

Hopping perturbation treatment of the periodic Anderson model around the atomic limit

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(Received 17 May 2000; revised manuscript received 13 February 2001; published 8 June 2001)

The periodic Anderson model with two strongly correlated subsystems of d and f electrons and local on-site hybridization is investigated by considering the hopping of d electrons between lattice sites as perturbation. In zero order without the intersite transfer term, the system of correlated d and f electrons can be treated exactly. The delocalization of electrons and the corresponding renormalization of the one-particle Green's functions are analyzed by using a special diagram technique from which the Dyson equations for the Green's functions are established. We discuss the physics of the delocalized electrons in the simplest approximation corresponding to a Hubbard I-like decoupling giving rise to eight different energy bands, which depend in a non-trivial way on the exact eigenvalues of the local model. These bands are discussed for the symmetrical case in which the energies of doubly occupied d and f states are equal to each other.

DOI: 10.1103/PhysRevB.63.245119

PACS number(s): 71.28.+d, 71.27.+a

I. INTRODUCTION

The periodic Anderson model (PAM) (Ref. 1) is one of the main models for studying strongly correlated electrons in heavy-fermion systems, mixed-valence compounds, narrow energy-band materials, and high-temperature superconductors. Recent results of experimental and theoretical investigations of mixed-valent and heavy-fermion systems can be found in Refs. 2–6. Usually the simplest variant of the PAM is used, which consists of correlated localized f electrons with only one spin degree of freedom and uncorrelated conduction electrons. In this work, we consider an extended version with the corresponding Hamiltonian given by

$$\begin{aligned}
 H^0 = & \epsilon_d \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + U_d \sum_i n_{i\uparrow}^d n_{i\downarrow}^d + \epsilon_f \sum_{i\sigma} f_{i\sigma}^\dagger f_{i\sigma} \\
 & + U_f \sum_i n_{i\uparrow}^f n_{i\downarrow}^f + V \sum_{i\sigma} (f_{i\sigma}^\dagger d_{i\sigma} + d_{i\sigma}^\dagger f_{i\sigma}) \\
 & + G \sum_i (n_{i\uparrow}^d + n_{i\downarrow}^d)(n_{i\uparrow}^f + n_{i\downarrow}^f), \quad (1a)
 \end{aligned}$$

$$H^1 = \sum_{ij\sigma} t(j-i) d_{j\sigma}^\dagger d_{i\sigma}, \quad (1b)$$

where $a_{i\sigma}^\dagger$ ($a_{i\sigma}$) with $a=d, f$ is the creation (annihilation) operator of itinerant and localized electrons, respectively; ϵ_a is the corresponding local energies taken relative to the

chemical potential, i.e., $\epsilon_a = \bar{\epsilon}_a - \mu$; U_a are the on-site Coulomb repulsions; and $n_{i\sigma}^a = a_{i\sigma}^\dagger a_{i\sigma}$ are the number operators of the electrons. For simplicity, the hybridization between itinerant and localized states is taken to be a local quantity. The last term in Eq. (1a) is the so-called Falicov-Kimball term. In this paper, we take Eq. (1a) as the zero-order problem, which can be diagonalized exactly, and we use the hopping or transfer term in Eq. (1b) as perturbation. The main purpose of this paper is to see in detail how the hopping of the conduction electrons will change the ionic quantum transitions.

This type of Hamiltonian has been investigated by many authors, mostly for the simpler case in which $U_d = G = 0$.^{2–12} Alascio *et al.*⁷ (in the limit of $U_f \rightarrow \infty$) and mainly Mancini, Marinaro *et al.*,^{8,9} Noce and Romano,^{10,11} and Long¹² reduced the problem (for $U_d = G = 0$) to a system of independent sites, in which case the correlated f electrons and their hybridization can be treated exactly. The Hamiltonian (1a) has 16 quantum states and the corresponding matrix can be easily diagonalized. For $U_d = G = 0$, the resulting eigenvalues E_λ ($\lambda = 1, \dots, 16$) can be found in Refs. 7–12. In the limit of strong Coulomb repulsion ($U_f \rightarrow \infty$), as discussed in Ref. 7, only 12 quantum states are available for the electrons because double occupancy of a single site by two f electrons is forbidden. Knowledge of the energy spectrum allowed the authors^{7–11} to obtain the partition function Z_0 of the system and its relevant thermodynamical quantities, and to prove that many of the most characteristic features of the interme-

diate valence state (experimental trends) are already present in the limit of zero-band width.

II. PERTURBATIVE TREATMENT

From a theoretical point of view, the zero-band width model is of further interest. It was proved in Refs. 8 and 9 that, because of the nonapplicability of Wick's theorem for the single-site Hamiltonian (1a), the n -point Green's function cannot be factorized in terms of two-point Green's functions. The authors formulated the rules to build up a diagrammatic representation for any Green's function of the Hamiltonian (1a) (for $U_d=G=0$) and obtained by means of the path-integral formalism the corresponding exact analytic expressions. The role of the kinetic energy of the conduction electrons in the process of delocalization and in the renormalization of the dynamical quantities was not discussed. We have addressed this question in Refs. 13 and 14, where the Hamiltonian (1a) and (1b) was investigated for $U_d=G=0$ by assuming that decoupled f and conduction electrons (limit of zero hybridization) are a good starting point for a perturbation expansion in powers of the hybridization. In this context, we formulated the Dyson equations for the renormalized one-particle Green's functions for the normal and superconducting state, respectively.

Because of the above-mentioned nonapplicability of Wick's theorem of conventional quantum-field theory to strongly correlated systems, we proposed in Refs. 15–22 an alternative perturbative treatment in terms of the hopping integral of conduction electrons. To this we formulated a generalized Wick's theorem (GWT) and corresponding diagram technique, which allowed us to reduce averages to n -particle Matsubara Green's functions of the atomic system, which can be further factorized by using the GWT (see Refs. 15–22 for details).

The perturbation theory is formulated in the interaction representation by using grand-canonical ensemble averages for the chronological products of interactions. These averages are reduced to n -particle local Matsubara Green's functions $G_n^{(0)}(1, \dots, n | 1', \dots, n')$ depending on $2n$ groups of arguments ($1 = \text{site } i, \text{ time } \tau, \text{ spin } \sigma$). In the absence of correlations, the functions factorize and can be represented by a sum of products of n independent one-particle Green's functions (standard Wick theorem). In the presence of correlations, new terms appear in addition to the previous ones. All new terms contain one or more on-site many-particle irreducible Green's functions $G_m^{(0)}(1, \dots, m | 1', \dots, m')$ with $m \leq n$, the structure of which is of Kubo's cumulant type. All site indices of the individual irreducible functions are the same; they are strictly local functions. The decomposition of the local n -particle Green's functions $G_n^{(0)}$ is the sum of different contributions that can contain n_1 one-particle, n_2 two-particle irreducible, n_3 three-particle irreducible, etc., Green's functions, whereby the structures are conditioned by the conservation law for particle numbers $n = n_1 + 2n_2 + 3n_3 + \dots$ with details determined by the GWT. These irreducible functions being diagonal with respect to their site indices, have, however, different time and spin labels. The diagrammatic representation of the perturbation se-

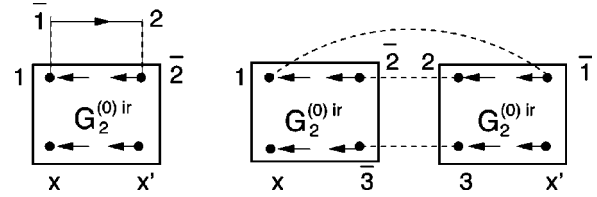


FIG. 1. A typical Feynman diagram of second (left) and third (right) order of the perturbation theory for the d -electron correlation function Z^{dd} . The solid line is the d -electron propagator; squares represent the irreducible two-particle Green's functions $G_2^{(0)ir}(x1|\bar{2}x')$, $G_2^{(0)ir}(x1|\bar{2}\bar{3})$, and $G_2^{(0)ir}(3\bar{2}|\bar{1}x')$. Dotted lines stand for the hopping matrix elements.

ries contains new elements, as indicated in Fig. 1. These new elements can be gathered together in a function, the correlation function $Z_{\sigma\sigma'}(x-x')$. Z is the sum of all *strongly connected irreducible diagrams*, each of which has two external vertices x and x' , where x stands for (i, τ, σ) . In the general case, the correlation function Z is not diagonal with respect to the site indices (in the simplest case of second-order perturbation with respect to hopping, the two-particle correlation function appears, which, however, is diagonal). The nice feature of this perturbation expansion is that the renormalized one-particle Green's function can be formulated in terms of Z only. The correlation function Z and corresponding Dyson equation had not been established in previous expansions.^{23–25}

The novelty of the diagram technique is that the GWT allows us to generate all contributions of the perturbation expansion for correlated electron systems by using the simple algebra of usual fermion operators instead of the algebra of Hubbard transfer (projection) operators used previously by Stasyuk, Zaitsev, and Izyumov.^{23–25} The technique of projection operators is only used at the final stage of the calculations in order to find the simplest irreducible functions. In contrast with Refs. 23–25, we have only one kind of vertex, one localized zero-order Green's function, and only one kind of irreducible n -particle Green's function. Previous diagrammatical formulations contain a variety of such quantities. A Dyson-type equation for the delocalized one-particle Green's function using this technique was first formulated in Refs. 15 and 16. A numerical investigation (yet to be undertaken) of the simplest contribution (the two-particle irreducible diagram $Z^{(2)}$ shown in Fig. 1) will allow us to discuss metal-insulator and superconducting transitions.^{16–18,26} The function $Z^{(2)}$ is of primary interest when going beyond the Hubbard I approximation.

We will now briefly investigate the properties of the PAM in the atomic limit when the contribution of the hopping of the d electrons is absent, and we will subsequently investigate the impact of hopping on the ionic quantum transitions by employing the new perturbation theory.

III. THE LOCAL MODEL (ATOMIC LIMIT)

In the case of zero conduction-band width, we have to diagonalize Eq. (1a). Since there are four states for the d and f electrons, respectively, we have altogether 16 quantum

states at each lattice site, which, for completeness, are listed as follows (the site index has been omitted):

$$\begin{aligned}
|\Psi_1\rangle &= |0\rangle, & |\Psi_9\rangle &= d_{\uparrow}^{\dagger} f_{\uparrow}^{\dagger} |0\rangle, \\
|\Psi_2\rangle &= d_{\uparrow}^{\dagger} |0\rangle, & |\Psi_{10}\rangle &= \frac{1}{\sqrt{2}}(d_{\uparrow}^{\dagger} f_{\uparrow}^{\dagger} + d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger}) |0\rangle, \\
|\Psi_3\rangle &= f_{\uparrow}^{\dagger} |0\rangle, & |\Psi_{11}\rangle &= d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger} |0\rangle, \\
|\Psi_4\rangle &= d_{\uparrow}^{\dagger} |0\rangle, & |\Psi_{12}\rangle &= d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger} |0\rangle, \\
|\Psi_5\rangle &= f_{\uparrow}^{\dagger} |0\rangle, & |\Psi_{13}\rangle &= d_{\uparrow}^{\dagger} f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} |0\rangle, \\
|\Psi_6\rangle &= d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} |0\rangle, & |\Psi_{14}\rangle &= d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger} |0\rangle, \\
|\Psi_7\rangle &= \frac{1}{\sqrt{2}}(d_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} - d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger}) |0\rangle, & |\Psi_{15}\rangle &= d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} |0\rangle, \\
|\Psi_8\rangle &= f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} |0\rangle, & |\Psi_{16}\rangle &= d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} |0\rangle,
\end{aligned} \tag{2}$$

where $|0\rangle$ is the vacuum state of the ion corresponding to an empty lattice site. The states $|\Psi_2\rangle \dots |\Psi_5\rangle$ are single-particle states with $N=1$ electron, spin $S=\frac{1}{2}$, and $S_z = \pm\frac{1}{2}$; $|\Psi_6\rangle$, $|\Psi_7\rangle$, and $|\Psi_8\rangle$ are the singlet states with $N=2$ electrons and spin $S=0$; the next three states are the triplet states with $N=2$, $S=1$, and $S_z = -1, 0, +1$; then there are four states— $|\Psi_{12}\rangle$, $|\Psi_{13}\rangle$, $|\Psi_{14}\rangle$, and $|\Psi_{15}\rangle$ —with $N=3$, $S=\frac{1}{2}$, and $S_z = \pm\frac{1}{2}$. The last state $|\Psi_{16}\rangle$ corresponds to $N=4$ and $S=0$.

The action of the Hamiltonian (1a) on the ionic states (2) gives rise to a 16×16 matrix, \mathbf{H}^0 , for each lattice site, which has nearly diagonal structure. In order to diagonalize this matrix, we make use of the complete orthonormalized system of eigenfunctions, $\Phi_n(E_\lambda)$, determined by the matrix equation,

$$\mathbf{H}^0 \Phi(E_\lambda) = E_\lambda \Phi(E_\lambda), \tag{3}$$

where $\Phi(E_\lambda)$ is a column vector with the usual orthonormalization conditions,

$$\sum_{\lambda=1}^{16} \Phi_n^*(E_\lambda) \Phi_m(E_\lambda) = \delta_{m,n}, \tag{4a}$$

$$\sum_{n=1}^{16} \Phi_n^*(E_\lambda) \Phi_n(E_{\lambda'}) = \delta_{\lambda,\lambda'}. \tag{4b}$$

The set of column vectors $\Phi(E_\lambda)$ ($\lambda=1, \dots, 16$) can be used as elements for the \mathbf{S} matrix, which diagonalizes the local Hamiltonian (this method is different from the method used so far^{8,9} and does not require additional computational work) by

$$\tilde{\mathbf{H}}^0 = \mathbf{S}^{-1} \mathbf{H}^0 \mathbf{S}, \tag{5}$$

the eigenfunctions of which, $|E_\lambda\rangle$, allow us to formulate the transformation of the wave functions between the different representations,

$$|\Psi_n\rangle = \sum_{\lambda} \Phi_n(E_\lambda) |E_\lambda\rangle, \quad \langle \Psi_n | = \sum_{\lambda} \langle E_\lambda | \Phi_n^*(E_\lambda), \tag{6a}$$

$$|E_\lambda\rangle = \sum_n \Phi_n^*(E_\lambda) |\Psi_n\rangle, \quad \langle E_\lambda | = \sum_n \langle \Psi_n | \Phi_n(E_\lambda). \tag{6b}$$

Using Eq. (6b) and the properties of $\Phi_n(E_\lambda)$ listed in the Appendix allows us to obtain the eigenfunctions of the local Hamiltonian,

$$\begin{aligned}
|E_1\rangle &= |0\rangle, & |E_9\rangle &= |\Psi_9\rangle, \\
|E_2\rangle &= \Phi_2(E_2) |\Psi_2\rangle + \Phi_3(E_2) |\Psi_3\rangle, & |E_{10}\rangle &= |\Psi_{10}\rangle, \\
|E_3\rangle &= \Phi_2(E_3) |\Psi_2\rangle + \Phi_3(E_3) |\Psi_3\rangle, & |E_{11}\rangle &= |\Psi_{11}\rangle, \\
|E_4\rangle &= \Phi_4(E_4) |\Psi_4\rangle + \Phi_5(E_4) |\Psi_5\rangle, \\
|E_{12}\rangle &= \Phi_{12}(E_{12}) |\Psi_{12}\rangle + \Phi_{13}(E_{12}) |\Psi_{13}\rangle, \\
|E_5\rangle &= \Phi_4(E_5) |\Psi_4\rangle + \Phi_5(E_5) |\Psi_5\rangle, \\
|E_{13}\rangle &= \Phi_{12}(E_{13}) |\Psi_{12}\rangle + \Phi_{13}(E_{13}) |\Psi_{13}\rangle, \\
|E_6\rangle &= \Phi_6(E_6) |\Psi_6\rangle + \Phi_7(E_6) |\Psi_7\rangle + \Phi_8(E_6) |\Psi_8\rangle, \\
|E_{14}\rangle &= \Phi_{14}(E_{14}) |\Psi_{14}\rangle + \Phi_{15}(E_{14}) |\Psi_{15}\rangle, \\
|E_7\rangle &= \Phi_6(E_7) |\Psi_6\rangle + \Phi_7(E_7) |\Psi_7\rangle + \Phi_8(E_7) |\Psi_8\rangle, \\
|E_{15}\rangle &= \Phi_{14}(E_{15}) |\Psi_{14}\rangle + \Phi_{15}(E_{15}) |\Psi_{15}\rangle, \\
|E_8\rangle &= \Phi_6(E_8) |\Psi_6\rangle + \Phi_7(E_8) |\Psi_7\rangle + \Phi_8(E_8) |\Psi_8\rangle, \\
|E_{16}\rangle &= |\Psi_{16}\rangle.
\end{aligned} \tag{7}$$

These kinds of functions have been listed in Refs. 7 and 10–12 for the case $U_d=0$ and in Ref. 12 for $U_d=G=0$. One of these functions should have the lowest energy corresponding to the ground state of the system. A candidate for the ground state is one of the three singlet functions with $N=2$, $S=0$, and energy E_a , $a=6, \dots, 8$.

Knowledge of the energy spectrum in the atomic limit (listed in the Appendix) gives us the possibility to find the corresponding partition function Z_0 ,^{7,10,11}

$$\begin{aligned}
Z_0 &= \sum_{\lambda=1}^{16} e^{-\beta E_\lambda} = 1 + 2e^{-\beta E_2} + 2e^{-\beta E_3} + \sum_{a=6,7,8} e^{-\beta E_a} \\
&\quad + 3e^{-\beta E_9} + 2e^{-\beta E_{12}} + 2e^{-\beta E_{13}} + e^{-\beta E_{16}}
\end{aligned} \tag{8}$$

with $\beta = (k_B T)^{-1}$. By using the equation

$$\frac{\partial E_\lambda}{\partial \mu} = -N, \tag{9}$$

where N is the number of particles in the correlated state $|E_\lambda\rangle$, we can obtain from Eq. (8) the following property:

$$n^d + n^f = \langle n_{\uparrow}^d + n_{\downarrow}^d + n_{\uparrow}^f + n_{\downarrow}^f \rangle = \frac{1}{\beta} \frac{\partial \ln Z_0}{\partial \mu}, \quad (10)$$

which can be rewritten as

$$n^d + n^f = \frac{2}{Z_0} [(e^{-\beta E_{16}} - 1) + (e^{-\beta E_{12}} - e^{-\beta E_2}) + (e^{-\beta E_{13}} - e^{-\beta E_3})], \quad (11)$$

For the symmetrical case (14) defined below, for which

$$E_{12,13} = E_{2,3} + \frac{1}{2} E_{16} \quad (12)$$

holds, Eq. (11) simplifies to

$$n^d + n^f - 2 = \frac{2}{Z_0} (e^{-\beta E_{16}/2} - 1) (1 + e^{-\beta E_2} + e^{-\beta E_3} + e^{-\beta E_{16}/2}). \quad (13)$$

It is interesting to note that the average number of electrons is $n_d + n_f = 2$ if, in addition to the condition of symmetry (equal energies of doubly occupied d and f states, see the Appendix),

$$2\epsilon_d + U_d = 2\epsilon_f + U_f, \quad (14)$$

E_{16} is identically zero. In this case, the chemical potential takes the value

$$2\mu = \bar{\epsilon}_d + \bar{\epsilon}_f + U + 2G, \quad (15)$$

which is the condition for half-filling. If $\mu \rightarrow -\infty$, the quantity $n_d + n_f$ goes to zero, and if $\mu \rightarrow +\infty$, this number approaches 4.

We now introduce Hubbard transfer operators for the ionic quantum transitions $X^{mn} = |\Psi_m\rangle\langle\Psi_n|$ and express the annihilation operators of d and f electrons in terms of them,

$$d_{\sigma} = X^{1,3-\sigma} + \sigma X^{3+\sigma,6} + \frac{1}{\sqrt{2}} (\sigma X^{4+\sigma,7} + X^{4+\sigma,10}) + \frac{1}{\sqrt{2}} (\sigma X^{10,13-\sigma} - X^{7,13-\sigma}) + \sigma X^{10+\sigma,13+\sigma} + X^{4-\sigma,10-\sigma} + X^{8,14-\sigma} + \sigma X^{14+\sigma,16} \quad (16)$$

and

$$f_{\sigma} = X^{1,4-\sigma} + \sigma X^{4+\sigma,8} + \frac{1}{\sqrt{2}} (\sigma X^{3+\sigma,7} - X^{3+\sigma,10}) - X^{3-\sigma,10-\sigma} + X^{6,13-\sigma} - \frac{1}{\sqrt{2}} (X^{7,14-\sigma} + \sigma X^{10,14-\sigma}) + \sigma (-X^{10+\sigma,14+\sigma} + X^{13+\sigma,16}). \quad (17)$$

In the case in which we have only correlated d electrons with four states at each site,

$$|\Psi_1\rangle = |0\rangle, \quad |\Psi_2\rangle = d_{\uparrow}^{\dagger}|0\rangle, \quad |\Psi_3\rangle = d_{\downarrow}^{\dagger}|0\rangle,$$

$$|\Psi_4\rangle = d_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger}|0\rangle, \quad (18)$$

the definition of d annihilation operators by means of Hubbard operators is simply

$$d_{\sigma} = |\Psi_1\rangle\langle\Psi_{2+(1-\sigma)/2}| + \sigma |\Psi_{2+(1+\sigma)/2}\rangle\langle\Psi_4|. \quad (19)$$

The complicated form of Eqs. (16) and (17) compared to Eq. (18) is due to the complicated form of our zero-order Hamiltonian (1a) (similar operator expressions for the two-site but single-band Hubbard model¹⁷ can be found in Ref. 28).

The Hubbard transfer operators $Y^{\lambda\lambda'} = |E_{\lambda}\rangle\langle E_{\lambda}'|$ between states of the diagonalized Hamiltonian are more convenient to use than the primary Hubbard operators X^{mn} . On the basis of Eqs. (6a) and (6b) we find for the transformation of Hubbard operators,

$$X^{mn} = \sum_{\lambda\lambda'} \Phi_m(E_{\lambda}) \Phi_n^*(E_{\lambda}') Y^{\lambda\lambda'}, \quad (20a)$$

$$Y^{\lambda\lambda'} = \sum_{mn} \Phi_m^*(E_{\lambda}) \Phi_n(E_{\lambda}') X^{mn}. \quad (20b)$$

Taking into account Eqs. (16), (17), (20a), and (20b), we obtain

$$d_{\uparrow} = \sum_{\lambda=2,3} \Phi_2(E_{\lambda}) Y^{1,\lambda} + \sum_{\lambda=2,3} \Phi_3(E_{\lambda}) Y^{\lambda,9} + \frac{1}{\sqrt{2}} \sum_{\lambda=4,5} \Phi_5(E_{\lambda}) Y^{\lambda,10} + \sum_{a=6,7,8} \sum_{\lambda=4,5} \left[\Phi_5(E_{\lambda}) \frac{1}{\sqrt{2}} \Phi_7(E_a) + \Phi_4(E_{\lambda}) \Phi_6(E_a) \right] Y^{\lambda,a} + \sum_{a=6,7,8} \sum_{\lambda=12,13} \left[-\frac{1}{\sqrt{2}} \Phi_7(E_a) \Phi_{12}(E_{\lambda}) + \Phi_8(E_a) \Phi_{13}(E_{\lambda}) \right] Y^{a,\lambda} + \frac{1}{\sqrt{2}} \sum_{\lambda=12,13} \Phi_{12}(E_{\lambda}) Y^{10,\lambda} + \sum_{\lambda=14,15} [\Phi_{14}(E_{\lambda}) Y^{11,\lambda} + \Phi_{15}(E_{\lambda}) Y^{\lambda,16}] \quad (21)$$

and

$$\begin{aligned}
f_{\uparrow} = & \sum_{\lambda=2,3} [\Phi_3(E_{\lambda})Y^{1,\lambda} - \Phi_2(E_{\lambda})Y^{\lambda,9}] \\
& - \frac{1}{\sqrt{2}} \sum_{\lambda=4,5} \Phi_4(E_{\lambda})Y^{\lambda,10} \\
& + \sum_{a=6,7,8} \sum_{\lambda=4,5} \left[\Phi_4(E_{\lambda}) \frac{1}{\sqrt{2}} \Phi_7(E_a) \right. \\
& \left. + \Phi_5(E_{\lambda})\Phi_8(E_a) \right] Y^{\lambda,a} \\
& + \sum_{a=6,7,8} \sum_{\lambda=12,13} \left[-\frac{1}{\sqrt{2}} \Phi_7(E_a)\Phi_{13}(E_{\lambda}) \right. \\
& \left. + \Phi_6(E_a)\Phi_{12}(E_{\lambda}) \right] Y^{a,\lambda} - \frac{1}{\sqrt{2}} \sum_{\lambda=12,13} \Phi_{13}(E_{\lambda})Y^{10,\lambda} \\
& + \sum_{\lambda=14,15} [-\Phi_{15}(E_{\lambda})Y^{11,\lambda} + \Phi_{14}(E_{\lambda})Y^{\lambda,16}]. \quad (22)
\end{aligned}$$

With the help of these equations, it is easy to determine the average number of d and f electrons in the local model,

$$\begin{aligned}
\langle d_{\uparrow}^{\dagger}d_{\uparrow} \rangle_0 = & \frac{1}{Z_0} \left\{ \sum_{\lambda=2,3} \Phi_2^2(E_{\lambda})e^{-\beta E_{\lambda}} \right. \\
& + \sum_{a=6,7,8} \left[\Phi_6^2(E_a) + \frac{1}{2}\Phi_7^2(E_a) \right] e^{-\beta E_a} + \frac{3}{2}e^{-\beta E_9} \\
& \left. + \sum_{\lambda=12,13} [1 + \Phi_{12}^2(E_{\lambda})]e^{-\beta E_{\lambda}} + e^{-\beta E_{16}} \right\} \quad (23)
\end{aligned}$$

and

$$\begin{aligned}
\langle f_{\uparrow}^{\dagger}f_{\uparrow} \rangle_0 = & \frac{1}{Z_0} \left\{ \sum_{\lambda=2,3} \Phi_3^2(E_{\lambda})e^{-\beta E_{\lambda}} \right. \\
& + \sum_{a=6,7,8} \left[\frac{1}{2}\Phi_7^2(E_a) + \Phi_8^2(E_a) \right] e^{-\beta E_a} + \frac{3}{2}e^{-\beta E_9} \\
& \left. + \sum_{\lambda=12,13} [1 + \Phi_{13}^2(E_{\lambda})]e^{-\beta E_{\lambda}} + e^{-\beta E_{16}} \right\}. \quad (24)
\end{aligned}$$

The sum of these two equations gives us the average number of d and f -electrons for one spin direction. Because of the mixing of the d - and f -electron states, the value $\langle f_{\uparrow}^{\dagger}d_{\uparrow} \rangle$ is different from zero,

$$\begin{aligned}
\langle f_{\uparrow}^{\dagger}d_{\uparrow} \rangle_0 = & \frac{1}{Z_0} \left\{ \sum_{\lambda=2,3} \Phi_2(E_{\lambda})\Phi_3(E_{\lambda})e^{-\beta E_{\lambda}} \right. \\
& - \sum_{\lambda=14,15} \Phi_{14}(E_{\lambda})\Phi_{15}(E_{\lambda})e^{-\beta E_{\lambda}} \\
& \left. + \frac{1}{\sqrt{2}} \sum_{a=6,7,8} \Phi_7(E_a)[\Phi_6(E_a) + \Phi_8(E_a)]e^{-\beta E_a} \right\} \quad (25)
\end{aligned}$$

We will now determine the Matsubara one-particle Green's functions of localized d and f electrons:

$$G_{\sigma}^{dd(0)}(\tau - \tau') = -\langle Td_{\sigma}(\tau)\bar{d}_{\sigma}(\tau') \rangle_0, \quad (26a)$$

$$G_{\sigma}^{ff(0)}(\tau - \tau') = -\langle Tf_{\sigma}(\tau)\bar{f}_{\sigma}(\tau') \rangle_0, \quad (26b)$$

$$G_{\sigma}^{df(0)}(\tau - \tau') = -\langle Td_{\sigma}(\tau)\bar{f}_{\sigma}(\tau') \rangle_0, \quad (26c)$$

where $d(\tau) = e^{\tau H_0}d e^{-\tau H_0}$, $\bar{d}(\tau) = e^{\tau H_0}d^{\dagger} e^{-\tau H_0}$, etc., and their Fourier components,

$$G_{\sigma}(\tau) = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n\tau} G_{\sigma}(i\omega_n), \quad \omega_n = \frac{\pi}{\beta}(2n+1).$$

By using Eqs. (21), (26a), and the properties of the Hubbard operators, we obtain the following equation for the d -electron Green's function:

$$\begin{aligned}
G_{\uparrow}^{dd(0)}(i\omega_n) = & \frac{1}{Z_0} \left\{ \sum_{\lambda=2,3} \Phi_2^2(E_{\lambda}) \frac{e^{-\beta E_1} + e^{-\beta E_{\lambda}}}{i\omega_n + E_1 - E_{\lambda}} + \frac{3}{2} \sum_{\lambda=2,3} \Phi_3^2(E_{\lambda}) \frac{e^{-\beta E_{\lambda}} + e^{-\beta E_9}}{i\omega_n + E_{\lambda} - E_9} \right. \\
& + \sum_{a=6,7,8} \sum_{\lambda=2,3} \left(\Phi_3(E_{\lambda}) \frac{1}{\sqrt{2}} \Phi_7(E_a) + \Phi_2(E_{\lambda})\Phi_6(E_a) \right)^2 \frac{e^{-\beta E_{\lambda}} + e^{-\beta E_a}}{i\omega_n + E_{\lambda} - E_a} \\
& + \frac{3}{2} \sum_{\lambda=12,13} \Phi_{12}^2(E_{\lambda}) \frac{e^{-\beta E_9} + e^{-\beta E_{\lambda}}}{i\omega_n + E_9 - E_{\lambda}} + \sum_{\lambda=12,13} \Phi_{13}^2(E_{\lambda}) \frac{e^{-\beta E_{\lambda}} + e^{-\beta E_{16}}}{i\omega_n + E_{\lambda} - E_{16}} \\
& \left. + \sum_{a=6,7,8} \sum_{\lambda=12,13} \left(-\frac{1}{\sqrt{2}} \Phi_7(E_a)\Phi_{12}(E_{\lambda}) + \Phi_8(E_a)\Phi_{13}(E_{\lambda}) \right)^2 \frac{e^{-\beta E_{\lambda}} + e^{-\beta E_a}}{i\omega_n + E_a - E_{\lambda}} \right\}; \quad (27)
\end{aligned}$$

for f electrons we have

$$\begin{aligned}
G_{\uparrow}^{ff(0)}(i\omega_n) = & \frac{1}{Z_0} \left\{ \sum_{\lambda=2,3} \Phi_3^2(E_\lambda) \frac{e^{-\beta E_1} + e^{-\beta E_\lambda}}{i\omega_n + E_1 - E_\lambda} + \frac{3}{2} \sum_{\lambda=2,3} \Phi_2^2(E_\lambda) \frac{e^{-\beta E_\lambda} + e^{-\beta E_9}}{i\omega_n + E_\lambda - E_9} \right. \\
& + \sum_{a=6,7,8} \sum_{\lambda=2,3} \left(\Phi_2(E_\lambda) \frac{1}{\sqrt{2}} \Phi_7(E_a) + \Phi_3(E_\lambda) \Phi_8(E_a) \right)^2 \frac{e^{-\beta E_\lambda} + e^{-\beta E_a}}{i\omega_n + E_\lambda - E_a} \\
& + \frac{3}{2} \sum_{\lambda=12,13} \Phi_{13}^2(E_\lambda) \frac{e^{-\beta E_9} + e^{-\beta E_\lambda}}{i\omega_n + E_9 - E_\lambda} + \sum_{\lambda=12,13} \Phi_{12}^2(E_\lambda) \frac{e^{-\beta E_\lambda} + e^{-\beta E_{16}}}{i\omega_n + E_\lambda - E_{16}} \\
& \left. + \sum_{a=6,7,8} \sum_{\lambda=12,13} \left(-\frac{1}{\sqrt{2}} \Phi_7(E_a) \Phi_{13}(E_\lambda) + \Phi_6(E_a) \Phi_{12}(E_\lambda) \right)^2 \frac{e^{-\beta E_\lambda} + e^{-\beta E_a}}{i\omega_n + E_a - E_\lambda} \right\}; \quad (28)
\end{aligned}$$

and finally for the mixed local Green's function it follows that

$$\begin{aligned}
G_{\uparrow}^{df(0)}(i\omega_n) = & \frac{1}{Z_0} \left\{ \sum_{\lambda=2,3} \Phi_2(E_\lambda) \Phi_3(E_\lambda) \left(\frac{e^{-\beta E_1} + e^{-\beta E_\lambda}}{i\omega_n + E_1 - E_\lambda} - \frac{3}{2} \frac{e^{-\beta E_9} + e^{-\beta E_\lambda}}{i\omega_n + E_\lambda - E_9} \right) \right. \\
& + \sum_{\lambda=12,13} \Phi_{12}(E_\lambda) \Phi_{13}(E_\lambda) \left(-\frac{3}{2} \frac{e^{-\beta E_9} + e^{-\beta E_\lambda}}{i\omega_n + E_9 - E_\lambda} + \frac{e^{-\beta E_\lambda} + e^{-\beta E_{16}}}{i\omega_n + E_\lambda - E_{16}} \right) \\
& + \sum_{a=6,7,8} \sum_{\lambda=2,3} \left(\Phi_3(E_\lambda) \frac{1}{\sqrt{2}} \Phi_7(E_a) + \Phi_2(E_\lambda) \Phi_6(E_a) \right) \left(\Phi_2(E_\lambda) \frac{1}{\sqrt{2}} \Phi_7(E_a) + \Phi_3(E_\lambda) \Phi_8(E_a) \right) \\
& \times \frac{e^{-\beta E_\lambda} + e^{-\beta E_a}}{i\omega_n + E_\lambda - E_a} + \sum_{a=6,7,8} \sum_{\lambda=12,13} \left(-\frac{1}{\sqrt{2}} \Phi_7(E_a) \Phi_{13}(E_\lambda) + \Phi_6(E_a) \Phi_{12}(E_\lambda) \right) \\
& \times \left(-\frac{1}{\sqrt{2}} \Phi_7(E_a) \Phi_{12}(E_\lambda) + \Phi_8(E_a) \Phi_{13}(E_\lambda) \right) \frac{e^{-\beta E_\lambda} + e^{-\beta E_a}}{i\omega_n + E_a - E_\lambda} \left. \right\}. \quad (29)
\end{aligned}$$

When the symmetry condition (14) holds, we have the following simplifications:

$$\Phi_{12}(E_{12,13}) = \Phi_2(E_{3,2}), \quad \Phi_{13}(E_{12,13}) = \Phi_3(E_{3,2}).$$

If in addition $E_{16}=0$ is fulfilled and we make use of Eq. (15) for the chemical potential at half-filling, the following symmetry properties are easily verified:

$$G_{\sigma}^{aa(0)}(-i\omega_n) = -G_{\sigma}^{aa(0)}(i\omega_n), \quad a=(d,f), \quad (30a)$$

$$G_{\sigma}^{df(0)}(-i\omega_n) = G_{\sigma}^{df(0)}(i\omega_n). \quad (30b)$$

The diagonal local functions (27) and (28) are even and the mixed functions (29) are odd with respect to the change of sign of the hybridization. Therefore, we have the following antisymmetry relation valid for all local Green's functions for the case when Eq. (14) holds and $E_{16}=0$,

$$G_{\sigma}^{ab(0)}(-i\omega_n, -V) = -G_{\sigma}^{ab(0)}(i\omega_n, V). \quad (31)$$

IV. THE DELOCALIZATION PROCESS

The renormalization of the local Green's function due to d -electron hopping is now discussed in a rather compact fashion, since many elements of the perturbation theory developed earlier for the Hubbard model^{15,16} can be used here.

The full Matsubara Green's functions in the interaction representation are defined by

$$G_{\sigma\sigma'}^{dd}(x-x') = -\langle T d_{x\sigma}^{\dagger}(\tau) \bar{d}_{x'\sigma'}(\tau') U(\beta) \rangle_0^c, \quad (32a)$$

$$G_{\sigma\sigma'}^{ff}(x-x') = -\langle T f_{x\sigma}^{\dagger}(\tau) \bar{f}_{x'\sigma'}(\tau') U(\beta) \rangle_0^c, \quad (32b)$$

$$G_{\sigma\sigma'}^{df}(x-x') = -\langle T d_{x\sigma}^{\dagger}(\tau) \bar{f}_{x'\sigma'}(\tau') U(\beta) \rangle_0^c \quad (32c)$$

with $x=(\vec{x}, \tau)$. The evolution operator

$$U(\beta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\beta} d\tau_1 \cdots \int_0^{\beta} d\tau_n T H'(\tau_1) \cdots H'(\tau_n)$$

has the same form as in the case of the one-band Hubbard model for d electrons with hopping t_{ij} in Eq. (1b) as perturbation. The statistical averages in Eq. (32) will be evaluated with the partition function of the local model. The index c in Eq. (32) means that only connected diagrams have to be taken into account. The GWT and corresponding diagram technique¹⁵⁻²² will be used to obtain the Green's functions. Because the first Green's function in Eqs. (32) formally coincides with the corresponding one of the one-band Hubbard model,^{15,16} we may write the Dyson equation as

$$G_{\sigma\sigma'}^{dd}(x-x') = \Lambda_{\sigma\sigma'}^{dd}(x-x') + \sum_{\sigma_1} \sum_{12} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \\ \times \Lambda_{\sigma_1\sigma'}^{dd}(x-1)t(1-2)G_{\sigma_1\sigma'}^{dd}(2-x'), \quad (33)$$

where $t(1-2) = t(\vec{1}-\vec{2})\delta(\tau_1-\tau_2)$ and

$$\Lambda_{\sigma\sigma'}^{dd}(x-x') = G_{\sigma\sigma'}^{dd(0)}(x-x') + Z_{\sigma\sigma'}^{dd}(x-x'). \quad (34)$$

Here $Z_{\sigma\sigma'}^{dd}$ is the correlation function first obtained in Refs. 14 and 15 as the sum of all *strongly connected diagrams* that contain irreducible Green's functions. Figure 1 shows some of the lower order Feynman diagrams for the correlation function $Z_{\sigma\sigma'}^{dd}$ of the d electrons. Retaining all terms in lowest order leads to^{15,16}

$$Z_{\sigma\sigma'}^{dd(2)}(x-x') = -\delta_{\vec{x},\vec{x}'} \sum_{\sigma_1\sigma_2} \sum_{12} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 G_2^{(0)ir} \\ \times (\sigma\tau, \sigma_1\tau_1 | \sigma_2\tau_2, \sigma'\tau') t(\vec{x}-\vec{2})t \\ \times (\vec{1}-\vec{x})G_{\sigma_1\sigma_2}^{dd(0)}(2-1). \quad (35)$$

If we take into account only the chain diagrams and neglect all contributions that contain irreducible Green's functions, we obtain the Hubbard I-like approximation of our model. The Fourier transform of the d -electron Green's function is then of the form

$$G_{\sigma}^{ddl}(\vec{k}, i\omega) = G_{\sigma}^{dd(0)}(i\omega)[1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(i\omega)]^{-1}. \quad (36)$$

In the same approximation, the propagator of the f electrons and of the d - f transfer can be expressed as

$$G_{\sigma}^{ffl}(\vec{k}, i\omega) = G_{\sigma}^{ff(0)}(i\omega) + \frac{G_{\sigma}^{fd(0)}(i\omega)\epsilon(\vec{k})G_{\sigma}^{df(0)}}{1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(i\omega)} \quad (37)$$

and

$$G_{\sigma}^{dfl}(\vec{k}, i\omega) = G_{\sigma}^{df(0)}(i\omega)[1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(i\omega)]^{-1}, \quad (38a)$$

$$G_{\sigma}^{fdl}(\vec{k}, i\omega) = G_{\sigma}^{fd(0)}(i\omega)[1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(i\omega)]^{-1}. \quad (38b)$$

It is clear that in this approximation the energy spectrum of delocalized states of the PAM is determined by the equation

$$1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(E) = 0, \quad (39)$$

where $G_{\sigma}^{dd(0)}(E)$ is the analytical continuation of the Matsubara function from the discrete number of points, $i\omega_n$, into the complex E plane. For the one-band Hubbard model, the Hubbard I approximation gives two branches, the lower and upper Hubbard subbands. But in our case, due to the complicated structure of Eq. (27), Eq. (39) will be nontrivial and will have as many roots as there are distinct energy differences for all possible quantum transitions on the ion.

In order to simplify the problem of finding the energy subbands, we will discuss only the case of the symmetrical PAM given by the condition (14). Additionally, we assume that the Falicov-Kimball term is zero, $G=0$. In this case, we find from the denominators of the Green's functions (27) and (28) that some of the 20 energy differences coincide and only eight of them remain different,

$$E_1 - E_2 = E_3 - E_9 = E_7 - E_{12} = -E_f, \\ E_1 - E_3 = E_2 - E_9 = E_7 - E_{13} = -E_d, \\ E_2 - E_6 = E_8 - E_{13} = -E_d + \alpha^2 U, \\ E_3 - E_6 = E_8 - E_{12} = -E_f + \alpha^2 U, \quad (40)$$

$$E_2 - E_7 = E_9 - E_{13} = E_{12} - E_{16} = -E_d - U,$$

$$E_3 - E_7 = E_9 - E_{12} = E_{13} - E_{16} = -E_f - U,$$

$$E_2 - E_8 = E_6 - E_{13} = -E_d - U - \alpha^2 U,$$

$$E_3 - E_8 = E_6 - E_{12} = -E_f - U - \alpha^2 U,$$

where

$$E_d = \epsilon_d + \frac{\Phi^2}{1-2\Phi^2}(\epsilon_d - \epsilon_f),$$

$$E_f = \epsilon_f - \frac{\Phi^2}{1-2\Phi^2}(\epsilon_d - \epsilon_f),$$

$$\Phi^2 = \frac{1}{2} \left[1 - \frac{1}{\sqrt{1 + [2V/(\epsilon_d - \epsilon_f)]^2}} \right],$$

$$\alpha^2 = \frac{\Psi^2}{1-2\Psi^2},$$

$$\Psi^2 = \frac{1}{2} \left[1 - \frac{1}{\sqrt{1 + (4V/U)^2}} \right],$$

$$D^2 = \frac{1}{2} \left[\Phi^2 + \Psi^2 - 2\Phi^2\Psi^2 - \frac{4V^2(1-2\Phi^2)(1-2\Psi^2)}{U(\epsilon_d - \epsilon_f)} \right].$$

In this case, the Green's function (27) takes the form

$$G_{\uparrow}^{dd(0)}(E) = \frac{(1-\Phi^2)A_1}{E-E_d} + \frac{1}{2} \frac{(1-2D^2)A_2}{E-E_d+\alpha^2 U} + \frac{(1-\Phi^2)A_3}{E-E_f-U} \\ + \frac{1}{2} \frac{(1-2D^2)A_4}{E-E_f-U-\alpha^2 U} + \frac{\Phi^2 A_5}{E-E_f} + \frac{\Phi^2 A_6}{E-E_d-U} \\ + \frac{D^2 A_7}{E-E_d-U-\alpha^2 U} + \frac{D^2 A_8}{E-E_f+\alpha^2 U}. \quad (41)$$

The values of the coefficients A_n are equal to

$$\begin{aligned}
Z_0 A_1 &= e^{-\beta E_1} + e^{-\beta E_3} + \frac{3}{2}(e^{-\beta E_2} + e^{-\beta E_9}) \\
&\quad + \frac{1}{2}(e^{-\beta E_7} + e^{-\beta E_{13}}), \\
Z_0 A_2 &= e^{-\beta E_2} + e^{-\beta E_6} + e^{-\beta E_8} + e^{-\beta E_{13}}, \\
Z_0 A_3 &= \frac{1}{2}(e^{-\beta E_3} + e^{-\beta E_7}) + \frac{3}{2}(e^{-\beta E_9} + e^{-\beta E_{12}}) \\
&\quad + e^{-\beta E_{13}} + e^{-\beta E_{16}}, \\
Z_0 A_4 &= e^{-\beta E_3} + e^{-\beta E_8} + e^{-\beta E_6} + e^{-\beta E_{12}}, \quad (42) \\
Z_0 A_5 &= e^{-\beta E_1} + e^{-\beta E_2} + \frac{3}{2}(e^{-\beta E_9} + e^{-\beta E_3}) \\
&\quad + \frac{1}{2}(e^{-\beta E_7} + e^{-\beta E_{12}}), \\
Z_0 A_6 &= e^{-\beta E_{12}} + e^{-\beta E_{16}} + \frac{3}{2}(e^{-\beta E_9} + e^{-\beta E_{13}}) \\
&\quad + \frac{1}{2}(e^{-\beta E_2} + e^{-\beta E_7}), \\
A_7 &= A_2, \quad A_8 = A_4.
\end{aligned}$$

In the following, we show that the energy spectrum for the symmetrical case can be discussed analytically for energies close to the local energies E_f and $E_d + U$ and for weak hybridization (exact numerical results are discussed at the end). Close to E_f , the main contributions to the Green's function (41) are terms that contain the coefficients A_5 and A_8 . Because the numerators of these terms contain small parameters, it is necessary to keep only the terms of the same order of smallness in the denominators, i.e., $V/U, V/(\epsilon_d - \epsilon_f) \ll 1$. This leads close to E_f to two energy subbands,

$$E = E_f + \Phi^2 \lambda_1 + O(\Phi^4), \quad \Phi^2 \ll 1, \quad (43)$$

where λ_1 is determined from

$$\frac{A_5}{\lambda_1} + \frac{D^2}{\Phi^2} \frac{A_8}{\lambda_1 + \alpha^2 U / \Phi^2} + \frac{A_1 + \frac{1}{2} A_2}{\epsilon_f - \epsilon_d} - \frac{A_3 + \frac{1}{2} A_4}{U} = \frac{1}{\epsilon(\vec{k})}. \quad (44)$$

Near the local energy $E_d + U$ we obtain also two subbands,

$$E = E_d + U + \Phi^2 \lambda_2 + O(\Phi^4), \quad \Phi^2 \ll 1, \quad (45)$$

where λ_2 is determined by

$$\frac{A_6}{\lambda_2} + \frac{D^2}{\Phi^2} \frac{A_7}{\lambda_2 - \alpha^2 U / \Phi^2} + \frac{A_1 + \frac{1}{2} A_2}{U} + \frac{A_3 + \frac{1}{2} A_4}{\epsilon_d - \epsilon_f} = \frac{1}{\epsilon(\vec{k})}. \quad (46)$$

We will now try to find the four missing solutions of Eq. (39). There are contributions from those terms in Eq. (41) that contain in the denominators $E - E_d$ and $E - E_f - U$. All of them have no small parameters in the numerators. Therefore, it is necessary to find first the solutions of Eq. (39) for the case in which all small parameters are equal to zero. This equation is of the form,

$$\frac{A_1 + \frac{1}{2} A_2}{\lambda^{(0)} - \epsilon_d} + \frac{A_3 + \frac{1}{2} A_4}{\lambda^{(0)} - \epsilon_f - U} = \frac{1}{\epsilon(\vec{k})}. \quad (47)$$

After solving this equation, we determine the corrections conditioned by the small parameters. From Eq. (47), one obtains

$$\begin{aligned}
\lambda_{\pm}^{(0)} &= \frac{1}{2}(\epsilon_d + \epsilon_f + U + \epsilon(\vec{k}))(A_1 + \frac{1}{2} A_2 + A_3 + \frac{1}{2} A_4) \\
&\quad \pm \{[\epsilon_d - \epsilon_f - U + \epsilon(\vec{k}))(A_1 + \frac{1}{2} A_2 - A_3 - \frac{1}{2} A_4)]^2 \\
&\quad + 4\epsilon^2(\vec{k})(A_1 + \frac{1}{2} A_2)(A_3 + \frac{1}{2} A_4)\}^{1/2}. \quad (48)
\end{aligned}$$

The improved solutions have the form

$$E_{\pm} = \lambda_{\pm}^{(0)} + \Phi^2 \lambda_{\pm}^{(1)} + O(\Phi^4), \quad (49)$$

where $\lambda^{(1)}$ is determined from

$$\begin{aligned}
\lambda_{\pm}^{(1)} &\left\{ \frac{A_1 + \frac{1}{2} A_2}{(\lambda_{\pm}^{(0)} - \epsilon_d)^2} + \frac{A_3 + \frac{1}{2} A_4}{(\lambda_{\pm}^{(0)} - \epsilon_f - U)^2} \right\} = - \frac{A_1 + A_2 D^2 / \Phi^2}{\lambda_{\pm}^{(0)} - \epsilon_d} \\
&\quad - \frac{\frac{1}{2} A_2 U \alpha^2 / \Phi^2}{(\lambda_{\pm}^{(0)} - \epsilon_d)^2} - \frac{A_3 + A_4 D^2 / \Phi^2}{\lambda_{\pm}^{(0)} - \epsilon_f - U} + \frac{\frac{1}{2} A_4 U \alpha^2 / \Phi^2}{(\lambda_{\pm}^{(0)} - \epsilon_f - U)^2} \\
&\quad + \frac{(\epsilon_d - \epsilon_f)(A_1 + \frac{1}{2} A_2)}{(\lambda_{\pm}^{(0)} - \epsilon_d)^2} + \frac{A_5 + A_8 D^2 / \Phi^2}{\lambda_{\pm}^{(0)} - \epsilon_f} \\
&\quad - \frac{A_6 + A_7 D^2 / \Phi^2}{\lambda_{\pm}^{(0)} - \epsilon_d - U} - \frac{(\epsilon_d - \epsilon_f)(A_3 + \frac{1}{2} A_4)}{(\lambda_{\pm}^{(0)} - \epsilon_f - U)^2}. \quad (50)
\end{aligned}$$

Two further solutions remain to be found. We suppose that one of them is close to E_d and can be written in the form

$$E = E_d + \Phi^2 \lambda_1 + O(\Phi^4). \quad (51)$$

The second one is close to $E_f + U$,

$$E = E_f + U + \Phi^2 \lambda_2 + O(\Phi^4). \quad (52)$$

When evaluating λ_1 and λ_2 , special care must be taken when $\epsilon(\vec{k}) = 0$. If we use $\epsilon(\vec{k}) = \Phi^2 \bar{\epsilon}(\vec{k})$, essential energetic contributions are transferred to the main part of the expansion ensuring its existence also for $\vec{k} = 0$. The result is

$$\begin{aligned}
\lambda_1 &= \frac{1}{2} \bar{\epsilon}(\vec{k})(A_1 + \frac{1}{2} A_2) - \alpha^2 U / (2\Phi^2) \\
&\quad - \frac{1}{2} \text{sgn} \bar{\epsilon}(\vec{k}) [\{\bar{\epsilon}(\vec{k})(A_1 + \frac{1}{2} A_2)\}^2 \\
&\quad + 2U \bar{\epsilon}(\vec{k})(A_1 - \frac{1}{2} A_2) \alpha^2 / \Phi^2 + (\alpha^2 U / \Phi^2)^2]^{1/2}. \quad (53)
\end{aligned}$$

From the two possible solutions for λ_1 , we take that one for which $\bar{\epsilon} = \epsilon / \Phi^2 \rightarrow \infty$ gives us the correct solution. In the same way, we obtain the following for λ_2 :

$$\begin{aligned}
\lambda_2 &= \frac{1}{2} \bar{\epsilon}(\vec{k})(A_3 + \frac{1}{2} A_4) - \alpha^2 U / (2\Phi^2) \\
&\quad - \frac{1}{2} \text{sgn} \bar{\epsilon}(\vec{k}) [\{\bar{\epsilon}(\vec{k})(A_3 + \frac{1}{2} A_4)\}^2 \\
&\quad + 2U \bar{\epsilon}(\vec{k})(\frac{1}{2} A_4 - A_3) \alpha^2 / \Phi^2 + (\alpha^2 U / \Phi^2)^2]^{1/2} \quad (54)
\end{aligned}$$

Both quantities λ_1 and λ_2 now have correct values for all band energies $\epsilon(\vec{k})$.

V. COMPUTATION OF QUASIPARTICLE BANDS

The Hamiltonian of our model contains two different types of matrix elements, namely the on-site hybridization of d and f electrons and the d -electron transfer term between nearest neighbor sites. The first one is, among other things, responsible for pairing fluctuations of electrons.^{13,14,29} This term is taken into account exactly in zero order, where it is already responsible for the appearance of singlet pairs, see $|\Psi_7\rangle$ in Eq. (2). The second type of interaction is responsible for the delocalization of the electrons and contributes to conductivity processes.

The local model has been treated exactly by using a new form of canonical transformation on the basis of the complete set of orthonormalized functions $\Phi_n(E_\lambda)$ determined by Eqs. (4) and (5). These functions allow us to classify the eigenvalues and eigenfunctions of the local Hamiltonian (1a). We have obtained 10 different renormalized values of the bare on-site energies, which can be classified by using the number of particles that participates in the corresponding quantum state as well as the spin and its projections. The renormalized vacuum state $|E_1\rangle = |0\rangle$ is not altered by the hybridization. But all one-, two-, and three-particle states with spin $S = \frac{1}{2}, 0$ and 1 are essentially changed. For example, instead of the two one-particle states with energies ϵ_d and ϵ_f , $|E_2\rangle$ and $|E_3\rangle$ appear (and also $|E_4\rangle$ and E_5) having bonding and antibonding character, respectively. The corresponding operators that create the bonding and antibonding states are determined by the canonical transformation,¹⁰⁻¹²

$$b_{\sigma}^{\dagger} = \Phi_2(E_2)d_{\sigma}^{\dagger} + \Phi_3(E_2)f_{\sigma}^{\dagger}, \quad (55a)$$

$$a_{\sigma}^{\dagger} = \Phi_2(E_3)d_{\sigma}^{\dagger} + \Phi_3(E_3)f_{\sigma}^{\dagger}. \quad (55b)$$

For the energies of the three two-electron singlet states with $N=2$ and $S=0$, we find in the limit of weak hybridization

$$E_6 \approx \epsilon_d + \epsilon_f + G - \frac{4V^2(U-G)}{(U-G)^2 - [\epsilon_d - \epsilon_f + \frac{1}{2}(U_d - U_f)]^2}, \quad (56a)$$

$$E_7 \approx 2\epsilon_d + U_d + \frac{2V^2}{\epsilon_d - \epsilon_f + U_d - G}, \quad (56b)$$

$$E_8 \approx 2\epsilon_f + U_f + \frac{2V^2}{\epsilon_f - \epsilon_d + U_f - G}, \quad (56c)$$

where $U = \frac{1}{2}(U_d + U_f)$, $E_{2d} = 2\epsilon_d + U_d$, and $E_{2f} = 2\epsilon_f + U_f$ (the latter two quantities are the energies of the doublet states). From Eqs. (56) it follows that E_6 is much lower in energy than E_7 and E_8 . If the hybridization is not weak, the same observation follows from Eqs. (A4) and (A5) in the Appendix. The lowest renormalized state $|E_6\rangle$ is the superposition of the original ionic singlet states,

$$|E_6\rangle = \Phi_6(E_6)d_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger}|0\rangle + \frac{1}{\sqrt{2}}\Phi_7(E_6)(d_{\uparrow}^{\dagger}f_{\downarrow}^{\dagger} - d_{\downarrow}^{\dagger}d_{\uparrow}^{\dagger})|0\rangle + \Phi_8(E_6)f_{\uparrow}^{\dagger}f_{\downarrow}^{\dagger}|0\rangle, \quad (57)$$

where the functions $\Phi_n(E_6)$ are the probability amplitudes that the ionic states are involved in the renormalization. Only for very special cases can the singlet state of lowest energy be presented by two bonding states, $b_{\uparrow}^{\dagger}b_{\downarrow}^{\dagger}|0\rangle$.

Three triplet states, $|E_9, \dots, 11\rangle$, are situated above this singlet state all having the same energy $E_9 = \epsilon_d + \epsilon_f + G$. The corresponding energy difference determines some critical temperature,

$$k_B T^* = E_9 - E_6, \quad (58)$$

being equal to the energy gain associated with the formation of the singlet state $|E_6\rangle$. This temperature is crucial for understanding the magnetic properties of the model. For temperatures $T \ll T^*$ and low enough electron concentration, it is mainly the singlet state that is populated, giving rise to zero magnetic moment. With increasing temperature, the triplet states can be populated, giving rise to a nonvanishing magnetic moment.⁶ For strong correlations, the energy spectrum can be separated into a low-energy part containing the states $|E_\lambda\rangle$ ($\lambda = 1, \dots, 6, 9, \dots, 11$) and a high-energy part ($\lambda = 7, 8, 12, \dots, 16$) with a separation in energy that is proportional to the Coulomb interaction.

We now discuss the resulting renormalization of the on-site transitions (40) by using Eqs. (36) and (39) for the case

$$\epsilon_f < \epsilon_d = 0, \quad G = 0, \quad U_f, U_d, \epsilon_d - \epsilon_f \gg |V| \quad (59)$$

leading to $0 > E_9 > E_2 > E_6$. This allows us to estimate the values of A_n in the low-temperature limit. $T \rightarrow 0$,

$$\begin{aligned} A_1 &\approx \frac{3}{2}g, \quad A_2 \approx 1 - g, \quad A_3 \approx \frac{3}{2}g_1, \\ A_4 &\approx 1 - 2g, \quad A_5 \approx g, \quad A_6 \approx \frac{1}{2}g, \\ g &= e^{-\beta(E_2 - E_6)}, \quad g_1 = e^{-\beta(E_9 - E_6)}, \end{aligned} \quad (60)$$

where g and g_1 are very small quantities. For small hybridization, also the quantities Φ^2 , Ψ^2 , and D^2 become small and can be approximated by

$$\begin{aligned} \Phi^2 &\approx \frac{V^2}{(\epsilon_d - \epsilon_f)^2}, \quad \alpha^2 \approx \Psi^2 \approx \frac{4V^2}{U^2}, \\ D^2 &\approx \frac{V^2}{2} \left(\frac{1}{\epsilon_d - \epsilon_f} - \frac{2}{U} \right). \end{aligned} \quad (61)$$

For such typical values of the parameters as $\epsilon_d = 0$, $\epsilon_f = -1$ eV, $U = 1 - 4$ eV, $U_d = 0 - 1$ eV, and $|V| = (10)^{-1/2}$ eV, the coefficients in Eq. (61) are of the order of 10^{-1} . Using the smallness of (g, g_1) and (Φ^2, α^2, D^2) , we can obtain from Eqs. (43) and (44) a simplified expression for two subbands,

$$E_{\pm}^{(1)} = \epsilon_f - \Phi^2(\epsilon_d - \epsilon_f) + \Phi^2 \lambda_1^{(\pm)}, \quad (62)$$

where

$$\lambda_1^{(-)} = -\frac{\alpha^2 U}{\Phi^2} \left\{ 1 - \frac{D^2}{\alpha^2} \frac{\epsilon(\vec{k})}{U + \frac{1}{2}\epsilon(\vec{k})(\gamma+1)} \right\} - g\epsilon(\vec{k})U \left\{ \frac{1}{U + \frac{1}{2}\epsilon(\vec{k})(\gamma+1 - 2D^2/\alpha^2)} - \frac{1 - D^2/\Phi^2}{1 + \frac{1}{2}\epsilon(\vec{k})(\gamma+1)} + \frac{\alpha^2 D^2}{\Phi^2} \frac{\epsilon(\vec{k})(\gamma + g_1/g - \frac{1}{2})}{\Phi^2 [U + \frac{1}{2}\epsilon(\vec{k})(\gamma+1)]^2} \right\}, \quad (63a)$$

$$\lambda_1^{(+)} = \frac{g\epsilon(\vec{k})U}{U + \frac{1}{2}\epsilon(\vec{k})(\gamma+1 - 2D^2/\alpha^2)}, \quad (63b)$$

$$\gamma = \frac{U}{\epsilon_d - \epsilon_f}, \quad \frac{D^2}{\Phi^2} = \frac{1}{2} \left(1 - \frac{2}{\gamma} \right)^2, \quad \frac{D^2}{\alpha^2} = \frac{1}{8} (\gamma - 2)^2.$$

For $T=0$, the subband $E_-^{(1)}$ remains broadened while $E_+^{(1)}$ is reduced to the initial local energy. The two simplified solutions behave in much the same way. They can be obtained from Eqs. (45) and (48),

$$E_{\pm}^{(2)} = \epsilon_d + U + \Phi^2(\epsilon_d - \epsilon_f) + \Phi^2 \lambda_2^{(\pm)}, \quad (64)$$

where

$$\lambda_2^{(-)} = (2 - \gamma)^2 \frac{gU}{4} \frac{\epsilon(\vec{k})}{\epsilon(\vec{k})(1 + \gamma) - 2U} \times \left\{ 1 - \frac{\epsilon(\vec{k})}{2[U - \epsilon(\vec{k})(1 - \frac{1}{8}\gamma)]} \right\}, \quad (65a)$$

$$\lambda_2^{(+)} = \frac{U}{\gamma^2} \left\{ 4 - (\gamma - 2)^2 \frac{\epsilon(\vec{k})}{\epsilon(\vec{k})(1 + \gamma) - 2U} \right\} \frac{g\epsilon(\vec{k})}{2} \times \left\{ \frac{U}{U - \epsilon(\vec{k})\gamma(1 - \frac{1}{8}\gamma)} + \frac{4}{\gamma} \frac{\epsilon(\vec{k})(1 - \gamma)(\gamma - 2)^2 U}{[\epsilon(\vec{k})(1 + \gamma) - 2U]^2} \right\}. \quad (65b)$$

For $T \rightarrow 0$, $E_-^{(2)}$ is reduced to the ionic level, whereas $E_+^{(2)}$ keeps some dispersion.

Using the same simplifications as before, two further subbands can be obtained from Eqs. (47)–(50),

$$E_{\pm}^{(3)} = \lambda_0^{(\pm)} + \Phi^2 \lambda_1^{(\pm)}. \quad (66)$$

with

$$\lambda_0^{(\pm)} = \frac{1}{2} \{ \epsilon_d + \epsilon_f + U + \epsilon(\vec{k})(1 + \frac{3}{2}g_1) \pm [(\epsilon_d - \epsilon_f - U)^2 + \epsilon^2(\vec{k})(1 + 3g_1) + 4g\epsilon(\vec{k})(\epsilon_d - \epsilon_f - U)]^{1/2} \}, \quad (67a)$$

$$\lambda_1^{(\pm)} \left\{ \frac{1 + 2g}{(\lambda_0^{(\pm)} - \epsilon_d)^2} + \frac{1 - 2g + 3g_1}{(\lambda_0^{(\pm)} - \epsilon_f - U)^2} \right\} = \frac{2D^2}{\Phi^2} \left\{ \frac{1}{\lambda_0^{(\pm)} - \epsilon_f} + \frac{1}{\lambda_0^{(\pm)} - \epsilon_d - U} - \frac{1}{\lambda_0^{(\pm)} - \epsilon_d} - \frac{1}{\lambda_0^{(\pm)} - \epsilon_f - U} \right\} + (\epsilon_d - \epsilon_f - \alpha^2 U / \Phi^2) \times \left\{ \frac{1}{(\lambda_0^{(\pm)} - \epsilon_f)^2} - \frac{1}{(\lambda_0^{(\pm)} - \epsilon_f - U)^2} \right\} + g \left\{ -\frac{3 - 2D^2/\Phi^2}{\lambda_0^{(\pm)} - \epsilon_d} + \frac{2(\epsilon_d - \epsilon_f) + \alpha^2 U / \Phi^2}{(\lambda_0^{(\pm)} - \epsilon_d)^2} - \frac{(\epsilon_d - \epsilon_f)(3g_1/g - 2) + \alpha^2 U / \Phi^2}{(\lambda_0^{(\pm)} - \epsilon_f - U)^2} - \frac{3g_1/g - 4D^2/\Phi^2}{\lambda_0^{(\pm)} - \epsilon_f - U} + \frac{2(1 - 2D^2/\Phi^2)}{\lambda_0^{(\pm)} - \epsilon_f} + \frac{1 - 2D^2/\Phi^2}{\lambda_0^{(\pm)} - \epsilon_d - U} \right\}. \quad (67b)$$

In this case, both subbands survive in the limit $T=0$ K.

From Eqs. (51), (53) and (52), (54), respectively, we obtain two further subbands, both of which do not survive for $T \rightarrow 0$,

$$E^{(4)} = \epsilon_d + \Phi^2(\epsilon_d - \epsilon_f) + \Phi^2 \lambda_1, \quad (68a)$$

$$E^{(5)} = \epsilon_f + U - \Phi^2(\epsilon_d - \epsilon_f) + \Phi^2 \lambda_2 \quad (68b)$$

with

$$\lambda_1 = -3g \frac{\alpha^2 U}{\Phi^2} \frac{\epsilon(\vec{k})}{\epsilon(\vec{k}) - 2\alpha^2 U}, \quad (69a)$$

$$\lambda_2 = -3g_1 \frac{\alpha^2 U}{\Phi^2} \frac{\epsilon(\vec{k})}{\epsilon(\vec{k}) + 2\alpha^2 U}. \quad (69b)$$

The renormalization of the eight one-particle quantum transitions due to correlation and hybridization effects is shown in Figs. 2–4 for different temperatures. Figure 2 shows those bands that survive in the limit $T \rightarrow 0$, while the remaining figures show the complete set of eight bands and their variation if T is increased. With respect to the zero-temperature solutions, the individual bands (from bottom to top) correspond to the following transitions:

$$E_-^{(3)} : E_3 - E_6 = E_6 - E_{12} = -E_f + \alpha^2 U,$$

$$E_-^{(3)} : E_2 - E_6 = E_8 - E_{13} = -E_d + \alpha^2 U,$$

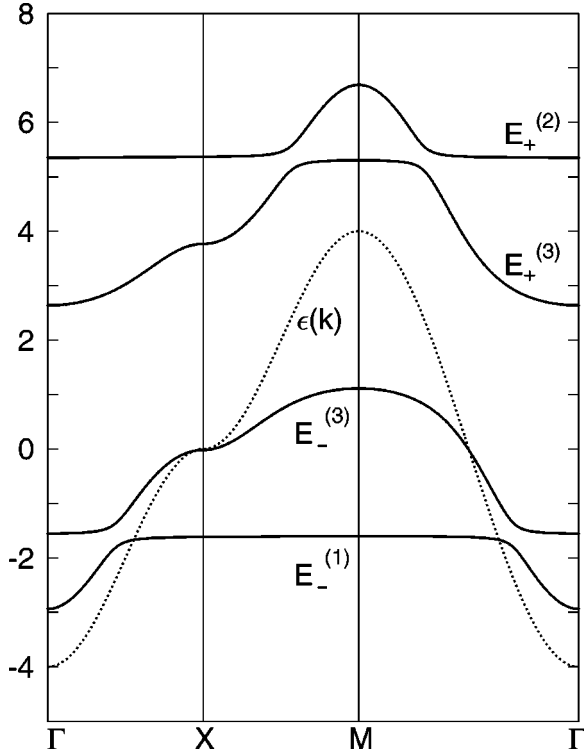


FIG. 2. Results for quasiparticle bands as they result from the solution of Eq. (39), $1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(E) = 0$, at zero temperature for the simple case of an underlying two-dimensional square lattice for the d electrons with tight-binding dispersion $\epsilon(\vec{k})$. The labeling of the bands follows the notation in the approximate expressions given by Eqs. (62), (64), and (66). Although the effect of hopping is taken into account only in a Hubbard I-like fashion, there are strong renormalization effects observable between X and Γ . Parameter values are $\epsilon_d = 0$, $\epsilon_f = -1.25$, $t = 1$, $V = 0.5$, and $U = 5$ (in units of eV).

$$E_+^{(3)}: E_3 - E_8 = E_6 - E_{12} = -E_f - U - \alpha^2 U,$$

$$E_+^{(2)}: E_2 - E_8 = E_6 - E_{13} = -E_d - U - \alpha^2 U.$$

For finite temperatures, the situation is more complicated because additional hybridization and repulsion effects appear due to four additional bands, which correspond to the following quantum transitions (with energies from bottom to top):

$$E_1 - E_2 = E_3 - E_9 = E_7 - E_{12} = -E_f \approx -\epsilon_f,$$

$$E_1 - E_3 = E_2 - E_9 = E_7 - E_{13} = -E_d \approx -\epsilon_d,$$

$$E_3 - E_7 = E_9 - E_{12} = E_{13} - E_{16} = -E_f - U \approx -\epsilon_f - U,$$

$$E_2 - E_7 = E_9 - E_{13} = E_{12} - E_{16} = -E_d - U \approx \epsilon_d - U.$$

In view of the nature of the states in Eqs. (2) and (7) and because the one-particle Green's functions in Eqs. (27)–(29) can only describe quantum transitions with change of particle number by $N=1$, the latter describe the transitions $|E_1\rangle \rightleftharpoons |E_2\rangle$ or $|E_3\rangle$, $|E_{2,3}\rangle \rightleftharpoons |E_9\rangle$, $|E_{14,15}\rangle \rightleftharpoons |E_{6,7,8}\rangle$, $|E_{10}\rangle \rightleftharpoons |E_{12,13}\rangle$, $|E_{14,15}\rangle \rightleftharpoons |E_{16}\rangle$, and $|E_{6,7,8}\rangle \rightleftharpoons |E_{12,13}\rangle$. Corresponding to 20 transitions altogether. For the symmetrical

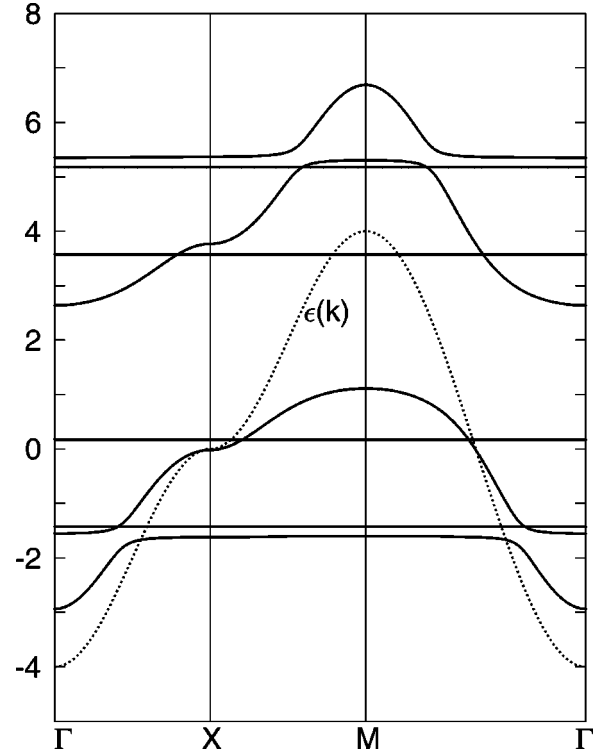


FIG. 3. Results for quasiparticle bands as they result from the solution of Eq. (39), $1 - \epsilon(\vec{k})G_{\sigma}^{dd(0)}(E) = 0$, for nonzero temperature ($T = 5$ K). Parameter values are the same as in Fig. 2.

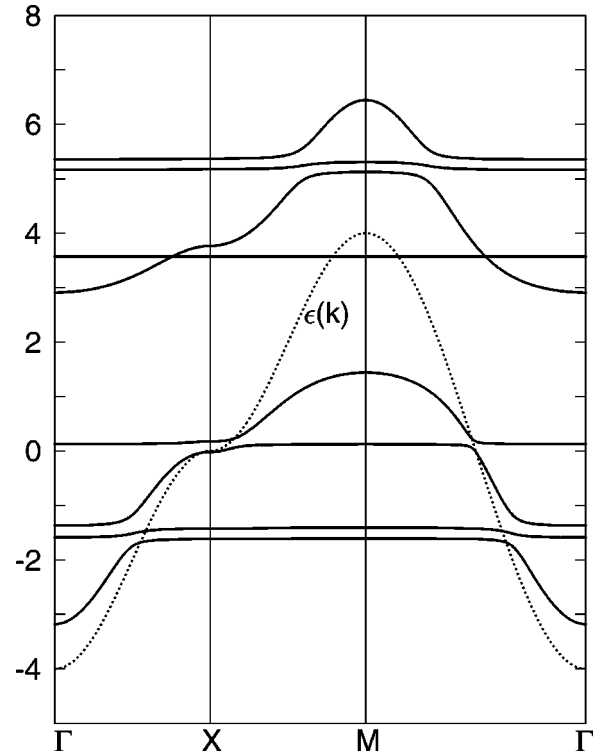


FIG. 4. Quasiparticle bands for $T = 1000$ K, otherwise the same parameter values as in Fig. 3.

case, only the eight different transitions in Eqs. (40) survive, from which four vanish for $T \rightarrow 0$.

VI. DISCUSSION

In this paper, we have exactly solved the ionic problem of correlated d and f electrons, including for simplicity only a local hybridization. The problem of delocalization due to electron hopping cannot be solved exactly. In order to see the influence of hopping on the ionic quantum states, we have used for simplicity the Hubbard I-like approximation (which means that important features such as Kondo- and heavy-fermion behavior, etc., cannot be described, although, depending on the parameters localized, and less localized ionic states are observed). The final result for the Hubbard I-like approximation is that from the eight subbands of the symmetrical model, only four subbands survive at low temperatures. The physical picture of these one-particle transitions will change in a complicated way when going beyond the Hubbard I approximation.

ACKNOWLEDGMENTS

The authors (V.A.M. and N.B.P.) would like to thank Professor Plakida for his interest and discussions. This work has been supported by a grant from the Steering Committee of the Heisenberg-Landau Program (V.A.M. and P.E.). V.A.M. thanks the theory group of the University of Duisburg for its hospitality.

APPENDIX: ATOMIC LIMIT RESULTS

Because of the quasideagonal character of the eigenvalue problem (3) in matrix form, the system of equations for the 16 atomic eigenfunctions ($n=1, \dots, 16$) and eigenvalues ($\lambda=1, \dots, 16$) breaks up into 10 subsystems of equations which can be easily solved. There are five linear equations of the form $H_{nn}^0 \Phi_n(E_\lambda) = E_\lambda \Phi_n(E_\lambda)$ for $n=1, 9, 10, 11$, and 16. For $n=1$, we have the solution $E_1=0$, $\Phi_1(E_1)=1$, $\Phi_1(E_{\lambda \neq 1})=0$. Then there are four equations of second order for the group of functions $n=2, \dots, 5, 12, \dots, 15$. Finally, there is one equation of third order for $n=6, \dots, 8$. It is clear that the functions of one group are equal to zero when the values of energies E_λ belong to other groups and that the orthonormalization conditions (4) are fulfilled for each group separately. We now give a brief account of the atomic solutions as the finite-temperature quasiparticle bands rely on them.

For $n, \lambda=2,3$, we have

$$E_{2,3} = \frac{1}{2} [\epsilon_d + \epsilon_f \mp \sqrt{(\epsilon_d - \epsilon_f)^2 + 4V^2}], \quad (\text{A1a})$$

$$\Phi_2(E_{2,3}) = \frac{1}{\sqrt{2}} \left[1 \mp \frac{\epsilon_d - \epsilon_f}{\sqrt{(\epsilon_d - \epsilon_f)^2 + 4V^2}} \right]^{1/2}, \quad (\text{A1b})$$

$$\Phi_3(E_{2,3}) = \mp \frac{\text{sgn } V}{\sqrt{2}} \left[1 \pm \frac{\epsilon_d - \epsilon_f}{\sqrt{(\epsilon_d - \epsilon_f)^2 + 4V^2}} \right]^{1/2} \quad (\text{A1c})$$

with $\Phi_{2,3}(E_\lambda)=0$ for $\lambda \neq (2,3)$. In Eqs. (A1a)–(A1c) and in all following equations, the first number index refers to the upper sign, the second index to the lower sign. For $n, \lambda=4,5$ we find

$$E_{4,5} = E_{2,3}, \quad \Phi_4(E_{4,5}) = \Phi_2(E_{2,3}), \quad \Phi_5(E_{4,5}) = \Phi_3(E_{2,3}). \quad (\text{A2})$$

For the triple group of functions, the corresponding eigenvalues, E_λ ($\lambda=6,7,8$), have to be determined by the cubic equation

$$\begin{aligned} x^3 - x[(\epsilon_d + \epsilon_f + U)^2 - (2\epsilon_d + U_d)(2\epsilon_f + U_f)] \\ + \frac{1}{3}(G - U)^2 + 4V^2 + \frac{2}{3}(G - U)[(\epsilon_d + \epsilon_f + U)^2 \\ - (2\epsilon_d + U_d)(2\epsilon_f + U_f) - \frac{1}{9}(G - U)^2 - 2V^2] = 0, \end{aligned} \quad (\text{A3})$$

where $E = \epsilon_d + \epsilon_f + \frac{1}{3}(2U + G) + x$ has been used; $U = \frac{1}{2}(U_d + U_f)$. For the special case $G = U$, there are simple solutions,

$$E_{6,8} = \epsilon_d + \epsilon_f + U \mp \sqrt{(\Delta/2)^2 + (2V)^2}, \quad (\text{A4a})$$

$$E_7 = \epsilon_d + \epsilon_f + U, \quad (\text{A4b})$$

$$\Phi_6(E_7) = -\Phi_8(E_7) = \frac{\sqrt{2}|V|}{\sqrt{(\Delta/2)^2 + (2V)^2}}, \quad (\text{A4c})$$

$$\Phi_7(E_7) = -\frac{\text{sgn } V}{\sqrt{2}} \frac{\Delta/2}{\sqrt{(\Delta/2)^2 + (2V)^2}}, \quad (\text{A4d})$$

$$\Phi_6(E_{6,8}) = \Phi_8(E_{6,8}) = \frac{1}{2} \left[1 \mp \frac{\Delta/2}{\sqrt{(\Delta/2)^2 + (2V)^2}} \right], \quad (\text{A4e})$$

$$\Phi_7(E_{6,8}) = \mp \frac{\sqrt{2}V}{\sqrt{(\Delta/2)^2 + (2V)^2}} \quad (\text{A4f})$$

with $\Delta = 2\epsilon_d + U_d - (2\epsilon_f + U_f)$. For the symmetrical case $\Delta = 0$ (for which we have computed the quasiparticle bands), we find

$$E_{6,8} = \epsilon_d + \epsilon_f + \frac{1}{2}(U + G) \mp \frac{1}{2}\sqrt{(U - G)^2 + (4V)^2}, \quad (\text{A5a})$$

$$E_7 = \epsilon_d + \epsilon_f + U, \quad (\text{A5b})$$

$$\Phi_6(E_7) = -\Phi_8(E_7) = \frac{1}{\sqrt{2}}, \quad \Phi_7(E_7) = 0, \quad (\text{A5c})$$

$$\Phi_6(E_{6,8}) = \Phi_8(E_{6,8}) = \frac{1}{2} \left[1 \mp \frac{U - G}{\sqrt{(U - G)^2 + (4V)^2}} \right]^{1/2}, \quad (\text{A5d})$$

$$\Phi_7(E_{6,8}) = \mp \frac{\text{sgn } V}{\sqrt{2}} \left[1 \pm \frac{U-G}{\sqrt{(U-G)^2 + (4V)^2}} \right]^{1/2}. \quad (\text{A5e})$$

The three linear equations for $n=9, \dots, 11$ yield

$$E_\lambda = \epsilon_d + \epsilon_f + G, \quad \lambda = 9, \dots, 11, \quad \Phi_n(E_\lambda) = \delta_{n,\lambda}. \quad (\text{A6})$$

For $n=12, \dots, 15$ follows that

$$E_{12,13} = \frac{1}{2} [3(\epsilon_d + \epsilon_f) + 2U + 4G \mp \sqrt{(\Delta_1/2)^2 + (2V)^2}], \quad (\text{A7a})$$

$$\Phi_{12}(E_{12,13}) = \frac{1}{\sqrt{2}} \left[1 \mp \frac{\Delta_1}{\sqrt{(\Delta_1)^2 + (4V)^2}} \right]^{1/2}, \quad (\text{A7b})$$

$$\Phi_{13}(E_{12,13}) = \pm \frac{\text{sgn } V}{\sqrt{2}} \left[1 \pm \frac{\Delta_1}{\sqrt{(\Delta_1)^2 + (4V)^2}} \right]^{1/2}, \quad (\text{A7c})$$

$$\Phi_{12,13}(E_\lambda) = 0 \quad \text{for } \lambda \neq 12, 13, \quad (\text{A7d})$$

$$E_{14,15} = E_{12,13}, \quad \Phi_{14}(E_{14,15}) = \Phi_{12}(E_{12,13}), \quad (\text{A7e})$$

$$\Phi_{15}(E_{14,15}) = \Phi_{13}(E_{12,13}), \quad \Phi_{14,15}(E_\lambda) = 0, \quad \lambda \neq (14, 15) \quad (\text{A7f})$$

with $\Delta_1 = \Delta + U_d - U_f$. Finally, for $\Phi_{16}(E_\lambda)$ we obtain

$$E_{16} = 2(\epsilon_d + \epsilon_f) + 2U + 4G, \quad \Phi_{16}(E_\lambda) = \delta_{\lambda,16}. \quad (\text{A8})$$

The foregoing solutions correspond to a generalization of previous works⁵⁻¹² to the case of two correlated electron systems including a Falicov-Kimball term. They coincide with previous works for the case $U_d = G = 0$.

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