Equivalence of variational and slave-boson mean-field treatments of the periodic Anderson model

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We investigate Gutzwiller-correlated wave functions as variational ground states for the periodic Anderson model. We extend a recently developed technique for the Hubbard model to the case of two hybridized bands with degeneracy N. We calculate expectation values in the following limits: dilute system (single-impurity case), large degeneracy N, and large dimension d. The mean-field results using the slave-boson approach of Coleman and of Kotliar and Ruckenstein are reproduced in the large-N and large-d limit, respectively. These techniques, therefore, obey variational principles at $T=0$ in the respective limits and their applicability for $T>0$ is naturally limited to the Fermi-liquid regime. Evaluations of Gutzwiller-correlated wave functions using the "Gutzwiller approximation" are seen to become exact in the limit of large dimensions. A systematic expansion in $1/d$ can be performed for $N=2$. In general, corrections are small, of order $1/(dN)$.

I. INTRODUCTION

Electrons on a lattice with a strong, short-ranged interaction present a complicated many-body problem. It is difficult to make reliable statements about the physical contents even for simplifying model Hamiltonians like the Hubbard[1,2] or the periodic Anderson model.[3-5] Among the few analytical tools to study low-temperature properties of strongly correlated electron systems are slave-boson techniques along the lines of Coleman, Read and Newns,[6-9] and Kotliar and Ruckenstein.[10-16]. The slave-boson techniques have gained renewed interest for the description of high-T_c materials.[17-19]

The two approaches, however, do not give the same results at the mean-field level. Besides this ambiguity, it is not guaranteed within the approach that the dynamical constraints are fulfilled at the mean-field level. For these reasons a better understanding of the slave-boson mean-field approaches is clearly desirable. In this paper we show for the periodic Anderson model that both mean-field results can be obtained from the same class of Gutzwiller-correlated wave functions in the respective limits of large degeneracy N and large dimension d.

The expansion parameter $1/N$ was readily identified for the slave-boson approach to the periodic Anderson model used by Coleman[6] and by Read and Newns[7] since it represents the generalization of the single-impurity technique to the lattice case. To lowest order there are no differences between the results for the single-impurity and the lattice case.[6-9] Lattice effects show up in order $1/N$ for the specific heat, magnetic susceptibility, and correlation functions, while the Wilson ratios in the lattice and single-impurity case are the same to order $1/N$.[8,9] A $1/N$ expansion even without the use of slave bosons is also possible.[20]

Recently, Metzner and Vollhardt introduced the limit of large dimensions d for itinerant lattice fermions,[21] which allowed for the exact solution of the Falicov-Kimball model[22] on a d-dimensional hypercubic lattice[23] and a Bethe lattice with large coordination number.[24] Self-consistent calculations are now numerically feasible in this limit.[25,26] Furthermore, the expansion parameter $1/d$ is especially useful for the evaluation of Gutzwiller-correlated wave functions. Variational wave functions allow for an approximative description of the ground-state properties of a physical system. However, one frequently had to use semiclassical approximations ("Gutzwiller approximation") for their evaluation.[27] For the single-band Hubbard model without degeneracy it is seen that the Gutzwiller approximation becomes exact for $d=\infty$.[21,28] Furthermore, all Kotliar-Ruckenstein slave-boson results for the Hubbard model without orbital degeneracy are completely reproduced from the variational approach in this limit.[28] A compact formalism for a $1/d$ expansion has been developed in Ref. 28 (hereafter referred to as I).

In this paper we extend the formalism in I to the case of a two-band model with orbital degeneracy. In Sec. II we present the periodic Anderson model and introduce the class of Gutzwiller-correlated wave functions. In Sec. III we sketch their evaluation where details of the calculations are given in the Appendixes. In Sec. IV we discuss the exactly solvable cases: the dilute system (single-impurity problem), the large-N limit, and the large-d limit. Furthermore, we discuss the influence of $1/d$ and $1/N$ corrections. We summarize our results in Sec. V.

II. HAMILTON OPERATOR AND VARIATIONAL WAVE FUNCTIONS

In this section we introduce the periodic Anderson Hamiltonian, which is thought to include the essential physics of dense rare-earth compounds (for an experimental review, see Ref. 29). Then we specify the class of Gutzwiller-correlated wave functions, which were frequently used to study ground-state properties of the model.

The derivation of the model and the simplifications made are discussed, e.g., in Refs. 3–5. It describes N degenerate bands of conduction electrons with dispersion $\varepsilon(\mathbf{k})$ on a lattice with L lattice sites. Furthermore, there are f orbitals at L^f lattice sites with a bare energy level E_0^f. The f electrons are correlated by a Hubbard interaction U and hybridize with the conduction electrons via a matrix element $V_{\mathbf{k}}$. The same degeneracy is chosen for the c and f electrons so that the model has a $1/N$ expansion. In second quantization the model Hamiltonian reads

$$\hat{H}=\sum_{\mathbf{k},\alpha}\varepsilon(\mathbf{k})\hat{c}^{\dagger}_{\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\alpha}+E_0^f\sum_{\mathbf{i},\alpha}\hat{n}^f_{\mathbf{i}\alpha}+\frac{U}{2}\sum_{\mathbf{i}}\sum_{\substack{\alpha,\beta\\(\alpha\neq\beta)}}\hat{n}^f_{\mathbf{i}\alpha}\hat{n}^f_{\mathbf{i}\beta}$$
$$-\frac{1}{\sqrt{NL}}\sum_{\mathbf{k},\mathbf{i},\alpha}V_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{i}}(\hat{c}^{\dagger}_{\mathbf{k}\alpha}\hat{f}_{\mathbf{i}\alpha}+\text{H.c.})\ . \tag{1}$$

Here, $\hat{n}^f_{\mathbf{i}\alpha}=\hat{f}^{\dagger}_{\mathbf{i}\alpha}\hat{f}_{\mathbf{i}\alpha}$, and α,β are combined orbital and spin indices running from 1 to N. In the case $L^f=L$ one obtains the periodic Anderson model, while in the case $L^f=1$ the single-impurity model with an impurity at the origin is recovered. Usually the limit of strong correlations ($U\rightarrow\infty$) is considered, which implies

$$\sum_{\alpha}\langle\hat{n}^f_{\mathbf{i}\alpha}\rangle\leq 1\quad\text{for } U=\infty \tag{2}$$

at *each* individual site $\mathbf{i}$. The treatment of the constraint (2) is a crucial point in any analytical approach to the periodic Anderson model in the strongly correlated regime.[6–9,30–32]

Most likely the simplest way to formulate correlated wave functions for a model Hamiltonian with a Hubbard-type interaction is due to Gutzwiller.[2] In the case of the periodic Anderson model his ideas were generalized by Varma, Weber, and Randall,[33] Brandow,[34] Fazekas,[35,36] Rice and Ueda,[37] and Vulović and Abrahams.[38] For arbitrary degeneracy N one considers the class of wave functions

$$|\Psi_g\rangle=g^{\hat{D}^f}|\Psi_0\rangle=\prod_{\mathbf{i}}\prod_{\alpha<\beta}[1+(g-1)\hat{n}^f_{\mathbf{i}\alpha}\hat{n}^f_{\mathbf{i}\beta}]|\Psi_0\rangle\ , \tag{3}$$

where $\hat{D}^f=\sum_{\mathbf{i},\alpha<\beta}\hat{n}^f_{\mathbf{i}\alpha}\hat{n}^f_{\mathbf{i}\beta}$ is given by the interaction term between the f electrons in Eq. (1), and $|\Psi_0\rangle$ is an arbitrary one-particle product wave function.[39] $0\leq g\leq 1$ is a variational parameter and the correlation operator in Eq. (3) reduces configurations with multiply occupied f-electron levels in $|\Psi_0\rangle$. In the strongly correlated regime ($U=\infty$) one has $g=0$ so that only empty or singly occupied f levels at each lattice site are allowed.

$|\Psi_0\rangle$ is chosen as a lattice generalization of the Varma-Yafet state[40] (or lowest-order Gunnarsson-Schönhammer state[41]), which was designed for the single-impurity case. Starting from a filled Fermi sea of conduction electrons, a one-particle operator simulates the hybridization of conduction electrons and f electrons. Explicitly we write

$$|\Psi_0\rangle=\exp\left[\frac{1}{\sqrt{NL}}\sum_{\mathbf{i},\mathbf{k},\alpha}e^{i\mathbf{k}\cdot\mathbf{i}}a_{\mathbf{k}\alpha}\hat{f}^{\dagger}_{\mathbf{i}\alpha}\hat{c}_{\mathbf{k}\alpha}\right]|c\text{FS}\rangle\ , \tag{4}$$

where $|c\text{FS}\rangle$ is a state where the f levels are empty and all electrons fill the Fermi sea up to the Fermi wave vector k_F. The parameters $a_{\mathbf{k}\alpha}$ describe the degree of hybridization between the conduction and f electrons and have to be determined variationally.

III. EVALUATION OF THE WAVE FUNCTION

The task is to calculate expectation values with the wave functions defined in Eq. (3), $\langle\hat{O}\rangle=\langle\Psi_g|\hat{O}|\Psi_g\rangle/\langle\Psi_g|\Psi_g\rangle$. The general formalism to deal with this problem in a controlled expansion in $1/d$ (for $N=2$) has been outlined in I. Here we present its generalization to the case of arbitrary degeneracy. We sketch the important steps and discuss some technical points in Appendix A.

As in I, we rewrite $|\Psi_g\rangle$ in Eq. (3) as

$$|\Psi_g\rangle=g^{\hat{D}^f}|\Psi_0\rangle=g^{\hat{K}^f}|\Phi_0\rangle \tag{5a}$$

with

$$\hat{K}^f=\sum_{\mathbf{i}}\hat{K}^f_{\mathbf{i}}=\sum_{\mathbf{i}}\sum_{\alpha<\beta}(\hat{n}^f_{\mathbf{i}\alpha}\hat{n}^f_{\mathbf{i}\beta}-\mu_{\mathbf{i}\alpha}\hat{n}^f_{\mathbf{i}\alpha}-\mu_{\mathbf{i}\beta}\hat{n}^f_{\mathbf{i}\beta}+\eta_{\mathbf{i}})\ . \tag{5b}$$

The wave function $|\Phi_0\rangle$ is a one-particle product wave function like $|\Psi_0\rangle$ since the operator $\hat{K}^f-\hat{D}^f$ is a one-particle operator. We choose $|\Phi_0\rangle$ to be normalized to unity.

According to I, we have to subtract all trivial Hartree contributions in the expansion of the correlation operator. We denote $\langle\cdots\rangle_0$ as the expectation value with respect to $|\Phi_0\rangle$, and choose $\mu_{\mathbf{i}\nu}$ ($\nu=1,2,\ldots,N$) and $\eta_{\mathbf{i}}$ so that

$$g^{2\hat{K}^f_{\mathbf{i}}}=1+\sum_{r=2}^{N}\frac{1}{r!}{\sum_{\alpha_1,\ldots,\alpha_r=1}^{N}}'x_{i,\alpha_1\cdots\alpha_r}\times\prod_{p=1}^{r}(\hat{n}_{\mathbf{i},\alpha_p}-\langle\hat{n}_{\mathbf{i},\alpha_p}\rangle_0)$$
$$\equiv 1+\hat{\Gamma}_{\mathbf{i}} \tag{6}$$

holds. Here, the $x_{\mathbf{i},\alpha_1\cdots\alpha_r}$ are symmetric under interchange of two indices, and the prime on the sum implies the omission of terms where two of them are equal, i.e., $\alpha_1\neq\alpha_2\neq\cdots\neq\alpha_r$. The number of parameters $\{x_{i,\alpha}\}$ is 2^N-N-1 so that we have 2^N unknown quantities altogether. In fact, Eq. (6) is a set of 2^N equations since each orbital ν can be either occupied or empty. All parameters are therefore uniquely obtained from (6). For $N=2$ there is only one $x_{\mathbf{i}}=x_{\mathbf{i},1,2}=x_{\mathbf{i},2,1}$. The solution for this case is given in Appendix B. Of course, it is impossible to give an explicit solution of this set of equations for $N>2$ and arbitrary g, $\langle\hat{n}^f_{\mathbf{i}\nu}\rangle_0$.

As we will see later, we do not need the information provided by the $\{x_{\mathbf{i},\alpha}\}$ in the limit of large dimension and/or large degeneracy but only the quantities $\mu_{\mathbf{i}\nu}$ and $\eta_{\mathbf{i}}$. To determine these quantities, we take the expectation value of both sides of Eq. (6) with respect to $|\Phi_0\rangle$. This gives

$$\langle \Phi_0 | g^{2\hat{K}_i^f} | \Phi_0 \rangle = 1 \ . \tag{7a}$$

Furthermore, we obtain N equations by multiplying both sides of Eq. (6) with $\hat{n}_{i\nu}^f$ and taking again the expectation value with respect to $|\Phi_0\rangle$,

$$\langle \Phi_0 | \hat{n}_{i\nu}^f g^{2\hat{K}_i^f} | \Phi_0 \rangle = \langle \hat{n}_{i\nu}^f \rangle_0 \ . \tag{7b}$$

Equations (7) form a set of $N+1$ equations to determine $\mu_{i\nu}$ and η_i.

However, even this set of $N+1$ algebraic equations is still too complicated to solve for $N>2$ and arbitrary g, $\langle \hat{n}_{i\nu}^f \rangle_0$. For the strongly correlated case we have $g=0$, so that a closed solution is possible since each lattice point can be only singly occupied or empty. In this case one easily obtains

$$g^{N(N-1)\eta_i}\big|_{g=0} = (1-\langle \hat{n}_i^f \rangle_0) \Big/ \left[\prod_{\alpha=1}^{N} (1-\langle \hat{n}_{i\alpha}^f \rangle_0) \right] \tag{8a}$$

and

$$g^{N(N-1)\eta_i} g^{-2(N-1)\mu_{i\nu}}\big|_{g=0} = (1-\langle \hat{n}_{i\nu}^f \rangle_0) \Big/ \left[\prod_{\alpha=1}^{N} (1-\langle \hat{n}_{i\alpha}^f \rangle_0) \right] , \tag{8b}$$

where $\langle \hat{n}_i^f \rangle_0 = \sum_{\alpha=1}^{N} \langle \hat{n}_{i\alpha}^f \rangle_0$. Here, we have to assure that $\langle \hat{n}_i^f \rangle_0 \le 1$, which is the generalization of the usual "less than half-filling" condition to the case $N>2$ and is necessary to fulfill the constraint, Eq. (2).

We proceed as in I. We have to calculate the one-particle density matrix for the c electrons $P_\nu^c(\mathbf{i},\mathbf{j}) = \langle \hat{c}_{i\nu}^\dagger \hat{c}_{j\nu} \rangle$, the f electrons $P_\nu^f(\mathbf{i},\mathbf{j}) = \langle \hat{f}_{i\nu}^\dagger \hat{f}_{j\nu} \rangle$, the mixing matrix element $P_\nu^x(\mathbf{i},\mathbf{j}) = \langle \hat{c}_{i\nu}^\dagger \hat{f}_{j\nu} \rangle$, and the mean f-electron double occupancy $\bar{d}_{i\lambda\nu}^f = \langle \hat{n}_{i\lambda}^f \hat{n}_{i\nu}^f \rangle$. These quantities are evaluated through an expansion in terms of $\hat{\Gamma}_i$ [see Eq. (6)]. One can apply Wick's theorem to calculate the different orders in the expansion because $|\Phi_0\rangle$ is a one-particle product wave function. The corresponding contributions are represented graphically and it is possible to show that the linked cluster theorem applies (see I and Appendix A for further details). During this procedure one has to guarantee that there will be no Hartree contributions at the external vertices. The corresponding algebraic manipulations lead to the introduction of renormalization factors $q_{i\nu}$, which are defined in terms of the $\mu_{i\nu}$, η_i as

$$\sqrt{q_{i\nu}} = \langle \Phi_0 | g^{\hat{Q}_{i\nu}} | \Phi_0 \rangle \tag{9a}$$

$$\hat{Q}_{i\nu} = 2 \sum_{\alpha<\beta}{}' (\hat{n}_{i\alpha}^f \hat{n}_{i\beta}^f - \mu_{i\alpha}\hat{n}_{i\alpha}^f - \mu_{i\beta}\hat{n}_{i\beta}^f + \eta_i) + \sum_{\alpha}{}' [(1-2\mu_{i\alpha})\hat{n}_{i\alpha}^f - \mu_{i\nu} + 2\eta_i] \ . \tag{9b}$$

The prime on the sums implies the omission of terms with $\alpha=\nu$ or $\beta=\nu$. The one-particle density matrices and the mean double occupancy are then expressed in terms of the noninteracting quantities, $P_\nu^{f,0}(\mathbf{i},\mathbf{j})$, etc., renormalization factors like $q_{i\nu}$, and a "self-energy" $S_\nu^f(\mathbf{i},\mathbf{j})$ which is defined in terms of connected graphs.

The essential point of these considerations is the following: the self-energy *vanishes* in the limits of large dimension and/or energy large degeneracy. Explicitly,

$$S_\nu^f(\mathbf{i},\mathbf{j}) \equiv \begin{cases} 0 \ \text{for} \ d=\infty \\ 0 \ \text{for} \ N=\infty \ . \end{cases} \tag{10}$$

To see this we consider the graph expression for $S_\nu^f(\mathbf{i},\mathbf{j})$. There are on Hartree bubbles in the graph expansion of $S_\nu^f(\mathbf{i},\mathbf{j})$; instead the lines are given by

$$\tilde{P}_\nu^{f,0}(\mathbf{i},\mathbf{j}) = P_\nu^{f,0}(\mathbf{i},\mathbf{j}) - \delta_{\mathbf{i},\mathbf{j}} P_\nu^{f,0}(\mathbf{i},\mathbf{i}) \ . \tag{11}$$

Especially, $\tilde{P}_\nu^{f,0}(\mathbf{i},\mathbf{i})=0$, which means that two lattice points in a graph never coincide. For large dimensions on a hypercubic lattice we have[21,26,42]

$$P_\nu^{f,0}(\mathbf{i},\mathbf{j}) \simeq O((\sqrt{1/d}\,)^r) \ , \tag{12}$$

where $r=|\mathbf{i}-\mathbf{j}|=\sum_{l=1}^{d}|i_l-j_l|$ is the distance of $\mathbf{i}$ and $\mathbf{j}$ measured by the number of nearest-neighbor steps from $\mathbf{i}$ to $\mathbf{j}$. There are always two points in a graph that are connected by at least three separate paths. Two typical lowest-order graphs for $S_\nu^f(\mathbf{i},\mathbf{j})$ are shown in Figs. 1(a) and 1(b). As an example, consider the graph in Fig. 1(a). Due to the special choice of lines, this graph is of order $1/d$ since there are four lines joining $\mathbf{i}$ and $\mathbf{g}$. We have $\mathbf{i}\neq\mathbf{g}$ so that the dominant contribution comes from the $2d$ nearest neighbors of $\mathbf{g}$. Therefore, it is of order $d(1/d)^2 = 1/d$. Furthermore, each line is proportional to the density of electrons per line, i.e., proportional to $1/N$. This means, e.g., that the graph in Fig. 1(b), which has a free summation over an orbital index, is proportional to

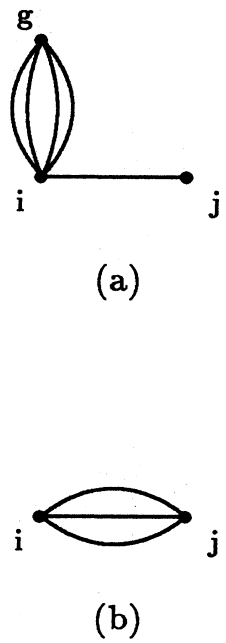

FIG. 1. Two diagrams for the self-energy; both are of order $1/(dN)$.

$N(1/N)^2$ and is therefore of order $1/N$. These arguments apply for all self-energy graphs so that $S_\nu^f(\mathbf{i},\mathbf{j})$ vanishes in the limits $d=\infty$ and $N=\infty$ separately, i.e., $S_\nu^f(\mathbf{i},\mathbf{j})\simeq O(1/(dN))$. Note that there are no restrictions on $|\Phi_0\rangle$ so that this result is valid for completely general one-particle product wave functions $|\Phi_0\rangle$.

Of course, there is another exactly solvable limit: the limit of a single impurity since $S_\nu^f(\mathbf{i},\mathbf{j})$ is zero by definition. This limit may be viewed as the dilute limit of the model where $S_\nu^f(\mathbf{i},\mathbf{j})$ vanishes with some power of the f-atom concentration.

IV. RESULTS FOR THE EXACTLY TREATABLE LIMITS

As derived in the preceding section, the Gutzwiller-correlated wave functions can be evaluated exactly in the following cases: (i) the dilute limit where only one impurity is considered; (ii) the limit of large degeneracy ($N=\infty$); and (iii) the limit of large dimension ($d=\infty$). In all three cases the self-energy vanishes and we get the following expressions for the one-particle density matrices for the c and f electrons, the mixing between c and f electrons, and for the mean f double occupancy (see I and Appendix A):

$$P_\nu^c(\mathbf{i},\mathbf{j})=P_\nu^{c,0}(\mathbf{i},\mathbf{j}) , \tag{13a}$$

$$P_\nu^f(\mathbf{i},\mathbf{j})=\sqrt{q_{\mathbf{j}\nu}}\sqrt{q_{\mathbf{j}\nu}}P_\nu^{f,0}(\mathbf{i},\mathbf{j})+\delta_{\mathbf{ij}}(1-q_{\mathbf{i}\nu})\langle\hat{n}_{\mathbf{i}\nu}^f\rangle_0 , \tag{13b}$$

$$P_\nu^x(\mathbf{i},\mathbf{j})=\sqrt{q_{\mathbf{j}\nu}}P_\nu^{x,0}(\mathbf{i},\mathbf{j}) , \tag{13c}$$

$$g^2=\frac{\bar{d}_{\mathbf{i}\lambda\nu}^f g^{2\mu_{\mathbf{i}\lambda}+2\mu_{\mathbf{i}\nu}-2\eta_{\mathbf{i}}}}{\bar{d}_{\mathbf{i}\lambda\nu}^{f,0}z_{\mathbf{i}\lambda\nu}} \quad (\lambda\neq\nu) , \tag{13d}$$

where $q_{\mathbf{i}\nu}$ is defined in Eq. (9), $\bar{d}_{\mathbf{i}\lambda\nu}^{f,0}=\langle\hat{n}_{\mathbf{i}\lambda}^f\rangle_0\langle\hat{n}_{\mathbf{i}\nu}^f\rangle_0$, and we defined

$$z_{\mathbf{i}\lambda\nu}=\langle\Phi_0|g^{\hat{Z}_{\mathbf{i}\lambda\nu}}|\Phi_0\rangle , \tag{14a}$$

$$\hat{Z}_{\mathbf{i}\lambda\nu}=2\sum_{\alpha<\beta}{}''(\hat{n}_{\mathbf{i}\alpha}^f\hat{n}_{\mathbf{i}\beta}^f-\mu_{\mathbf{i}\alpha}\hat{n}_{\mathbf{i}\alpha}^f-\mu_{\mathbf{i}\beta}\hat{n}_{\mathbf{i}\beta}^f+\eta_{\mathbf{i}}) +2\sum_\alpha{}''[(2-2\mu_{\mathbf{i}\alpha})\hat{n}_{\mathbf{i}\alpha}^f-\mu_{\mathbf{i}\nu}-\mu_{\mathbf{i}\lambda}+2\eta_{\mathbf{i}}] . \tag{14b}$$

The double prime on the sum in Eq. (14b) implies the exclusion of $\alpha=\lambda,\nu$ and $\beta=\lambda,\nu$. For $N=2$ we have $z_{\mathbf{i}\lambda\nu}\equiv 1$.

We will now discuss the three different cases separately.

A. Single impurity

First we want to make sure that the single-impurity results are reproduced correctly. We limit ourselves to the limit of strong correlations ($U=\infty$) and therefore set $g=0$ in the variational wave function $|\Psi_g\rangle$, Eq. (3). A very successful variation approach to this problem has been developed by Gunnarsson and Schönhammer,[41] who proved that $|\Psi_{g=0}\rangle$ becomes the exact ground-state wave function for the single-impurity case in the limit of large degeneracy, $N=\infty$. A detailed review on $1/N$-expansion techniques for the single-impurity model has been given by Bickers.[32]

For large U we have $\bar{d}_{\mathbf{i}\lambda\nu}^f=0$, i.e., the f orbitals are either empty or singly occupied. Denoting $n^f=\langle\hat{n}^f\rangle=N\langle\hat{n}_\nu^f\rangle$, we obtain from Eqs. (8) and (9)

$$q\equiv q_\nu=\frac{1-n^f}{1-n^f/N} . \tag{15}$$

Note that $\langle n_\nu^f\rangle=\langle\hat{n}_\nu^f\rangle_0$ holds. We can write Eq. (4) as

$$|\Phi_0\rangle=\prod_\alpha\left[1+\sqrt{1/(NL)}\sum_{\mathbf{k}}\tilde{\alpha}_{\mathbf{k}}\hat{f}_\alpha^\dagger\hat{c}_{\mathbf{k}\alpha}\right]|c\mathrm{FS}\rangle . \tag{16}$$

Using Eq. (13) we obtain

$$\langle\hat{H}\rangle=E_{\mathrm{FS}}+\Delta E ,$$

$$\Delta E\left[1+\frac{1}{NL}\sum_{\mathbf{k}}{}'\tilde{\alpha}_{\mathbf{k}}^2\right]=\frac{1}{L}\sum_{\mathbf{k}}{}'\{[E_0^f-\varepsilon(\mathbf{k})]\tilde{\alpha}_{\mathbf{k}}^2-2\sqrt{q}\,V_{\mathbf{k}}\tilde{\alpha}_{\mathbf{k}}\}, \tag{17a}$$

$$n^f=\frac{(1/L)\sum_{\mathbf{k}}{}'\tilde{\alpha}_{\mathbf{k}}^2}{1+(1/L)\sum_{\mathbf{k}}{}'\tilde{\alpha}_{\mathbf{k}}^2/N} . \tag{17b}$$

Here $E_{\mathrm{FS}}=\sum_{\mathbf{k}}{}'\varepsilon(\mathbf{k})$ is the energy of the unperturbed Fermi sea, and the prime on the $\mathbf{k}$ sum implies summing up to the Fermi energy.

The approach used here allows for a simple reinterpretation of the variational problem. $\langle\hat{H}\rangle$ is the variational ground-state energy for a system of c and *noninteracting* f electrons described by an effective single-impurity Hamiltonian

$$\hat{H}_{\mathrm{SI}}^{\mathrm{eff}}=\sum_{\mathbf{k},\alpha}\varepsilon(\mathbf{k})\hat{c}_{\mathbf{k}\alpha}^\dagger\hat{c}_{\mathbf{k}\alpha}+E^f\sum_\alpha\hat{f}_\alpha^\dagger\hat{f}_\alpha -\frac{1}{\sqrt{NL}}\sum_{\mathbf{k},\alpha}\tilde{V}_{\mathbf{k}}(\hat{c}_{\mathbf{k}\alpha}^\dagger\hat{f}_\alpha+\mathrm{H.c.})-\lambda n^f , \tag{18}$$

where the Lagrange parameter λ is implemented to guarantee Eq. (17b). The correlation between the f electrons shows up in the dependence of the effective hybridization, $\tilde{V}_{\mathbf{k}}=\sqrt{q}\,V_{\mathbf{k}}$, and the effective f level, $E^f=E_0^f+\lambda$, on the f-electron density n^f.

We will now minimize Eq. (17a). We are interested in the Kondo limit. In this limit, $E_0^f<0$ lies far below the Fermi energy ε_F of the conduction electrons, which are assumed to form a featureless band of width $W=2D$. Furthermore, $V_{\mathbf{k}}\equiv V$ is assumed to be small compared to W and E_0^f. Defining $\Delta\varepsilon$ as the binding energy compared to the case $V=0$ [$\Delta\varepsilon=\Delta E+(\varepsilon_F-E_0^f)$], we find (see Appendix D)

$$\Delta\varepsilon\equiv -T_K=-(D+\varepsilon_F)\exp\left[\frac{W}{V^2}(\varepsilon_F+|E_0^f|)\right] . \tag{19a}$$

The deviation from an integer value for n^f is

$$\delta \equiv 1-n^f = \frac{W}{V^2} T_K \tag{19b}$$

and the position of the effective f level is slightly above the Fermi energy at

$$E^f = \varepsilon_F + T_K \ . \tag{19c}$$

Here, T_K is the Kondo temperature. This expression provides a variational upper bound for the binding energy in the single-impurity model (at temperature $T=0$) and becomes exact in the limit of large degeneracy ($N=\infty$).[41] The results (19) show that the q factor in Eq. (15) for the effective Hamiltonian (18) gives the correct results for the single-impurity case. This was questioned earlier.[5]

One may extend the above analysis of $\hat{H}_{\rm SI}^{\rm eff}$ to finite temperatures as described in Appendix C (see I for the case of the Hubbard model). A variational "spectrum" may be derived by calculating expectation values of $\hat{H}_{\rm SI}^{\rm eff}$ with single-particle wave functions like $|\Phi_0\rangle$ in Eq. (16), where the Fermi sea of c electrons is replaced by its excited states (see Appendix C for a more-detailed discussion of this procedure). The corresponding "partition function" and "free energy" that are derived from this variational approach are completely equivalent to the saddle-point solution of the single-impurity model given by Schönhammer,[16] who used the slave-boson functional-integral approach by Kotliar and Ruckenstein.[10] This saddle-point solution, therefore, provides exact upper bounds for temperature $T=0$; its applicability is, however, limited to "low" temperatures (Fermi-liquid regime) due to its variational origin.

Finally, we would like to compare our results with the slave-boson saddle-point treatment of the single-impurity model by Coleman[6] and Read and Newns.[7] This treatment of the model becomes exact for low temperatures to lowest order in $1/N$.[7,32] It gives the same effective Hamiltonian as in Eq. (18) with $q=1-n^f$ and its free energy is equivalent to the variational expression in the case of large degeneracy. Hence, the variational approach also covers the mean-field results of the slave-boson approach by Coleman and Read and Newns.

B. Large degeneracy

We now consider the periodic Anderson model, i.e., $L^f=L$. We want to compare our results to those of the slave-boson approach by Coleman,[6] Read and Newns,[7] Auerbach and Levin,[8] and Millis and Lee,[9] who studied the strongly correlated case $U=\infty$ ($g=0$).

It is well known that the limit of large degeneracy $N=\infty$ suppresses lattice effects and the physics of the single-impurity problem is widely recovered.[6-9] In fact, the same happens in our variational approach since the self-energy, which includes lattice effects in the correlator $g^{\hat{K}^f}$, vanishes identically for $N=\infty$. Assuming translational invariance, we obtain the following expression for the variational ground-state energy:

$$\langle \hat{H} \rangle = \sum_{\mathbf{k},\alpha} \left[\varepsilon(\mathbf{k}) \langle \hat{n}^c_{\mathbf{k}\alpha} \rangle_0 + E^f \langle \hat{n}^f_{\mathbf{k}\alpha} \rangle_0 - \frac{2}{\sqrt{N}} \tilde{V}_{\mathbf{k}} \langle \hat{n}^x_{\mathbf{k}\alpha} \rangle_0 \right] - \lambda n^f L \ , \tag{20}$$

where $q=1-n^f$, $n^f=Nn^f_\nu$, and $n^f_\nu=(1/L)\sum_{\mathbf{k}} \langle \hat{n}^f_{\mathbf{k}\nu} \rangle_0$. As in the single-impurity case, we have included the Lagrange multiplier λ to establish the connection between n^f and $\tilde{a}_{\mathbf{k}}$. The momentum distributions $\langle \hat{n}^f_{\mathbf{k}\nu} \rangle_0$, $\langle \hat{n}^c_{\mathbf{k}\nu} \rangle_0$, and $\langle \hat{n}^x_{\mathbf{k}\nu} \rangle_0$ are the Fourier transforms of the noninteracting one-particle density matrices, see Eqs. (13). They are given in terms of the $\tilde{a}_{\mathbf{k}}$ as $\langle \hat{n}^f_{\mathbf{k}\nu} \rangle_0 = (\tilde{a}^2_{\mathbf{k}}/N)/(1+\tilde{a}^2_{\mathbf{k}}/N)$, $\langle \hat{n}^c_{\mathbf{k}\nu} \rangle_0 = 1-\langle \hat{n}^f_{\mathbf{k}\nu} \rangle_0$, and $\langle \hat{n}^x_{\mathbf{k}\nu} \rangle_0 = (\tilde{a}_{\mathbf{k}}/\sqrt{N})/(1+\tilde{a}^2_{\mathbf{k}}/N)$, respectively.

Again, the minimization problem corresponds to the diagonalization of an effective Hamiltonian with renormalized parameters,

$$\tilde{V}_{\mathbf{k}} = \sqrt{q}\, V_{\mathbf{k}} \ , \tag{21a}$$

$$E^f = E^f_0 + \lambda \ . \tag{21b}$$

The effective Hamiltonian is the same as that obtained from a mean-field treatment of the periodic Anderson model using the slave-boson approach by Coleman and Read and Newns.[6-9] It describes two quasiparticle bands with dispersion relations

$$E^{\pm}_{\mathbf{k}} = \tfrac{1}{2}\{ \varepsilon(\mathbf{k}) + E^f \pm \sqrt{[\varepsilon(\mathbf{k})-E^f]^2 + 4\tilde{V}^2_{\mathbf{k}}/N} \} \ . \tag{22}$$

If one strictly takes the limit $N\to\infty$, Eq. (22) reduces to $E_{\mathbf{k}}=\varepsilon(\mathbf{k})$ and $E_{\mathbf{k}}=E^f$, respectively. Furthermore, one may easily verify that the lattice problem, Eq. (20), is identical to the single-impurity problem, Eq. (17), in the same limit. Hence, the binding energy, the Sommerfeld coefficient for the specific heat, and the expression for the magnetic susceptibility are the same as in the single-impurity problem for $N=\infty$. Corrections to these quantities using the slave-boson approach have been derived by Auerbach and Levin[8] and Millis and Lee.[9]

It is therefore seen that the limit of large degeneracy not only suppresses the lattice effects arising from the correlator $g^{\hat{K}^f}$ but also those that are present in $|\Phi_0\rangle$.

C. Large dimensions

The limit of large dimensions ($d=\infty$) provides another limit in which the Gutzwiller-correlated wave functions $|\Psi_g\rangle = g^{\hat{K}^f}|\Phi_0\rangle$ can be evaluated exactly. Again, the self-energy vanishes so that the general expressions given in Eqs. (13) hold in $d=\infty$. We consider $U=\infty$ and set $g=0$, i.e., the f levels may only be empty or singly occupied (for arbitrary g and $N=2$, see Appendix B). The variational problem for $g=0$ and $d=\infty$ is given by the same equation as for $N=\infty$, Eq. (20). However, the renormalization factor for the hybridization is now given by

$$q \equiv q_\nu = \frac{1-n^f}{1-n^f/N} \ . \tag{23}$$

Of course, Eqs. (13) not only cover the translational in-

variant case but are completely general. For instance, they may also be applied to the case of antiferromagnetism.

The variational approach used here gives the same results as the slave-boson saddle-point approximation by Kotliar and Ruckenstein,[10] which is therefore seen to obey a variational principle at $T=0$ in $d=\infty$. As in the case of the single-impurity problem (Sec. IV A) or the Hubbard model (see I), the saddle-point free-energy obtained from their slave-boson approach is limited to the Fermi-liquid regime due to its variational origin (see Appendix C).

Furthermore, Eqs. (20) and (23) prove results of counting-type approximations for $|\Psi_g\rangle$ ("Gutzwiller approximation"), which were applied to the periodic Anderson model in the translational invariant case by Varma, Weber, and Randall,[33] Brandow,[34] Fazekas,[34,36] Rice and Ueda,[37] and Vulović and Abrahams[38] (for a clear description of the method, see Vollhardt[27]). These approximate evaluations of $|\Psi_g\rangle$ are now seen to become exact in $d=\infty$.[43] Recently, Oleś and Zaanen[44] extended the Gutzwiller approximation to the case of antiferromagnetism ($N=2$). Although the method yields the correct q factors and the correct form of the effective Hamiltonian, the results are strictly valid only for $|\Psi_g\rangle$ in the form $|\Psi_g\rangle=g^{\hat{K}^f}|\Phi_0\rangle$ instead of $|\Psi_g\rangle=g^{\hat{D}^f}|\Phi_0\rangle$ as stated in Refs. 33, 37, and 44.

The binding energy $\Delta\varepsilon$ as compared to vanishing hybridization ($V_{\mathbf{k}}=0$) may now be obtained as in the single-impurity case (see Appendix D). We assume a weak hybridization $V_{\mathbf{k}}\equiv V$ and look at the Kondo regime where the bare f level E_0^f lies well below the Fermi energy so that the f-level occupancy n^f is close to unity. We calculate with a constant density of states (bandwidth W) instead of the exact Gaussian density of states in $d=\infty$.[21] From Appendix D we obtain for the binding energy per lattice site

$$\Delta\varepsilon\equiv -T_K^* = -(D+\varepsilon_F)\exp\left[-\frac{W}{V^2}\left[1-\frac{1}{N}\right](\varepsilon_F+|E_0^f|)\right] . \tag{24a}$$

For the deviation from an integer value for n^f we find

$$\delta\equiv 1-n^f=\frac{W}{V^2}\left[1-\frac{1}{N}\right]T_K^* \tag{24b}$$

and the effective f level lies slightly above the Fermi energy at

$$E^f=\varepsilon_F+T_K^* . \tag{24c}$$

These results may be compared to the single-impurity case, Eqs. (19). The exponent for the binding energy in the lattice case turns out to be *smaller* by a factor $1-1/N$ as compared to the single-impurity case, i.e., the binding is strongly enhanced over the single impurity ($T_K^* \gg T_K$). The origin of this discrepancy was attributed to the uncontrolled Gutzwiller-approximation technique frequently used to evaluate $|\Psi_g\rangle$. In fact, we have now proven that the result is correct in the limit $d=\infty$ and therefore provides a variational upper bound in this limit. Furthermore, the form of the q factors turns out to be the *same* in the lattice and the single-impurity case. The limit $d=\infty$ may therefore be viewed as a "single-site approximation" for the correlator and no lattice effects are present in the form of the renormalization factors $q_{\mathbf{i}\nu}$.

The reason for the appearance of the additional factor $1-1/N$ in T_K^* is a genuine lattice effect that is present in $|\Phi_0\rangle$. The binding increases in the lattice case because the f electrons in $|\Phi_0\rangle$ occupy Bloch states themselves, which lowers their kinetic energy and therefore increases the total binding energy. The validity of these considerations is confirmed by recent numerical investigations of the one-dimensional problem by Fye and Scalapino,[45] who find qualitative agreement with the results of Eqs. (24). The additional factor $1-1/N$ becomes equal to unity in the limit $N\to\infty$, where lattice effects become unimportant and the physics of the single impurity is recovered (see the discussion in Sec. IV B).

D. Magnetic instabilities and influence of corrections

In the preceding three subsections we have addressed the limits in which the Gutzwiller-correlated wave functions can be evaluated exactly. We found that the large-N limit underestimates lattice effects and reproduces the single-impurity results in lowest order in the $1/N$ expansion. On the other hand, the limit of large dimensions gives a much larger binding energy reflecting the coherent motion of the f electrons in quasiparticle bands.

However, we confined ourselves to the paramagnetic case. This is allowed in the limit of large degeneracy since neither lattice effects are important nor are there exchange effects that arise from the Pauli principle. The situation changes when one goes to low degeneracy, for example, $N=2$. In this case the Pauli principle is very important. Opposite to the limit of large degeneracy, the limit of large dimensions does not completely eliminate lattice and exchange effects. Actually, only the lattice effects present in the correlator $g^{\hat{K}^f}$ are eliminated but not those present in $|\Phi_0\rangle$; the f and c electrons still form quasiparticle bands. The exchange effects show up in the denominator of the renormalization factors for the effective hybridization at site $\mathbf{i}$, $q_{\mathbf{i}\nu}=(1-n_{\mathbf{i}}^f)/(1-n_{\mathbf{i}\nu}^f)$. The numerator $1-n_{\mathbf{i}}^f$ is simply given by the probability for $U=\infty$ that there is no f electron at $\mathbf{i}$ to make the hybridization process $\hat{c}_{\mathbf{i}\nu}^\dagger\to\hat{f}_{\mathbf{i}\nu}^\dagger$ possible. It is also present in a large-N approach. However, one has to calculate the total renormalization factor for $U=\infty$ *relative* to the respective probability at $U=0$. This probability is given by the denominator as $1-\hat{n}_{\mathbf{i}\nu}^f$ since the process is already forbidden by the Pauli principle for all values of U, if there is an f electron with the same quantum numbers at site $\mathbf{i}$. A trivial limit to check these arguments is given in the case of a total polarized band where there is no interaction at all. In this case one has $q_{\mathbf{i}\nu}=1$, which is certainly the correct result.

The dependence of the effective hybridization on the

magnetization has severe consequences on the stability of the paramagnetic ground state. In fact, as first shown by Rice and Ueda,[37] the paramagnetic state becomes unstable against ferromagnetic ordering in the Kondo regime. As investigated by Oleś and Zaanen,[44] an antiferromagnetic rather than ferromagnetic ordering is stable in the Kondo limit for $N=2$. Rice and Ueda derived a lower bound for the existence of paramagnetism from the ratio of magnetic exchange energy and Kondo energy.[37]

The limit of large degeneracy underestimates the influence of lattice and exchange effects. On the other hand, these effects are overestimated in the limit of large dimensions. The calculation of $1/d$ corrections is possible for $N=2$ (Ref. 46) and leads to a remarkable agreement with numerical (variational Monte Carlo) investigations by Shiba[47] even in $d=1$ dimension. In fact, these corrections show that the binding energy, i.e., T_K^*, is reduced from its value in $d=\infty$. Furthermore, all calculations were done for infinite repulsion between the f electrons. As shown by Vulović and Abrahams,[38] the effect of finite U is to reduce the binding energy as well. It is therefore seen that the tendency to magnetic ordering is reduced for degeneracy $N>2$ [see Eq. (24a)], finite-U corrections,[38] and finite-d corrections.[46,47] Furthermore, it is clear that lattice and exchange effects become less important in a dilute system, which has been studied in the framework of Gutzwiller-correlated wave functions by Fazekas.[35]

V. SUMMARY

We investigated general Gutzwiller-correlated wave functions $|\Psi_g\rangle=g^{\hat{D}^f}|\Psi_0\rangle=g^{\hat{K}^f}|\Phi_0\rangle$ for the periodic Anderson model, especially in the limit of strong correlations ($g=0$). The approximation-free evaluation of expectation values is a complicated many-body problem. For this purpose we extend the formalism in Ref. 28 to the present case of degenerate bands. Simple and explicit results can then be obtained in three cases: (i) the dilute limit (single-impurity case); (ii) the limit of large dimensions ($N=\infty$); (iii) the limit of large dimensions ($d=\infty$).

In the first case the wave function reduces to the Varma-Yafet[40] or lowest-order Gunnarsson-Schönhammer[41] state since the Gutzwiller correlator acts on one lattice site only. We obtain complete agreement with their results. For the lattice case we completely reproduce the results of the slave-boson mean-field solution of Coleman,[6] Read and Newns,[7] Auerbach and Levin,[8] and Millis and Lee[9] in the limit of large degeneracy. In the limit of large dimensions we completely reproduce the results of the slave-boson mean-field theory of Kotliar and Ruckenstein.[10] The two seemingly different slave-boson mean-field results are therefore obtained from the analysis of the same class of correlated wave functions. The variational approach proves that the constraint of no multiple f-level occupancy is strictly fulfilled at temperature $T=0$ and that the results provide variational bounds in the respective limits. The extension of these mean-field treatments to finite temperatures is restricted to the Fermi-liquid regime due to their variational origin.

In addition, we prove formulas that were derived for these wave functions from counting-type approximations ("Gutzwiller approximation") by several authors[33–38,44] to become correct in the limit of large dimensions. Our approach shows that the results in fact belong to $|\Psi_g\rangle$ in the form $|\Psi_g\rangle=g^{\hat{K}^f}|\Phi_0\rangle$ instead of $|\Psi_g\rangle=g^{\hat{D}^f}|\Phi_0\rangle$ as stated in Refs. 33, 37, and 44. Furthermore, an explicit calculation of $1/d$ corrections and equal-time correlation functions as in I is feasible[46] and shows remarkable agreement with numerical data given by Shiba.[47]

Both in the large-N and the large-d limit, the effects of the correlator are described by local renormalization factors $\sqrt{q_{i\nu}}$ for the hybridization. However, the limit of large degeneracy eliminates all lattice coherence effects and all exchange effects that arise from the Pauli principle. Hence, for large degeneracy the single-impurity results are widely recovered. The limit of large dimensions does not suppress these effects. The result is a much larger binding energy in the Kondo limit for the lattice than for the single impurity. This finding is confirmed by recent quantum Monte Carlo investigations on the one-dimensional Kondo lattice.[45] For small degeneracy ($N=2$) the paramagnetic state is unstable against (anti)ferromagnetic order in the Kondo limit. This tendency is reduced by finite-d and finite-U corrections and is generally weakened for large degeneracy and dilute systems. Although magnetically ordered states are realistic for dense Kondo systems with an effective degeneracy $N=2$, this effect is certainly overestimated in $|\Psi_g\rangle$. The one-particle product wave function $|\Phi_0\rangle$ is a quasiparticle vacuum and does not contain excitations. Their inclusion stabilizes the paramagnetic Fermi liquid.[35] A treatment of those more complicated variational wave functions lies beyond the scope of this work.

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APPENDIX A: CALCULATION OF THE ONE-PARTICLE DENSITY MATRICES

The calculation of the one-particle density matrices is performed as in I. As an example we evaluate this quantity for the f electrons.

We have to calculate

$$P_\nu^f(\mathbf{i},\mathbf{j})=\langle \hat{f}_{\mathbf{i}\nu}^\dagger \hat{f}_{\mathbf{j}\nu}\rangle=\frac{\langle \Psi_g|\hat{f}_{\mathbf{i}\nu}^\dagger \hat{f}_{\mathbf{j}\nu}|\Psi_g\rangle}{\langle \Psi_g|\Psi_g\rangle} \tag{A1}$$

for $\mathbf{i}\neq\mathbf{j}$. The numerator may be rewritten as [see Eqs. (5b) and (6)]

$$\langle \Phi_0|(g^{\hat{K}_\mathbf{i}^f}\hat{f}_{\mathbf{i}\nu}^\dagger g^{\hat{K}_\mathbf{i}^f})(g^{\hat{K}_\mathbf{j}^f}\hat{f}_{\mathbf{j}\nu}g^{\hat{K}_\mathbf{j}^f})\prod_{\mathbf{g}\,(\neq\mathbf{i},\mathbf{j})}(1+\hat{\Gamma}_\mathbf{g})|\Phi_0\rangle\ . \tag{A2}$$

The product may be expanded as

$$\prod_{\mathbf{g}\,(\neq \mathbf{i},\mathbf{j})}(1+\hat{\Gamma}_{\mathbf{g}})=1+\sum_{m=1}^{\infty}\frac{1}{m!}{\sum_{\substack{\mathbf{g}_1,\ldots,\mathbf{g}_m\\(\neq \mathbf{i},\mathbf{j})}}}'\hat{\Gamma}_{\mathbf{g}_1}\cdots\hat{\Gamma}_{\mathbf{g}_m} \tag{A3}$$

where the prime on the sum implies that all lattice vectors are different from each other. The number of operators $\hat{\Gamma}_{\mathbf{g}}$ involved is called the "order" of the expansion.

The restriction of the lattice sums and the expansion of $\hat{\Gamma}_{\mathbf{g}}$ itself, Eq. (6), assures that there will be no Hartree bubbles at any "inner vertex" $\mathbf{g}_m$. We have to get rid of the Hartree terms since they are always of order unity for all dimensions d and degeneracies N. We now eliminate these contributions at the "external vertices" i, j. First, we write

$$g^{\hat{K}_{\mathbf{i}}^{f}}\hat{f}_{\mathbf{i}\nu}^{\dagger}g^{\hat{K}_{\mathbf{i}}^{f}}=\hat{f}_{\mathbf{i}\nu}^{\dagger}g^{\hat{Q}_{\mathbf{i}\nu}}\,, \tag{A4}$$

where $\hat{Q}_{\mathbf{i}\nu}$ is given in Eq. (9b). We formally expand $g^{\hat{Q}_{\mathbf{i}\nu}}$ as

$$g^{\hat{Q}_{\mathbf{i}\nu}}=\sqrt{q_{\mathbf{i}\nu}}+\sum_{r=1}^{N}\frac{1}{r!}{\sum_{\alpha_1,\ldots,\alpha_r}}'y_{\mathbf{i},\alpha_1\cdots\alpha_r}^{(\nu)}\left[\sum_{p=1}^{r}(\hat{n}_{\mathbf{i}\alpha_p}^{f}-\langle\hat{n}_{\mathbf{i}\alpha_p}^{f}\rangle_0)\right]$$
$$\equiv\sqrt{q_{\mathbf{i}\nu}}(1+\hat{Y}_{\mathbf{i}\nu}) \tag{A5}$$

in analogy with the expansion of $g^{2\hat{K}_{\mathbf{i}}^{f}}$, Eq. (6). This expansion of $g^{\hat{Q}_{\mathbf{i}\nu}}$ guarantees that there will be no Hartree bubbles at site i. Equation (9a) can be proven by taking the expectation value of both sides in Eq. (A5) with $|\Phi_0\rangle$. Using this definition we find, for the numerator in mth order,

$$\sqrt{q_{\mathbf{i}\nu}}\sqrt{q_{\mathbf{j}\nu}}\langle\Phi_0|\hat{f}_{\mathbf{i}\nu}^{\dagger}\hat{f}_{\mathbf{j}\nu}(1+\hat{Y}_{\mathbf{i}\nu})(1+\hat{Y}_{\mathbf{j}\nu})\hat{\Gamma}_{\mathbf{g}_1}\cdots\hat{\Gamma}_{\mathbf{g}_m}|\Phi_0\rangle\,. \tag{A6}$$

We are now in the position to apply Wick's theorem. Since all lattice points in Eq. (A6) are different and all orbital indices in $\hat{\Gamma}_{\mathbf{g}}$ are different, also we may introduce "δ-less" contractions[48]

$$\{\hat{f}_{\mathbf{g}_1\mu}^{+}\hat{f}_{\mathbf{g}_2\nu}\}_0=\langle\hat{f}_{\mathbf{g}_1\mu}^{\dagger}\hat{f}_{\mathbf{g}_2\nu}\rangle_0=\delta_{\mu\nu}P_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_2)\,, \tag{A7}$$

$$\{\hat{f}_{\mathbf{g}_1\mu}\hat{f}_{\mathbf{g}_2\nu}^{\dagger}\}_0=-\langle\hat{f}_{\mathbf{g}_2\nu}^{+}\hat{f}_{\mathbf{g}_1\mu}\rangle_0=-\delta_{\mu\nu}P_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_2)\,. \tag{A8}$$

Furthermore, since all Hartree contributions were subtracted and all lattice sites and orbital indices were different, we may replace all contractions by

$$\tilde{P}_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_2)=P_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_2)-\delta_{\mathbf{g}_1,\mathbf{g}_2}P_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_1) \tag{A9}$$

without creating any new contributions (see I). Especially, $\tilde{P}_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_1)=0$ holds. We represent the terms arising from Wick's theorem graphically: (i) lines between two lattice points $\mathbf{g}_1,\mathbf{g}_2$ are given by $\tilde{P}_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_2)$; (ii) inner vertices are given by $x_{\mathbf{g},\alpha_1\cdots\alpha_r}$ when there are $2r$ lines at g; (iii) external vertices are given by $y_{\mathbf{i},\alpha_1\cdots\alpha_r}^{(\nu)}$ when there are $2r+1$ lines at i. According to the expansion of $\hat{\Gamma}_{\mathbf{g}}$ there are always at least four lines attached to any inner vertex g.

Now we have to deal with the restrictions on the orbital and lattice sums, which prevent the application of the linked cluster theorem. As in I, we may express the terms arising from Wick's theorem as sums over determinants. The restriction on the orbital sums may be released since the determinants are zero when two rows or columns are set equal. For $N=2$, the same argument applies for the lattice sums and the linked cluster theorem can be used. For $N>2$, however, the restriction on the lattice sum remains. A typical lowest-order disconnected graph is depicted in Fig. 2. The restriction $\mathbf{g}_1\neq\mathbf{g}_2$ may be released since the lattice points are connected by lines $\tilde{P}_{\nu}^{f,0}(\mathbf{g}_1,\mathbf{g}_2)$, which vanishes for $\mathbf{g}_1=\mathbf{g}_2$. However, there are additional contributions for $\mathbf{g}_1=\mathbf{i},\mathbf{j}$ and/or $\mathbf{g}_2=\mathbf{i},\mathbf{j}$. The resulting graphs are connected graphs again, so that all additional contributions can be absorbed into the vertices $x_{\mathbf{g},\alpha_1\cdots\alpha_r}$ and $y_{\mathbf{i},\alpha_1\cdots\alpha_r}^{(\nu)}$. One may introduce modified vertices $\tilde{x}_{\mathbf{g},\alpha_1\cdots\alpha_r}$ and $\tilde{y}_{\mathbf{i},\alpha_1\cdots\alpha_r}^{(\nu)}$ so that the restriction on the lattice sum may be released and the linked-cluster theorem applies. Since there are no disconnected graphs to order unity, the factors $q_{\mathbf{i}\nu}$, $q_{\mathbf{j}\nu}$ are unchanged by this procedure.

Finally, the one-particle density matrix is given as a sum over all connected graphs,

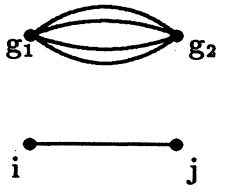

FIG. 2. Disconnected diagram for the self-energy.

$$P_\nu^f(\mathbf{i},\mathbf{j})=\sqrt{q_{\mathbf{i}\nu}}\sqrt{q_{\mathbf{j}\nu}}\left[f_{\mathbf{i}\nu}^\dagger f_{\mathbf{j}\nu}(1+\tilde{Y}_{\mathbf{i}}^{(\nu)})(1+\tilde{Y}_{\mathbf{j}}^{(\nu)})\left[1+\sum_{m=1}^{\infty}\frac{1}{m!}\sum_{\mathbf{g}_1,\ldots,\mathbf{g}_m}\tilde{\Gamma}_{\mathbf{g}_1}\cdots\tilde{\Gamma}_{\mathbf{g}_m}\right]\right]_0^c , \tag{A10}$$

which may be expressed in terms of the noninteracting one-particle density matrix $P_\nu^{f,0}(\mathbf{i},\mathbf{j})$ and a "self-energy" $S_\nu^f(\mathbf{g}_1,\mathbf{g}_2)$. There are at least two vertices in $S_\nu^f(\mathbf{g}_1,\mathbf{g}_2)$ that are connected by three or more separate paths (see I). For a vanishing self-energy, only the lowest-order graph contributes. Thus we find

$$P_\nu^f(\mathbf{i},\mathbf{j})=\sqrt{q_{\mathbf{i}\nu}}\sqrt{q_{\mathbf{j}\nu}}P_\nu^{f,0}(\mathbf{i},\mathbf{j}) \quad (\mathbf{i}\neq\mathbf{j}) \tag{A11}$$

for $d=\infty$ or $N=\infty$.

The calculation for the case $\mathbf{i}=\mathbf{j}$ is analogous and gives $\langle\hat{n}_{\mathbf{i}\nu}^f\rangle=\langle\hat{n}_{\mathbf{i}\nu}^f\rangle_0$ in the same limits. The other one-particle density matrices can be calculated along the same lines. The result becomes obvious when one realizes that the c-electron operators always commute with the correlation operator $g^{\hat{K}_\mathbf{i}^f}$, which only acts on the f electrons. The results for vanishing self-energy are then given in Eqs. (13).

APPENDIX B: RESULTS FOR NO ORBITAL DEGENERACY

Here we present results for the case where we have spin degeneracy only. In this case, one can easily solve Eq. (6), which explicitly reads (see I)

$$g^{2\eta_\mathbf{i}}=1+x_\mathbf{i}\langle\hat{n}_{\mathbf{i}\uparrow}^f\rangle_0\langle\hat{n}_{\mathbf{i}\downarrow}^f\rangle_0 , \tag{B1a}$$

$$g^{2\eta_\mathbf{i}}(g^{-2\mu_{\mathbf{i}\sigma}}-1)=-x_\mathbf{i}\langle\hat{n}_{\mathbf{i}-\sigma}^f\rangle_0, \quad \sigma=\uparrow,\downarrow \tag{B1b}$$

$$g^{2\eta_\mathbf{i}}(g^{2-2\mu_{\mathbf{i}\uparrow}-2\mu_{\mathbf{i}\downarrow}}-g^{-2\mu_{\mathbf{i}\downarrow}}-g^{-2\mu_{\mathbf{i}\uparrow}}+1)=x_\mathbf{i} . \tag{B1c}$$

This set of equations is easy to solve. One obtains

$$x_\mathbf{i}=\frac{1}{2(1-g^2)\bar{d}_{\mathbf{i},0}^f(1-n_{\mathbf{i},0}^f+\bar{d}_{\mathbf{i},0}^f)}\times\{-1+(1-g^2)(n_{\mathbf{i},0}^f-2\bar{d}_{\mathbf{i},0}^f)+\sqrt{1+(g^2-1)[n_{\mathbf{i},0}^f(2-n_{\mathbf{i},0}^f)+g^2(m_{\mathbf{i},0}^f)^2]}\} \tag{B2a}$$

and

$$g^{2\eta_\mathbf{i}}=1+x_\mathbf{i}\bar{d}_{\mathbf{i},0}^f , \tag{B2b}$$

$$g^{-2\mu_{\mathbf{i}\sigma}}=1-\frac{x_\mathbf{i}\langle\hat{n}_{\mathbf{i}-\sigma}^f\rangle_0}{1+x_\mathbf{i}\bar{d}_{\mathbf{i},0}^f} . \tag{B2c}$$

Here, $n_{\mathbf{i},0}^f=\langle\hat{n}_{\mathbf{i}\uparrow}^f\rangle_0+\langle\hat{n}_{\mathbf{i}\downarrow}^f\rangle_0$, $m_{\mathbf{i},0}^f=\langle\hat{n}_{\mathbf{i}\uparrow}^f\rangle_0-\langle\hat{n}_{\mathbf{i}\downarrow}^f\rangle_0$, and $\bar{d}_{\mathbf{i},0}^f=\langle\hat{n}_{\mathbf{i}\uparrow}^f\rangle_0\langle\hat{n}_{\mathbf{i}\downarrow}^f\rangle_0$ denote the local density, local magnetization, and local double occupancy for the f electrons in $|\Phi_0\rangle$, respectively.

These expressions now allow for an explicit representation of the q factors, which give the effective hybridization and the mean f-electron double occupancy for arbitrary g, $\langle\hat{n}_{\mathbf{i}\sigma}^f\rangle_0$. To determine $q_{\mathbf{i}\sigma}$ we have to evaluate Eq. (9). Equation (9b) reduces to $\hat{Q}_{\mathbf{i}\sigma}=(1-2\mu_{\mathbf{i}\sigma})\hat{n}_{\mathbf{i}-\sigma}^f-\mu_{\mathbf{i}\sigma}+2\eta_\mathbf{i}$. Using the definition of $q_{\mathbf{i}\sigma}$, Eq. (9a), and Eqs. (B2), we finally obtain

$$q_{\mathbf{i}\sigma}=\frac{1}{\langle\hat{n}_{\mathbf{i}\sigma}^f\rangle_0(1-\langle\hat{n}_{\mathbf{i}\sigma}^f\rangle_0)}\times[\sqrt{(1-n_{\mathbf{i},0}^f+\bar{d}_\mathbf{i}^f)(\langle\hat{n}_{\mathbf{i}\sigma}^f\rangle_0-\bar{d}_\mathbf{i}^f)}+\sqrt{\bar{d}_\mathbf{i}^f(\langle\hat{n}_{\mathbf{i}\sigma}^f\rangle_0-\bar{d}_\mathbf{i}^f)}]^2 . \tag{B3}$$

The mean double occupancy fulfills Eq. (13d). For $N=2$ we have $z_{\mathbf{i}\lambda\nu}\equiv 1$. Using Eqs. (B2) and dropping superfluous indices Eq. (13d) finally becomes

$$g^2=\frac{\bar{d}_\mathbf{i}^f(1-n_{\mathbf{i},0}^f+\bar{d}_\mathbf{i}^f)}{(\langle\hat{n}_{\mathbf{i}\uparrow}^f\rangle_0-\bar{d}_\mathbf{i}^f)(\langle\hat{n}_{\mathbf{i}\downarrow}^f\rangle_0-\bar{d}_\mathbf{i}^f)} . \tag{B4}$$

These results are exact in $d=\infty$ for general Gutzwiller-correlated wave functions $|\Psi_g\rangle$. Formulas that were obtained for these wave functions in the translational invariant case by using the Gutzwiller approximation are therefore seen to become exact in the limit of large dimension.[33–38,44] A detailed discussion of the results ($N=2$, arbitrary g) can be found in Refs. 37 and 38.

APPENDIX C: EXTENSION TO FINITE TEMPERATURE

The variational principle allows us to calculate upper bounds for the ground-state energy of a given Hamiltonian $\hat{H}$ and is therefore naturally limited to temperature $T=0$. On the other hand, one can make contact with Fermi-liquid theory by calculating Fermi-liquid parameters so that one can go beyond $T=0$ (see Vollhardt[27] for the application of the Gutzwiller wave function to normal fluid ^{3}He).

A formally different but conceptually equivalent way to extend the variational approach to finite temperature has been introduced in I. The ground state of $\hat{H}$ is approximated by the variational wave function $|\Psi_g\rangle=g^{\hat{K}^f}|\Phi_0\rangle$ to give a variational energy

$$E_0=\frac{\langle\Psi_g|\hat{H}|\Psi_g\rangle}{\langle\Psi_g|\Psi_g\rangle}=\langle\Phi_0|\hat{H}^{\rm eff}|\Phi_0\rangle \tag{C1}$$

while the latter equality is only exact in the limits discussed in Sec. III. $|\Phi_0\rangle$ may be chosen as the exact ground state of the *noninteracting* effective Hamiltonian $\hat{H}^{\rm eff}$ (lattice case) or as an approximative ground state

(singly-impurity case). From this point of view one may argue that *excited* states for $\hat{H}$ may easily be constructed as $|\Psi_g^n\rangle = g^{\hat{K}^f}|\Phi_n\rangle$, where $|\Phi_n\rangle$ $(n=1,2,\ldots)$ are excited states of $\hat{H}^{\text{eff}}$. Since the formalism presented here is completely general, we find in the limits discussed in Sec. III that

$$E_n = \frac{\langle \Psi_g^n|\hat{H}|\Psi_g^n\rangle}{\langle \Psi_g^n|\Psi_g^n\rangle} = \langle \Phi_n|\hat{H}^{\text{eff}}|\Phi_n\rangle \ . \tag{C2}$$

An excited state $|\Phi_n\rangle$ described in terms of the noninteracting Hamiltonian $\hat{H}^{\text{eff}}$ therefore corresponds to an excited stated $|\Psi_g^n\rangle = g^{\hat{K}^f}|\Phi_n\rangle$ in terms of the original interacting Hamiltonian $\hat{H}$ just like in the Fermi-liquid picture.

Therefore it seems natural to *define* the objects

$$Z_{\text{KR}} = \sum_{\{\Phi_n\}} e^{-\beta E_n} \ , \tag{C3a}$$

$$f_{\text{KR}} = -\frac{1}{\beta}\ln Z_{\text{KR}} \ , \tag{C3b}$$

where $\beta = 1/T$. The minimization procedure then has to be performed using f_{KR} for $T>0$ instead of E_0 at $T=0$. f_{KR} is then exactly the "free energy" and is Z_{KR} the "partition function" which follows from a saddle-point mean-field solution of $\hat{H}$ using the slave-boson treatment of Kotliar and Ruckenstein.[10,16] In the limit of large degeneracy it becomes equivalent to the free energy and partition function obtained from the saddle-point mean-field solution of $\hat{H}$ using the slave-boson treatment of Coleman and Read and Newns.[6,7]

However, it is clear from the construction that only low-lying excitations might be described in the same manner as the ground state. Higher-lying excitation, especially charge excitations, which are always suppressed by the correlation operator, cannot be described properly. Its variational origin limits the applicability of these slave-boson approaches to the Fermi-liquid regime.

APPENDIX D: MINIMIZATION PROCEDURES

1. Single-impurity case

We have to minimize Eq. (17a). We include (17b) by introducing a Lagrange parameter λ. Then we have to minimize

$$(\Delta E+\lambda n^f)\left[1+\frac{1}{NL}\sum_{\mathbf{k}}{}'\,\tilde{a}_{\mathbf{k}}^{\,2}\right] = \frac{1}{L}\sum_{\mathbf{k}}{}'\{[E^f-\varepsilon(\mathbf{k})]\tilde{a}_{\mathbf{k}}^{\,2}-2\tilde{V}_{\mathbf{k}}\tilde{a}_{\mathbf{k}}\} \tag{D1}$$

with respect to $\tilde{a}_{\mathbf{k}}$, λ, and n^f. Here, $\tilde{V}_{\mathbf{k}}=\sqrt{q}\,V_{\mathbf{k}}$, $q=(1-n^f)/(1-n^f/N)$, and $E^f=E_0^f+\lambda$. Minimization of ΔE with respect to $\tilde{a}_k$ gives

$$\tilde{a}_{\mathbf{k}} = \frac{\tilde{V}_{\mathbf{k}}}{E^f-\varepsilon(\mathbf{k})-(\Delta E+\lambda n^f)/N} \ . \tag{D2}$$

Reinserting this into (D1) gives

$$\Delta E+\lambda n^f = \frac{1}{L}\sum_{\mathbf{k}}{}'\frac{\tilde{V}_{\mathbf{k}}^{\,2}}{\varepsilon(\mathbf{k})-E^f+(\Delta E+\lambda n^f)/N} \ . \tag{D3}$$

Minimizing Eq. (D1) with respect to λ gives Eq. (17b)

$$n^f = \frac{(1/L)\sum_{\mathbf{k}}{}'\,\tilde{a}_{\mathbf{k}}^{\,2}}{1+(1/L)\sum_{\mathbf{k}}{}'\,\tilde{a}_{\mathbf{k}}^{\,2}/N} \ . \tag{D4}$$

The conduction electrons are assumed to form a featureless band of width W so that we can work with a constant density of states. $(1/L)\sum_{\mathbf{k}}{}'$ is then replaced by integrating in energy from the lower band edge $-D=-W/2$ up to ε_F. The total number of electrons is given by $n=N(\varepsilon_F+D)/W$. Equations (D3) and (D4) can now easily be evaluated. One finds

$$\Delta E = -\lambda n^f+\frac{\tilde{V}^2}{W}\ln\left|\frac{\varepsilon_F-E^f+(\Delta E+\lambda n^f)/N}{-D-E^f+(\Delta E+\lambda n^f)/N}\right| \ , \tag{D5a}$$

$$\frac{n^f}{1-n^f} = \frac{V^2(D+\varepsilon_F)}{W}\left[\left[\varepsilon_F-E^f+\frac{\Delta E+\lambda n^f}{N}\right]\times\left[-D-E^f+\frac{\Delta E+\lambda n^f}{N}\right]\right]^{-1} \ . \tag{D5b}$$

We may eliminate λ from Eq. (D5a) with the help of Eq. (D5b). For small V/W we obtain from (D5b)

$$\lambda = \frac{E_0^f-\varepsilon_F-\Delta E/N-V^2(1-n^f)/(n^fW)}{n^f/N-1} \tag{D6}$$

so that we find

$$\Delta E = n^f(E_0^f-\varepsilon_F) + \frac{V^2(1-n^f)}{W}\left[-1+\ln\left[\frac{V^2(1-n^f)}{n^fW(\varepsilon_F+D)}\right]\right] \ . \tag{D7}$$

The term $n^f(E_0^f-\varepsilon_F)$ in Eq. (D7) is independent of V and gives the energy of the occupied f level measured from the Fermi energy. Strictly speaking ε_F is altered by an amount of order n^f/L since the f level was supposed to be empty in our definition of ε_F. This plays no role in the single-impurity case but will be important in the following subsection.

We are interested in the Kondo limit where $\delta=1-n^f$ is a small quantity. Minimizing Eq. (D7) to lowest order in δ gives

$$\delta = 1-n^f = \frac{W(D+\varepsilon_F)}{V^2}\exp\left[-\frac{W}{V^2}(\varepsilon_F+|E_0^f|)\right] \tag{D8a}$$

and the binding energy $\Delta\varepsilon=\Delta E-n^f(E_0^f-\varepsilon_F)$ is given by

$$\Delta\varepsilon \equiv -T_K = -(\varepsilon_F + D)\exp\left[-\frac{W}{V^2}(\varepsilon_F + |E_0^f|)\right] . \tag{D8b}$$

The effective f level lies at $E^f = E_0^f + \lambda = \varepsilon_F + T_k$.

To make contact with the minimization problem in Refs. 40 and 41, one has to reexpress $|\Psi_g\rangle$ as $|\Psi_g\rangle = g^{\hat{D}^f}|\Psi_0\rangle$. From Eq. (5a) we have $\tilde{a}_k = g^{\mu} a_k$, which gives $\tilde{a}_k = \sqrt{q}\, a_k$ for $g = 0$. Using this one can easily obtain the minimization equations of Gunnarsson and Schönhammer if one identifies $V_k = \sqrt{NL}\, V(\varepsilon)$.

2. Lattice case

We have to minimize Eq. (20) with respect to $\tilde{a}_k$, λ, and n^f. Defining $\langle \hat{H} \rangle = E_{FS} + \Delta E$, we have to minimize

$$\Delta E + \lambda n^f L = \sum_k{}' \frac{\tilde{a}_k^2 [E^f - \varepsilon(\mathbf{k})] - 2\tilde{V}_k \tilde{a}_k}{1 + \tilde{a}_k^2/N} . \tag{D9}$$

Again, $\tilde{V}_k = \sqrt{q}\, V_k$, $q = (1-n^f)/(1-n^f/N)$, and $E^f = E_0^f + \lambda$. Minimization of ΔE with respect to $\tilde{a}_k$ gives

$$\tilde{a}_k = \frac{2\tilde{V}_k}{E^f - \varepsilon(\mathbf{k}) + \sqrt{[E^f - \varepsilon(\mathbf{k})]^2 + 4\tilde{V}_k^2/N}} . \tag{D10}$$

Taking the limit $N = \infty$ in Eqs. (D10) and (D2) one may easily see that both expressions agree in this case and give the same value for ΔE, i.e., lattice effects become unimportant in this limit.

Minimizing Eq. (D9) with respect to λ gives

$$n^f = \frac{1}{L} \sum_k{}' \frac{\tilde{a}_k^2}{1 + \tilde{a}_k^2/N} . \tag{D11}$$

We assume a featureless band of conduction electrons of width W and $V_k \equiv V \ll W$. The total number of electrons is given by $n = N(\varepsilon_0 + D)/W$, which is the actual definition of ε_0. Recall that we start from a filled c-electron Fermi sea and empty f levels [see Eq. (4)] so that ε_0 is equivalent to the Fermi vector k_F. We insert the optimized form of $\tilde{a}_k$, Eq. (D10), into Eqs. (D9) and (D11) and perform the elementary integrals. This yields

$$(\Delta E)/L = -\lambda n^f - \frac{N}{4W}\left[(\varepsilon_0 - E^f)^2 - (D + E^f)^2 + (\varepsilon_0 - E^f)\sqrt{(\varepsilon_0 - E^f)^2 + 4\tilde{V}^2/N} + (D + E^f)\sqrt{(D + E^f)^2 + 4\tilde{V}^2/N} - \frac{4\tilde{V}^2}{N}\ln\left|\frac{(\varepsilon_0 - E^f) - \sqrt{(\varepsilon_0 - E^f)^2 + 4\tilde{V}^2/N}}{(D + E^f) + \sqrt{(D + E^f)^2 + 4\tilde{V}^2/N}}\right|\right] , \tag{D12a}$$

$$n^f = \frac{N}{2W}\left[\varepsilon_0 + D + \sqrt{(\varepsilon_0 - E^f)^2 + 4\tilde{V}^2/N} - \sqrt{(D + E^f)^2 + 4\tilde{V}^2/N}\right] . \tag{D12b}$$

We may eliminate λ from Eq. (D12a) with the help of Eq. (D12b). For small V/W we obtain from (D12b)

$$\lambda = \varepsilon_0 - E_0^f - (Wn^f)/N + \lambda_1 \tilde{V}^2 , \tag{D13}$$

where λ_1 is an unimportant correction that does not show up in ΔE to order $\tilde{V}^2$. Retaining orders $\tilde{V}^2$ and $\tilde{V}^2 \ln \tilde{V}^2$ we obtain for ΔE

$$(\Delta E)/L = \frac{W(n^f)^2}{2N} - n^f(\varepsilon_0 - E_0^f) + \frac{\tilde{V}^2}{W}\left[-1 + \ln\left[\frac{\tilde{V}^2}{Wn^f(D + \varepsilon_0 - Wn^f/N)}\right]\right] . \tag{D14}$$

The term $(W(n^f)^2)/(2N) - n^f(\varepsilon_0 - E_0^f)$ in Eq. (D14) is independent of V and gives the energy of the occupied f levels. Including E_{FS} it may be written as $E(V=0) = N/(2W)[(\varepsilon_0')^2 - D^2] + E_0^f n^f$, where ε_0' is determined by $n - n^f = N(\varepsilon_0' + D)/W$. While ε_0 defines the Fermi momentum, the Fermi energy in the case $V = 0$ is given by $\varepsilon_0' = \varepsilon_0 - Wn^f/N$.

As soon as a finite hybridization is present, the f electrons become delocalized and two quasiparticle bands with dispersion relations

$$E_k^{\pm} = \tfrac{1}{2}\{\varepsilon(\mathbf{k}) + E^f \pm \sqrt{[\varepsilon(\mathbf{k}) - E^f]^2 + 4\tilde{V}_k^2/N}\} \tag{D15}$$

are formed. The Fermi energy ε_F lies in the lower band and fulfills the equation

$$\varepsilon_F = \tfrac{1}{2}\left[\varepsilon_0 + E^f - \sqrt{(\varepsilon_0 - E^f)^2 + 4\tilde{V}^2/N}\right] . \tag{D16}$$

This equation may be used to eliminate ε_0 in favor of the Fermi energy ε_F.

We are interested in the Kondo limit and therefore minimize the binding energy per lattice site $\Delta\varepsilon = [E(V) - E(V=0)]/L$ with respect to lowest order in δ. This gives

$$\delta \equiv 1 - n^f = \frac{W(1 - 1/N)}{V^2}(D + \varepsilon_F)\exp\left[-\frac{W(1 - 1/N)}{V^2} \times (\varepsilon_F + |E_0^f|)\right] \tag{D17a}$$

and the binding energy per lattice site reads

$$\Delta\varepsilon \equiv -T_K^* = -(D+\varepsilon_F)\exp\left[-\frac{W(1-1/N)}{V^2}(\varepsilon_F+|E_0^f|)\right], \tag{D17b}$$

where we used the lowest-order expression for the Fermi energy, $\varepsilon_F = E^f = E_0^f + \lambda = \varepsilon_0 - Wn^f/N$. Including the dominant correction in the Kondo limit, E^f reads

$$E^f = \varepsilon_F + T_K^* \ . \tag{D18}$$

For completeness we give the density of states at the Fermi energy ε_F, which is directly proportional to the effective mass

$$\rho^*(\varepsilon_F) = \frac{N}{W}\left[\frac{\partial E^-}{\partial\varepsilon}\right]^{-1}\Bigg|_{E^- = \varepsilon_F} = \rho_0 + \frac{1}{T_K^*} \ . \tag{D19}$$

The effective mass is clearly enhanced over the contribution for $V=0$, $\rho_0 = N/W$. The admixture of f-electron states for $V>0$ gives rise to the large contribution $1/T_K^*$.

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