hat{f}_{m}^{\dagger} f_m \right)_L - 2 \left( \hat{f}_{km}^{\dagger} f_k \right)_L \right\}
\end{equation}

To trace back all contributions to terms appearing in the unperturbed Hamiltonian \( \mathcal{H}_{0,\lambda} \), one has to replace all Hubbard operators by appropriate expressions in terms of usual Fermi operators. Thus, further approximations are needed for the local \( \left( \hat{f}_{km}^{\dagger} \hat{f}_{km} \right)_L \) and for the non-local \( f \) electron particle-hole excitations \( \left( \hat{f}_{km}^{\dagger} f_k \right)_L \). As was discussed before, due to the strong local Coulomb interaction, only empty and singly occupied \( f \) sites are of physical relevance. Thus the operator \( \left( \hat{f}_{km}^{\dagger} f_k \right)_L \) applied on physical states can not generate doubly occupied \( f \) sites. Therefore, the operator can be replaced by

\begin{equation}
\left( \hat{f}_{km}^{\dagger} f_k \right)_L \approx \left( \hat{f}_{km}^{\dagger} f_k \right)_L.
\end{equation}

The second operator, \( \left( \hat{f}_{km}^{\dagger} f_k \right)_L \), represents an \( f \) electron hopping between different sites without creating doubly occupied \( f \) sites. Thus, we may approximate

\begin{equation}
\left( \hat{f}_{km}^{\dagger} f_k \right)_L \approx \frac{1}{N} \sum_{i,j(\neq i)} \hat{f}_{ijm}^{\dagger} f_{jm} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} = \frac{1}{N} \sum_{i,j(\neq i)} D_{ijm} \hat{f}_{ijm}^{\dagger} f_{jm} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}
\end{equation}

\begin{equation}
\approx D \left( \hat{f}_{km}^{\dagger} f_k \right)_L
\end{equation}

where in the last equation the creation of doubly occupied sites is only fulfilled within a factorization approximation, \( D_{ijm} \approx D \).
Finally, by inserting (B27)–(B28) into (B1), and by using the approximations (B31) and (B32) one finds

\[
e^{X_{\lambda,\Delta\lambda}} c_{km}^\dagger c_{km} e^{-X_{\lambda,\Delta\lambda}} - c_{km}^\dagger c_{km} =
\]

\[
= - \frac{1}{2D} \Theta_k(\lambda, \Delta\lambda) A_k(\lambda, \Delta\lambda) \left\{ f_{km}^\dagger f_{km} + h.c. \right\} \left[ 1 - D - \sum_{\bar{m} \neq m} \left( f_{\bar{m}}^\dagger f_{\bar{m}} \right)_L \right]
\]

\[
- \frac{1}{2D} \Theta_k(\lambda, \Delta\lambda) \left\{ \cos \left[ 2\sqrt{D} A_k(\lambda, \Delta\lambda) \right] - 1 \right\} \left\{ D \left( f_{km}^\dagger f_{km} \right)_L + \left( f_{\bar{m}}^\dagger f_{\bar{m}} \right)_L \right\}
\]

\[
- D c_{km}^\dagger c_{km} - \left\{ c_{km}^\dagger c_{km} \right\} \left[ 1 - D - \sum_{\bar{m} \neq m} \left( f_{\bar{m}}^\dagger f_{\bar{m}} \right)_L \right]
\]

\[
+ \frac{1}{2\sqrt{D}} \Theta_k(\lambda, \Delta\lambda) \sin \left[ 2\sqrt{D} A_k(\lambda, \Delta\lambda) \right] \left\{ f_{km}^\dagger c_{km} + h.c. \right\}
\]

\[
+ \frac{1}{2D} \left\{ c_{km}^\dagger c_{km} + h.c. \right\} \left[ 1 - D - \sum_{\bar{m} \neq m} \left( f_{\bar{m}}^\dagger f_{\bar{m}} \right)_L \right]
\}

\]

Similar equations can be derived for the transformations of the remaining operators.

\[
e^{X_{\lambda,\Delta\lambda}} \left( f_{km}^\dagger f_{km} \right)_L e^{-X_{\lambda,\Delta\lambda}} - \left( f_{km}^\dagger f_{km} \right)_L =
\]

\[
= - D \left\{ e^{X_{\lambda,\Delta\lambda}} c_{km}^\dagger c_{km} e^{-X_{\lambda,\Delta\lambda}} - c_{km}^\dagger c_{km} \right\} + \Theta_k(\lambda, \Delta\lambda) A_k(\lambda, \Delta\lambda) \left\{ f_{km}^\dagger c_{km} + h.c. \right\}
\]

\[
\times \left[ 1 - D - \sum_{\bar{m} \neq m} \left( f_{\bar{m}}^\dagger f_{\bar{m}} \right)_L \right]
\]

\[
+ \frac{D}{N} \sum_{k'} \left\{ e^{X_{\lambda,\Delta\lambda}} c_{k'm}^\dagger c_{k'm} e^{-X_{\lambda,\Delta\lambda}} - c_{k'm}^\dagger c_{k'm} \right\}
\]

\[
+ \Theta_{k'}(\lambda, \Delta\lambda) A_{k'}(\lambda, \Delta\lambda) \left\{ f_{k'm}^\dagger c_{k'm} + h.c. \right\} \left[ 1 - D - \sum_{\bar{m} \neq m} \left( f_{\bar{m}}^\dagger f_{\bar{m}} \right)_L \right]
\}

\]

\[
e^{X_{\lambda,\Delta\lambda}} \left( f_{m}^\dagger f_{m} \right)_L e^{-X_{\lambda,\Delta\lambda}} - \left( f_{m}^\dagger f_{m} \right)_L = - \frac{1}{N} \sum_{k'} \left\{ e^{X_{\lambda,\Delta\lambda}} c_{k'm}^\dagger c_{k'm} e^{-X_{\lambda,\Delta\lambda}} - c_{k'm}^\dagger c_{k'm} \right\},
\]

\[
(B35)
\]
APPENDIX C: TRANSFORMATION OF THE ONE-PARTICLE OPERATORS

To determine the transformation of the one-particle operators we have again to apply the unitary transformation $\hat{e}$ which was used before to renormalize the Hamiltonian. As in Ref. 8 we first make the simplest operator ansatz for the $\lambda$ dependent $c$ creation operator

$$c_{km}^\dagger(\lambda) = u_{k,\lambda}c_{km}^\dagger + v_{k,\lambda}\hat{f}_{km}^\dagger$$  \hspace{1cm} (C1)

with the initial parameter values corresponding to the unrenormalized operators ($\lambda = \Lambda$)

$$u_{k,(\lambda = \Lambda)} = 1, \quad v_{k,(\lambda = \Lambda)} = 0.$$  \hspace{1cm} (C2)

Because the $\lambda$ dependent operators have to fulfill the same anticommutator relations as the unrenormalized operators, one concludes that

$$1 = |u_{k,\lambda}|^2 + D |v_{k,\lambda}|^2$$  \hspace{1cm} (C3)

holds for all $k$ and $\lambda$ values. Thus, the transformation of the $f$ electron creation operator is given by

$$\hat{f}_{km}^\dagger(\lambda) = -D v_{k,\lambda}c_{km}^\dagger + u_{k,\lambda}\hat{f}_{km}^\dagger.$$  \hspace{1cm} (C4)

Thereby, the approximation $[\hat{f}_{km}^\dagger, \hat{f}_{km}]_+ \approx D$ was used.

To derive renormalization equations for the parameters $u_{k,\lambda}$ and $v_{k,\lambda}$ of the one-particle operators we again consider the transformation step from $\lambda$ to $(\lambda - \Delta \lambda)$. As in the case of the Hamiltonian [compare Eqs. (31) and (35)] we obtain two equations for $c_{km}^\dagger(\lambda - \Delta \lambda)$

$$c_{km}^\dagger(\lambda - \Delta \lambda) = u_{k,(\lambda - \Delta \lambda)}c_{km}^\dagger + v_{k,(\lambda - \Delta \lambda)}\hat{f}_{km}^\dagger$$  \hspace{1cm} (C5)

where the first one is derived from ansatz (C4). The second equation follows from the application of the unitary transformation (15) to $c_{km}^\dagger(\lambda)$. To calculate the transformed operators in Eq. (C6) one has to retrace the procedure of appendix B so that we obtain

$$e^{X_{\lambda,\Delta \lambda}}c_{km}^\dagger e^{-X_{\lambda,\Delta \lambda}} = c_{km}^\dagger + \Theta_k(\lambda, \Delta \lambda) \left\{ \cos \left[ \sqrt{D}A_k(\lambda, \Delta \lambda) \right] - 1 \right\} c_{km}^\dagger$$  \hspace{1cm} (C7)

$$e^{X_{\lambda,\Delta \lambda}}\hat{f}_{km}^\dagger e^{-X_{\lambda,\Delta \lambda}} = \hat{f}_{km}^\dagger + \Theta_k(\lambda, \Delta \lambda) \left\{ \cos \left[ \sqrt{D}A_k(\lambda, \Delta \lambda) \right] - 1 \right\} \hat{f}_{km}^\dagger$$  \hspace{1cm} (C8)
Finally, inserting Eqs. (C7) and (C8) into (C6) we find the renormalization equations for the parameters $u_{k,\lambda}$ and $v_{k,\lambda}$:

\[
\begin{align*}
\frac{u_{k,\lambda}(\lambda-\Delta\lambda) - u_{k,\lambda}}{u_{k,\lambda}} &= \frac{1}{\sqrt{D}}v_{k,\lambda}\sin\sqrt{DA_k}\left(\lambda, \Delta\lambda\right), \\
\frac{v_{k,\lambda}(\lambda-\Delta\lambda) - v_{k,\lambda}}{v_{k,\lambda}} &= \frac{1}{\sqrt{D}}u_{k,\lambda}\sin\sqrt{DA_k}\left(\lambda, \Delta\lambda\right).
\end{align*}
\]

[1] H. R. Ott and Z. Fisk, in Handbook on the Physics and Chemistry of the Actinides, edited by A. J. Freeman and G. H. Lander (Elsevier, Amsterdam, 1987).
[2] P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Comments Cond. Mat. Phys. 12, 99 (1986).
[3] P.W. Anderson, Phys. Rev. 124, 41 (1961).
[4] U. Fano, Phys. Rev. 124, 1866 (1961).
[5] T. M. Rice and K. Ueda, Phys. Rev. Lett. 55, 995 (1985); T. M. Rice and K. Ueda, Phys. Rev. B 34, 6420 (1986).
[6] P. Coleman, Phys. Rev. B29, 3035 (1984).
[7] See, for example, P. Fulde, J. Keller, and G. Zwicknagl, in Solid State Physics, edited by H. Ehrenreich and D. Turnbull (Academic, San Diego, 1988), Vol. 41, p. 1.
[8] K. W. Becker, A. Hübsch, and T. Sommer, Phys. Rev. B 66, 235115 (2002).
[9] F. Wegner, Ann. Phys. (Leipzig) 3, 77 (1994).
[10] S. D. Glazek and K.G. Wilson, Phys. Rev. D 48, 5863 (1993); S. D. Glazek and K. G. Wilson, Phys. Rev. D 49, 4214 (1994).
[11] A. Hübsch and K. W. Becker, Eur. Phys. J. B 33, 391 (2003).
[12] R. Franco, M.S. Figueira, and M. E. Foglio, Phys. Rev. B 66, 045112 (2002).
[13] Y. Onishi and K. Miyake, J. Phy. Soc. Jpn. 69, 3955 (2000); A. T. Holmes, D. Jaccard, and K. Miyake, Phys. Rev. B 69, 024508 (2004).