Gutzwiller correlated wave functions in finite dimensions d: A systematic expansion in $1/d$

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(Received 3 November 1989)

We present a systematic formalism for the variational evaluation of ground-state properties of Hubbard-type models in finite dimensions d. The formalism starts from generalized Gutzwiller correlated wave functions, which are then studied in a systematic $(1/d)$ expansion around the limit of high dimensions ($d=\infty$). The limit of $d\to\infty$ has recently been introduced by Metzner and Vollhardt (MV) for itinerant lattice fermion systems. The approach, presented in this paper, is particularly efficient since results in $d=\infty$ are obtained without having to calculate a single graph. Our results confirm the finding of MV that counting approximations in the spirit of the Gutzwiller approximation become exact in $d=\infty$ for translationally invariant wave functions. This type of approximation is no longer exact for more complicated (e.g., antiferromagnetic) wave functions. In addition, we completely reproduce the results of the Kotliar-Ruckenstein path-integral approach to the Hubbard model. Performing a $(1/d)$ expansion for the Gutzwiller wave function, we show that the lowest orders in $(1/d)$ are sufficient to reproduce all numerical findings in $d=2,3$ *quantitatively*. We therefore conclude that the limit of $d=\infty$ is a very fruitful starting point for the study of finite-dimensional systems. On the basis of our study we propose new variational wave functions for the numerical investigation of antiferromagnetism in the Hubbard, the t-J, and the spin-$\frac{1}{2}$ Heisenberg model. For the first two models we calculate in $d=\infty$ only, for the Heisenberg model we also derive corrections up to order $(1/d)$. To this order we obtain complete agreement with linear spin-wave theory. Since our trial state is based on a fermionic description of the Heisenberg model, we interpret this analytically determined wave function as Fermi sea of spin-$\frac{1}{2}$ quasiparticles ("spinons").

I. INTRODUCTION

The description of ^{3}He, heavy-fermion materials, and, most recently, high-T_c superconductivity requires techniques that go beyond ordinary perturbation theory, because there are no small parameters in the system. Hence, the calculation of ground-state properties is a difficult problem even for simplified model Hamiltonians as the Hubbard[1] or the periodic Anderson model.[2] In this situation variational wave functions (VWF's) have proven to be very helpful. On one hand, they yield only an approximate description of the true ground state of a Hamiltonian or a physical system. On the other hand, the particular type of approximation is apparent from the explicit nature of such a trial state. Furthermore, the variational principle yields an exact upper bound for the ground-state energy and therefore provides a criterion for the quality of a VWF.

The calculation of expectation values is, however, still a complicated many-particle problem. Hence, one often uses approximate treatments which finally yield "physical" but essentially uncontrolled results. As a consequence one cannot decide whether a predicted physical effect is indeed included in the VWF or is due to the approximation. These basic problems also occur for the Gutzwiller wave function[3] (GWF) which is one of the simplest many-particle wave functions. The GWF consists of a correlation operator in position space acting on the Fermi sea of noninteracting particles. Gutzwiller invented an approximation[3] (GA) to treat this wave function. The results were then applied to several physical systems, e.g., the metal-insulator transition[4] and ^{3}He.[5]

An approximation-free solution was obtained only recently for the GWF in one dimension by Vollhardt and co-workers.[6,7] For higher dimensions, however, no complete analytical solution has been obtained so far. At the same time, numerical methods (e.g., variational Monte Carlo) cannot only be applied to $d=1$ (Refs. 8–10) but allow one to analyze the GWF in $d=2,3$ also.[8] This yields valuable insight into the physics described by the GWF. This technique can also be applied to more complicated VWF's (Refs. 8, 11, and 12) provided that finite-size effects are under control. Hence, the number of variational parameters is limited and the analytic dependence of a VWF on these parameters is an additional input.

Metzner and Vollhardt[13] (MV) recently introduced the limit of *high* dimensions which may play a key role for analytical investigations of correlated Fermi systems. This opened the possibility to study *finite*-dimensional systems via a systematic expansion around $d=\infty$, controlled by the parameter $(1/d)$. In the case of VWF's this concept is not limited to the GWF but can be applied to generalized Gutzwiller correlated VWF's. This class of wave functions consists of all one-particle product wave functions which are correlated by the Gutzwiller operator. As a first result they showed that the GA

yields the *exact* result for the GWF in $d=\infty$.[6,13] Furthermore they derived a graph formalism which, in principle, allows for the exact evaluation of expectation values for the whole class of Gutzwiller correlated VWF's in $d=\infty$. As an example they applied their method to a Gutzwiller correlated antiferromagnetic spin-density wave function (GSDW) in $d=\infty$.[13] Furthermore, one can calculate correlation functions in high dimensions exactly.[14] One can also apply their method to a Gutzwiller-type VWF for the periodic Anderson model[15–18] where the results of approximate treatments[15,16,18] and the exact result in $d=\infty$ (Ref. 19) are seen to agree. However, it is not a trivial task to derive the variational ground-state energy from the complete but implicit set of equations of MV for general wave functions. Furthermore, an explicit calculation of $(1/d)$ corrections is at least tedious even for the simple GWF.

The purpose of this paper is to present a formalism which utilizes the limit of high dimensions more economically. In Sec. II we derive expressions for the one-particle density matrix, the mean double occupancy, the variational ground-state energy, and several correlation functions. These formulas are valid for arbitrary dimensions d but simplify considerably in $d=\infty$ where all these quantities can be calculated exactly. The results are summed up in Sec. III. Since the formalism is valid for general Gutzwiller correlated VWF's we are able to compare the exact results in $d=\infty$ with the results of approximate methods in Sec. IV. In Sec. V we go beyond the GA for the GWF and calculate $(1/d)$ corrections for the GWF. These results are compared with numerical ($d=2,3$) and exact evaluations ($d=1$) in Sec. VI. In Sec. VII we use the concept of high dimensions to propose new VWF's for numerical studies in low dimensions. In this section we calculate the *optimal* Gutzwiller correlated spin-density wave function for the Hubbard and the t-J model[20–22] in $d=\infty$, and to order $(1/d)$ for the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg model. A summary in Sec. VIII closes the presentation.

II. GENERAL FORMALISM

In this section we consider the Hubbard model, which is the model of main interest in this paper. To investigate the ground-state properties of this model we analyze a large class of Gutzwiller correlated variational wave functions. We derive a general graph formalism to calculate expectation values with these VWF's and apply it to the evaluation of the one-particle density matrix, the potential energy, and several correlation functions (CF's). All these quantities allow insight into the physics described by the VWF's under concern. We show that their calculation is greatly simplified high dimensions because the formalism has the following advantages: (i) without calculating a single graph we can derive simple, exact results for all quantities in $d=\infty$, (ii) we need only a few graphs to calculate $(1/d)$ corrections.

A. Hubbard model and variational wave functions

One of the simplest models to treat correlation effects is the Hubbard model[1]

$$\hat{H}=\sum_{i,j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\ , \tag{1}$$

where $\hat{c}^{\dagger}_{i\sigma}$ creates an electron with spin σ on site $\mathbf{i}$, etc., and $\hat{n}_{i\sigma}=\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ is the number operator for σ electrons on site $\mathbf{i}$. The interaction in (1) is purely on site and can be written as $U\sum_i \hat{D}_i=U\hat{D}$, where $\hat{D}_i=\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ counts a double occupancy at site $\mathbf{i}$. We consider the model on d-dimensional hypercubic lattices with L lattice sites. We restrict ourselves to only nearest-neighbor hopping, i.e., $t_{ij}=-t$ for $\mathbf{i},\mathbf{j}$ nearest neighbors and $t_{ij}=0$ otherwise. For this choice of the hopping constants Metzner and Vollhardt[13] showed that one has to scale as

$$t=\frac{t^*}{\sqrt{2d}} \tag{2}$$

to obtain a nontrivial model in the limit $d\to\infty$. From now on we set $t^*\equiv 1$. The dispersion relation is then given by

$$\varepsilon(\mathbf{k})\equiv\frac{1}{L}\sum_{i,j}t_{ij}e^{i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}=-\left[\frac{2}{d}\right]^{1/2}\sum_{i=1}^{d}\cos k_i\ . \tag{3}$$

To study ground-state properties of models with strong on-site repulsion like the Hubbard model, we consider the class of Gutzwiller-type VWF's defined as

$$\begin{aligned}|\Psi_g\rangle&=g^{\hat{D}}|\Psi_0\rangle\\&=\prod_i[1-(1-g)\hat{D}_i]|\Psi_0\rangle\ ,\end{aligned} \tag{4}$$

where $0\le g\le 1$ is a variational parameter and $|\Psi_0\rangle$ is an arbitrary one-particle product wave function with fixed total number of particles.[23] Here $g^{\hat{D}}$ is the Gutzwiller correlator. We choose $|\Psi_0\rangle$ as any quasiparticle vacuum to ensure the applicability of Wick's theorem. For $|\Psi_0\rangle$ as the Fermi sea we recover the original Gutzwiller wave function[3] as a special case of (4). The Gutzwiller correlator globally reduces the weight of configurations in $|\Psi_0\rangle$ that give a large contribution to the on-site Coulomb interaction in the Hubbard model (1). Such VWF's therefore include substantial correlation effects induced by a strong on-site interaction in a natural way.

The task is now to calculate expectation values $\langle\hat{O}\rangle$ with the VWF (4) which are defined as

$$\langle\hat{O}\rangle=\langle\Psi_g|\hat{O}|\Psi_g\rangle/\langle\Psi_g|\Psi_g\rangle\ .$$

To carry out the variational procedure we have to calculate the one-particle density matrix

$$P_\sigma(\mathbf{i},\mathbf{j})=\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle \tag{5a}$$

and the mean double occupancy

$$\bar{d}_i=\langle\hat{D}_i\rangle\ . \tag{5b}$$

In the Hubbard model a lattice site may be empty, singly occupied by either an $\uparrow$ or $\downarrow$ electron, or doubly occupied. The correlations between these four entities are described by correlation functions of type

$$C^{XY}(\mathbf{j})=\frac{1}{L}\sum_i(\langle\hat{X}_i\hat{Y}_{i+j}\rangle-\langle\hat{X}_i\rangle\langle\hat{Y}_{i+j}\rangle)\ , \tag{6}$$

where $\hat{X}_i$ and $\hat{Y}_i$ are one of the following local operators:

$$\hat{S}_i^z \equiv (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})/2 , \tag{7a}$$

$$\hat{N}_i \equiv \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} , \tag{7b}$$

$$\hat{D}_i \equiv \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} , \tag{7c}$$

$$\hat{H}_i \equiv (1-\hat{n}_{i\uparrow})(1-\hat{n}_{i\downarrow}) , \tag{7d}$$

where $\hat{S}_i^z$ is the operator for the spin in z direction, $\hat{N}_i$ for the density, $\hat{D}_i$ for the doubly occupied site, and $\hat{H}_i$ for the empty site or "hole." Furthermore, we are interested in the spin-flip CF

$$C^{S^+S^-}(\mathbf{j}) = \frac{1}{L}\sum_i \langle \hat{S}_i^+ \hat{S}_{i+j}^- \rangle - \langle \hat{S}_i^+ \rangle \langle \hat{S}_{i+j}^- \rangle , \tag{7e}$$

where $\hat{S}_i^+ \equiv \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}$, $\hat{S}_i^- = (\hat{S}_i^+)^+$. The operators $\hat{S}_i^z$, $\hat{S}_i^+$, and $\hat{S}_i^-$ obey the commutation rules of a spin algebra for $S=\frac{1}{2}$ and can be used to construct the vector operator $\hat{\mathbf{S}}_i$ in the usual way. This CF yields additional information in the case of a broken spin symmetry in the VWF, e.g., in the case of a VWF for the antiferromagnetic Heisenberg model. As is easy to see, only seven of these CF's are independent.[7]

B. Generalized Gutzwiller correlated wave functions

Metzner and Vollhardt[6,13] expanded all expectation values in a power series in the parameter (g^2-1) using

$$g^{2\hat{D}} = \prod_i [1+(g^2-1)\hat{D}_i] . \tag{8}$$

They derived a graph formalism with lines representing the noninteracting one-particle density matrix

$$P_\sigma^0(\mathbf{i},\mathbf{j}) = \langle \Psi_0 | \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} | \Psi_0 \rangle$$

and vertices representing the expansion parameter (g^2-1). In this way the problem was solved exactly in $d=1$ (Refs. 6 and 7) for the GWF. For dimensions $d=2,3$ a closed solution has not been possible so far.

In this situation MV showed[13] that the limit of *high* dimensions again allows for exact, analytical calculations with Gutzwiller-type VWF's. Their diagrams are drastically simplified in $d=\infty$. Hence, they were able to write down a closed set of coupled equations for the one-particle density matrix. They obtained an explicit solution of their equations for the GWF ($|\Psi_0\rangle$ the Fermi sea) and for $|\Psi_0\rangle$ chosen as a general Gutzwiller correlated spin-density wave function. A straightforward application of their method yields all CF's for the GWF in $d=\infty$ (Ref. 14) and it can also be applied[19] to a VWF for the periodic Anderson model[15–18] in this limit.

However, their equations are so complicated that a solution for *general* $|\Psi_0\rangle$ is not possible in practice. Furthermore, within their formalism an explicit $(1/d)$ expansion is tedious even for the simple GWF and seems to be untractable for more complicated Gutzwiller correlated VWF's. For these reasons one desires a more effective formalism to treat the limit of high dimensions.

The main problem in the (g^2-1) expansion is that on-site contributions in the graphs do not vanish. The graphs do simplify in $d=\infty$ but nevertheless retain a nontrivial value due to $P_\sigma^0(\mathbf{i},\mathbf{i}) \neq 0$. Thus, the aim is to get rid of the on-site contributions in $P_\sigma^0(\mathbf{i},\mathbf{j})$. To fulfill this requirement we have at least to eliminate the trivial Hartree bubbles at site $\mathbf{i}$ with spin σ. These bubbles represent contributions

$$P_\sigma^0(\mathbf{i},\mathbf{i}) = \langle \Psi_0 | \hat{n}_{i\sigma} | \Psi_0 \rangle$$

and occur in the formalism of MV due to contractions of $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ in (8) at the same site $\mathbf{i}$. Hence, we want

$$g^{2\hat{K}} = \prod_i [1 + x_i(\hat{D}_i - \hat{D}_i^{\mathrm{HF}})] \tag{9}$$

with

$$\hat{D}_i^{\mathrm{HF}} = \hat{n}_{i\uparrow}\langle \hat{n}_{i\downarrow} \rangle_0 + \hat{n}_{i\downarrow}\langle \hat{n}_{i\uparrow} \rangle_0 - \langle \hat{n}_{i\uparrow} \rangle_0 \langle \hat{n}_{i\downarrow} \rangle_0$$

as the Hartree-Fock (HF) decomposition of $\hat{D}_i$. Here we introduced the *new, site-dependent* expansion parameter x_i, so that the vertex factor (g^2-1) of MV is replaced by x_i. Note that we also introduced the operator $\hat{K}$ which replaces $\hat{D}$ in Eq. (8). The subtraction of the Hartree bubbles is usually *not* sufficient to get rid of *all* on-site contributions in a graph formalism. In the special case of Gutzwiller correlated variational wave functions this is indeed the case if one expands the correlator as in Eq. (9). The full implications will become clear in the next subsection.

We now identify the expansion parameter x_i and the operator $\hat{K}$. Because $\hat{n}_{i\sigma}^2 = \hat{n}_{i\sigma}$, and $\hat{D}_i^2 = \hat{D}_i$ we can make the ansatz

$$\hat{K} = \sum_i \hat{K}_i = \sum_i (\hat{D}_i - \mu_{i\uparrow}\hat{n}_{i\uparrow} - \mu_{i\downarrow}\hat{n}_{i\downarrow} + \eta_i) , \tag{10a}$$

$$g^{2\hat{K}} = \prod_i [1 + x_i(\hat{D}_i - \hat{D}_i^{\mathrm{HF}})] . \tag{10b}$$

The real quantities $\mu_{i\uparrow}$, $\mu_{i\downarrow}$, and η_i in Eq. (10a) can be chosen at will but we choose them to fulfill Eq. (10b). Hence, we also use η_i which only results in a normalization factor. Expanding the exponential in (10b) we obtain the following set of four equations for the four unknowns $\mu_{i\uparrow}$, $\mu_{i\downarrow}$, η_i, and x_i:

$$g^{2\eta_i} = 1 + x_i \langle \hat{n}_{i\uparrow} \rangle_0 \langle \hat{n}_{i\downarrow} \rangle_0 , \tag{11a}$$

$$g^{2\eta_i}(g^{-2\mu_{i\sigma}} - 1) = -x_i \langle \hat{n}_{i-\sigma} \rangle_0, \quad \sigma = \uparrow, \downarrow , \tag{11b}$$

$$g^{2\eta_i}(g^{2-2\mu_{i\uparrow}-2\mu_{i\downarrow}} - g^{-2\mu_{i\uparrow}} - g^{-2\mu_{i\downarrow}} + 1) = x_i . \tag{11c}$$

Comparing Eqs. (4) and (10b) we see that Gutzwiller correlated wave functions can in general be written as

$$|\Psi_g\rangle = g^{\hat{K}}|\Phi_0\rangle = \left[\prod_i \hat{B}_i\right]|\Phi_0\rangle , \tag{12}$$

where $\hat{K} \equiv \sum_i \hat{D}_i - \mu_{i\uparrow}\hat{n}_{i\uparrow} - \mu_{i\downarrow}\hat{n}_{i\downarrow} + \eta_i$ and $\hat{B}_i = g^{\hat{K}_i} = g^{\hat{D}_i - \mu_{i\uparrow}\hat{n}_{i\uparrow} - \mu_{i\downarrow}\hat{n}_{i\downarrow} + \eta_i}$ is a Hermitian operator, with $\hat{B}_i^2 = 1 + x_i(\hat{D}_i - \hat{D}_i^{\mathrm{HF}})$ by construction. Thus, $|\Psi_0\rangle$ in (4) and $|\Phi_0\rangle$ in (12) are related by

$$|\Psi_0\rangle = g^{\hat{S}}|\Phi_0\rangle \tag{13}$$

where $\hat{S} = \hat{K} - \hat{D} \equiv \sum_i (-\mu_{i\uparrow}\hat{n}_{i\uparrow} - \mu_{i\downarrow}\hat{n}_{i\downarrow} + \eta_i)$. Note that

we have just rewritten $|\Psi_g\rangle$, i.e., we have

$$|\Psi_g\rangle = g^{\hat{D}}|\Psi_0\rangle = g^{\hat{K}}|\Phi_0\rangle \ .$$

Both forms are equivalent while the latter form is canonical for high dimensions (see below). In the original GWF $|\Psi_0\rangle$ and $|\Phi_0\rangle$ are identical (up to a trivial factor) where both are given by the Fermi sea. While for $g=1$ we always have $|\Psi_0\rangle \equiv |\Phi_0\rangle$ this is no longer true for $g<1$. However, only the correlated state $|\Psi_g\rangle$ is of any physical relevance, not $|\Psi_0\rangle$ or $|\Phi_0\rangle$. From now on, since we will work only with $|\Phi_0\rangle$, we always calculate expectation values in the uncorrelated state with $|\Phi_0\rangle$, (12), *instead of* $|\Psi_0\rangle$, (4). Such expectation values are indicated by $\langle \cdots \rangle_0$. Hence, we define

$$n_{i,0} = \langle \Phi_0|\hat{n}_{i\uparrow}|\Phi_0\rangle + \langle \Phi_0|\hat{n}_{i\downarrow}|\Phi_0\rangle = \langle \hat{n}_{i\uparrow}\rangle_0 + \langle \hat{n}_{i\downarrow}\rangle_0 \ ,$$

$$m_{i,0} = \langle \hat{n}_{i\uparrow}\rangle_0 - \langle \hat{n}_{i\downarrow}\rangle_0 \ ,$$

and

$$\bar{d}_{i,0} = \langle \hat{n}_{i\uparrow}\rangle_0 \langle \hat{n}_{i\downarrow}\rangle_0 \ .$$

With these definitions Eqs. (11a)–(11c) are easy to solve. The result is

$$x_i = \frac{1}{2(1-g^2)\bar{d}_{i,0}(1-n_{i,0}+\bar{d}_{i,0})} \times(-1+(1-g^2)(n_{i0}-2\bar{d}_{i,0}) + \{1+(g^2-1)[n_{i,0}(2-n_{i,0})+g^2 m_{i,0}^2]\}^{1/2}) \ . \quad (14a)$$

Furthermore,

$$g^{2\eta_i} = 1 + x_i \bar{d}_{i,0} \ , \quad (14b)$$

$$g^{-2\mu_{i\sigma}} = 1 - \frac{x_i \langle \hat{n}_{i-\sigma}\rangle_0}{1+x_i\bar{d}_{i,0}} \ . \quad (14c)$$

Equations (14a)–(14c) express the quantities $\mu_{i\uparrow}$, $\mu_{i\downarrow}$, η_i, and the requested expansion parameter x_i through the variational parameter g and the on-site particle densities in $|\Phi_0\rangle$. Note that we only rearranged the correlator and never had to specify $|\Phi_0\rangle$. Hence, the formalism is completely general.

C. Evaluation of $P_\sigma(\mathbf{i},\mathbf{j})$ and $\bar{d}_i$

We will now calculate the expectation values defined in Sec. II A. This is worked out explicitly for $P_\sigma(\mathbf{i},\mathbf{j})$, (5a). The results for all other quantities can be derived in a similar way and are just quoted at the end of this subsection.

For $\mathbf{i}\neq\mathbf{j}$ we have to calculate

$$P_\sigma(\mathbf{i},\mathbf{j}) = \langle \Psi_g|\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}|\Psi_g\rangle / \langle \Psi_g|\Psi_g\rangle \ .$$

In the numerator we have

$$\langle \Psi_g|\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}|\Psi_g\rangle = \left\langle (\hat{B}_i\hat{c}^\dagger_{i\sigma}\hat{B}_i)(\hat{B}_j\hat{c}_{j\sigma}\hat{B}_j)\prod_{f\neq i,j}[1+x_f(\hat{D}_f-\hat{D}^{HF}_f)]\right\rangle_0 \ , \quad (15)$$

where we used (12). Now,

$$\hat{B}_i\hat{c}^\dagger_{i\sigma}\hat{B}_i = \hat{c}^\dagger_{i\sigma}\sqrt{q_{i\sigma}}[1+x_i\alpha_{i\sigma}(\hat{n}_{i-\sigma}-\langle \hat{n}_{i-\sigma}\rangle_0)] \ , \quad (16a)$$

where we defined

$$\sqrt{q_{i\sigma}} \equiv g^{2\eta_i} g^{-\mu_{i\sigma}}[1+\langle \hat{n}_{i-\sigma}\rangle_0 (g^{1-2\mu_{i-\sigma}}-1)] \ , \quad (16b)$$

$$\alpha_{i\sigma} \equiv \frac{g^{1-2\mu_{i-\sigma}}-1}{x_i[1+\langle \hat{n}_{i-\sigma}\rangle_0(g^{1-2\mu_{i-\sigma}}-1)]} \ , \quad (16c)$$

with x_i given by Eq. (14a). In the case of the GWF $q_{i\sigma}$ is independent of i and σ and gives the discontinuity at the Fermi surface (see below). It is convenient to introduce $\sqrt{q_{i\sigma}}$ here. We arranged the terms in Eq. (16a) in such a way that there will be no Hartree bubble at site i after the application of Wick's theorem. We insert (16a)–(16c) into (15) and obtain

$$\langle \Psi_g|\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}|\Psi_g\rangle = \sqrt{q_{i\sigma}}\sqrt{q_{j\sigma}}\left[\langle \hat{O}_{i,j,\sigma}\rangle_0 + \sum_{m=1}^{L}\frac{1}{m!}\sum_{\substack{g_1\cdots g_m \\ (\neq i,j)}}{}' x_{g_1}\cdots x_{g_m}\langle \hat{O}_{i,j,\sigma}(\hat{D}_{g_1}-\hat{D}^{HF}_{g_1})\cdots(\hat{D}_{g_m}-\hat{D}^{HF}_{g_m})\rangle_0\right] \ , \quad (17a)$$

where

$$\hat{O}_{i,j,\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}[1+x_i\alpha_{i\sigma}(\hat{n}_{i-\sigma}-\langle \hat{n}_{i-\sigma}\rangle_0)][1+x_j\alpha_{j\sigma}(\hat{n}_{j-\sigma}-\langle \hat{n}_{j-\sigma}\rangle_0)] \ . \quad (17b)$$

Note that the prime on the lattice sum indicates that all lattice sites are *different*. We proceed as in Ref. 6. We apply Wick's theorem and a typical mth-order term reads

$$\sum_{\substack{g_1\cdots g_m \\ (\neq i,j)}}{}' \langle \hat{O}_{i,j,\sigma}(\hat{D}_{g_1}-\hat{D}^{HF}_{g_1})\cdots(\hat{D}_{g_m}-\hat{D}^{HF}_{g_m})\rangle_0 \quad (18a)$$

$$= \sum_{\substack{g_1\cdots g_m \\ (\neq i,j)}}{}' \{\hat{O}_{i,j,\sigma}(D_{g_1}-D^{HF}_{g_1})\cdots(D_{g_m}-D^{HF}_{g_m})\}_0 \ , \quad (18b)$$

where $\{\cdots\}_0$ denotes the sum over all possible pairs of contractions. Because all lattices sites are different when

Wick's theorem is applied, one can *define* the contractions as[6]

$$\{c^{\dagger}_{i\sigma}c_{j\sigma}\}_0 \equiv \langle \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle_0 , \tag{19a}$$

$$\{c_{j\sigma}c^{\dagger}_{i\sigma}\}_0 \equiv -\langle \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle_0 , \tag{19b}$$

where the usual δ_{ij} terms are *absent*. Given these contractions we can write Eq. (18b) as a sum over the products of two determinants.[6] For example, the first term in $O_{i,j,\sigma}$ can be written as

$$\sum_{\substack{\mathbf{g}_1\cdots\mathbf{g}_m \\ (\neq \mathbf{i},\mathbf{j})}}{}' \{c^{\dagger}_{i\sigma}c_{j\sigma}(D_{\mathbf{g}_1}-D^{\mathrm{HF}}_{\mathbf{g}_1})\cdots(D_{\mathbf{g}_m}-D^{\mathrm{HF}}_{\mathbf{g}_m})\}_0 = \sum_{\substack{\mathbf{g}_1\cdots\mathbf{g}_m \\ (\neq \mathbf{i},\mathbf{j})}}{}' \begin{vmatrix} P^0_{ij} & P^0_{i1} & \cdots & P^0_{im} \\ P^0_{1j} & 0 & \cdots & P^0_{1m} \\ \vdots & \vdots & & \vdots \\ P^0_{mj} & P^0_{m1} & \cdots & 0 \end{vmatrix}_{\sigma} \times \begin{vmatrix} 0 & P^0_{12} & \cdots & P^0_{1m} \\ P^0_{21} & 0 & \cdots & P^0_{2m} \\ \vdots & \vdots & & \vdots \\ P^0_{m1} & P^0_{m2} & \cdots & 0 \end{vmatrix}_{-\sigma} . \tag{20}$$

The diagonal elements in the determinants vanish at every inner vertex $\mathbf{g}_1\cdots\mathbf{g}_m$ because we subtracted $\hat{D}^{\mathrm{HF}}_{\mathbf{g}_1}$, etc., in the x_i expansion.

The elimination of the diagonal elements is the crucial step in our formalism and represents the essential difference to the method of MV:[13] we can substitute $P^0_{\sigma}(l,\mathbf{m})$ by $\tilde{P}^0_{\sigma}(l,\mathbf{m})$ defined by

$$\tilde{P}^0_{\sigma}(l,\mathbf{m}) = P^0_{\sigma}(l,\mathbf{m}) - \delta_{l,\mathbf{m}}P^0_{\sigma}(l,l) = \langle \hat{c}^{\dagger}_{l\sigma}\hat{c}_{\mathbf{m}\sigma}\rangle_0 - \delta_{l,\mathbf{m}}\langle \hat{c}^{\dagger}_{l\sigma}\hat{c}_{l\sigma}\rangle_0 . \tag{21}$$

Especially, $\tilde{P}^0_{\sigma}(l,l)=0$. In this step we do not create new contributions because the diagonal elements are already zero, and since all lattice sites are different (including $\mathbf{i}\neq\mathbf{j}$). *Now* we can release the restriction on the lattice sum (the determinants vanish when two rows or columns are set equal). The linked cluster theorem then applies[24] so that the denominator $\langle \Psi_g|\Psi_g\rangle$ cancels the disconnected graphs in (18b). Hence, we obtain the same graphs as MV but with lines joining the lattice points $\mathbf{i}$ and $\mathbf{j}$ interpreted as $\tilde{P}^0_{\sigma}(\mathbf{i},\mathbf{j})$, and inner vertices $\mathbf{i}$ interpreted as x_i.

The final result for the one-particle density matrix for $\mathbf{i}\neq\mathbf{j}$ is

$$P_{\sigma}(\mathbf{i},\mathbf{j}) = \sqrt{q_{i\sigma}}\sqrt{q_{j\sigma}}\{O_{i,j,\sigma}\tilde{\mathcal{D}}\}^c_0 , \tag{22}$$

where $\{\cdots\}^c_0$ denotes all connected graphs and

$$\tilde{\mathcal{D}} = 1 + \sum_{m=1}^{\infty}\frac{1}{m!}\sum_{\mathbf{g}_1\cdots\mathbf{g}_m} x_{\mathbf{g}_1}\cdots x_{\mathbf{g}_m}(D_{\mathbf{g}_1}-D^{\mathrm{HF}}_{\mathbf{g}_1})\cdots(D_{\mathbf{g}_m}-D^{\mathrm{HF}}_{\mathbf{g}_m}) . \tag{23}$$

The calculation of $P_{\sigma}(\mathbf{i},\mathbf{i}) = \langle \hat{n}_{i\sigma}\rangle$ proceeds along the same lines. One finds

$$\begin{aligned}\langle \hat{n}_{i\sigma}\rangle = {} & \langle \hat{n}_{i\sigma}\rangle_0 + \{(n_{i\sigma}-\langle \hat{n}_{i\sigma}\rangle_0)\tilde{\mathcal{D}}\}^c_0 + x_i(1-2\langle \hat{n}_{i\sigma}\rangle_0)\{(D_i-D^{\mathrm{HF}}_i)\tilde{\mathcal{D}}\}^c_0 \\ & + x_i(1-\langle \hat{n}_{i\sigma}\rangle_0)\langle \hat{n}_{i\sigma}\rangle_0\{(n_{i-\sigma}-\langle \hat{n}_{i-\sigma}\rangle_0)\tilde{\mathcal{D}}\}^c_0 .\end{aligned} \tag{24}$$

Using the same procedure we find for the mean double occupancy $\bar{d}_i$

$$\bar{d}_i = [1+x_i(1-n_{i,0}+\bar{d}_{i,0})]\left[\bar{d}_{i,0} + \sum_{\sigma}[\langle \hat{n}_{i\sigma}\rangle_0\{(n_{i-\sigma}-\langle \hat{n}_{i-\sigma}\rangle_0)\tilde{\mathcal{D}}\}^c_0 + \tfrac{1}{2}(1-x_i\bar{d}_{i,0})\{(D_i-D^{\mathrm{HF}}_i)\tilde{\mathcal{D}}\}^c_0]\right] . \tag{25}$$

To see the great advantage of the formalism we consider the self-energy $\tilde{S}_{\sigma}(\mathbf{g},\mathbf{h})$ defined as

$$\tilde{S}_{\sigma}(\mathbf{g},\mathbf{h}) = -x_{\mathbf{g}}\delta_{\mathbf{g},\mathbf{h}}\{(n_{\mathbf{g}-\sigma}-\langle \hat{n}_{\mathbf{g}-\sigma}\rangle_0)\tilde{\mathcal{D}}\}^c_0 + x_{\mathbf{g}}x_{\mathbf{h}}\{c^{\dagger}_{\mathbf{g}\sigma}c_{\mathbf{h}\sigma}(n_{\mathbf{g}-\sigma}-\langle \hat{n}_{\mathbf{g}-\sigma}\rangle_0)(n_{\mathbf{h}-\sigma}-\langle \hat{n}_{\mathbf{h}-\sigma}\rangle_0)\tilde{\mathcal{D}}\}^c_0 , \tag{26}$$

Using the fact that $\{(n_{i\sigma}-\langle \hat{n}_{i\sigma}\rangle_0)\tilde{\mathcal{D}}\}^c_0 = -(1/x_i)\tilde{S}_{-\sigma}(\mathbf{i},\mathbf{i})$ and $\{(D_i-D^{\mathrm{HF}}_i)\tilde{\mathcal{D}}\}^c_0 = -(1/x_i)\sum_{\mathbf{f}}\tilde{S}_{\sigma}(\mathbf{i},\mathbf{f})\tilde{P}^0_{\sigma}(\mathbf{f},\mathbf{i})$ ($\sigma=\uparrow,\downarrow$) one can write the one-particle density matrix ($\mathbf{i}\neq\mathbf{j}$), the local density, and the mean double occupancy as

$$P_{\sigma}(\mathbf{i},\mathbf{j}) = \sqrt{q_{i\sigma}}\sqrt{q_{j\sigma}}\left[\tilde{P}^0_{\sigma}(\mathbf{i},\mathbf{j}) + \sum_{\mathbf{g},\mathbf{h}}[\tilde{P}^0_{\sigma}(\mathbf{i},\mathbf{g})-\delta_{i,\mathbf{g}}\alpha_{i\sigma}]\tilde{S}_{\sigma}(\mathbf{g},\mathbf{h})[\tilde{P}^0_{\sigma}(\mathbf{h},\mathbf{j})-\delta_{\mathbf{h},j}\alpha_{j\sigma}]\right] , \tag{27}$$

$$\langle \hat{n}_{i\sigma}\rangle = \langle \hat{n}_{i\sigma}\rangle_0 - \frac{1}{x_i}\tilde{S}_{-\sigma}(\mathbf{i},\mathbf{i}) - (1-\langle \hat{n}_{i\sigma}\rangle_0)\langle \hat{n}_{i\sigma}\rangle_0\tilde{S}_{\sigma}(\mathbf{i},\mathbf{i}) - (1-2\langle \hat{n}_{i\sigma}\rangle_0)\sum_{\mathbf{f}}\tilde{S}_{\sigma}(\mathbf{i},\mathbf{f})\tilde{P}^0_{\sigma}(\mathbf{f},\mathbf{i}) , \tag{28}$$

$$\bar{d}_i = [1+x_i(1-n_{i,0}+\bar{d}_{i,0})]\left[\bar{d}_{i,0} - \frac{1}{x_i}\sum_{\sigma}\left[\langle \hat{n}_{i\sigma}\rangle_0\tilde{S}_{\sigma}(\mathbf{i},\mathbf{i}) + \tfrac{1}{2}(1-x_i\bar{d}_{i,0})\sum_{\mathbf{f}}\tilde{S}_{\sigma}(\mathbf{i},\mathbf{f})\tilde{P}^0_{\sigma}(\mathbf{f},\mathbf{i})\right]\right] . \tag{29}$$

On a d-dimensional hypercubic lattice we have for $d \gg 1$ (Refs. 13 and 14) $P_\sigma^0(\mathbf{i},\mathbf{j}) \simeq O((\sqrt{1/d}\,)^\nu)$, where

$$\nu = |\mathbf{i}-\mathbf{j}| = \sum_{l=1}^{d} |i_l - j_l|$$

is the so-called "New York" metric. It counts the number of nearest-neighbor steps from $\mathbf{i}$ to $\mathbf{j}$ on a d-dimensional hypercubic lattice. Since there are always three separate paths from $\mathbf{g}$ to $\mathbf{h}$ in $\tilde{S}_\sigma(\mathbf{g},\mathbf{h})$ the self-energy *vanishes* completely in infinite dimensions, i.e.,

$$\tilde{S}_\sigma(\mathbf{g},\mathbf{h}) \equiv 0 \quad \text{in } d=\infty \ . \tag{30}$$

This implies that in $d=\infty$ we do not have to calculate *any* graph to obtain the simple, exact result

$$P_\sigma(\mathbf{i},\mathbf{j}) = \sqrt{q_{\mathbf{i}\sigma}}\sqrt{q_{\mathbf{j}\sigma}}\,\tilde{P}_\sigma^0(\mathbf{i},\mathbf{j}) \quad (\mathbf{i}\neq\mathbf{j}) \ . \tag{31}$$

Equation (31) shows that the hopping amplitude from $\mathbf{i}$ to $\mathbf{j}$ to simply renormalized by two site-dependent factors $\sqrt{q_{\mathbf{i}\sigma}}\sqrt{q_{\mathbf{j}\sigma}}$.

Similarly, the expression (28) reduces in $d=\infty$ to

$$\langle \hat{n}_{\mathbf{i}\sigma} \rangle = \langle \hat{n}_{\mathbf{i}\sigma} \rangle_0 \tag{32}$$

independent of g. This shows explicitly that all the effects of the Gutzwiller correlator $g^{\hat{D}}$ on the local densities $\langle \hat{n}_{\mathbf{i}\sigma} \rangle$ can be absorbed in the local "fugacities" expressed as $g^{-\mu_{\mathbf{i}\uparrow}}$, $g^{-\mu_{\mathbf{i}\downarrow}}$, and $g^{\eta_{\mathbf{i}}}$ in (12). It is also possible to choose the local "fugacities" in a way that Eq. (32) holds in any dimension but it offers no calculational advantages. Equation (32) does not hold for the local densities in $|\Psi_0\rangle$. This was first noted explicitly by Vulović and Abrahams in their work on the periodic Anderson model.[18]

Lastly, the double occupancy is given in $d=\infty$ by

$$\bar{d}_{\mathbf{i}} = [1 + x_{\mathbf{i}}(1 - n_{\mathbf{i},0} + \bar{d}_{\mathbf{i},0})]\bar{d}_{\mathbf{i},0} \ . \tag{33}$$

D. Evaluation of correlation functions

We now analyze the CF's defined in Eqs. (7a)–(7e). These quantities were calculated exactly for the GWF in $d=1$ in Ref. 7 and in $d=\infty$ in Ref. 14. We are now able to go beyond the simple GWF and derive the exact formulas for arbitrary Gutzwiller projected wave functions in the limit of high dimensions.

For the CF's $C^{XY}(\mathbf{j})$ we do not consider the case $\mathbf{j}=0$ because in this case we can express them by sums over $\langle \hat{n}_{\mathbf{i}\sigma} \rangle_0$ and $\bar{d}_{\mathbf{i}}$. In complete analogy to Refs. 7 and 14 we introduce the functions ($\mathbf{g}\neq\mathbf{h}$)

$$\tilde{Y}_\sigma^{(1)}(\mathbf{g},\mathbf{h}) = \{(n_{\mathbf{g}\sigma} - \langle \hat{n}_{\mathbf{g}\sigma} \rangle_0)(n_{\mathbf{h}\sigma} - \langle \hat{n}_{\mathbf{h}\sigma} \rangle_0)\tilde{\mathcal{D}}\}_0^{\mathrm{FC}} \ , \tag{34a}$$

$$\tilde{Y}_\sigma^{(2)}(\mathbf{g},\mathbf{h}) = x_{\mathbf{h}}\{(n_{\mathbf{g}\sigma} - \langle \hat{n}_{\mathbf{g}\sigma} \rangle_0)(D_{\mathbf{h}} - D_{\mathbf{h}}^{\mathrm{HF}})\tilde{\mathcal{D}}\}_0^{\mathrm{FC}} \ , \tag{34b}$$

$$\tilde{Y}^{(3)}(\mathbf{g},\mathbf{h}) = x_{\mathbf{g}}x_{\mathbf{h}}\{(D_{\mathbf{g}} - D_{\mathbf{g}}^{\mathrm{HF}})(D_{\mathbf{h}} - D_{\mathbf{h}}^{\mathrm{HF}})\tilde{\mathcal{D}}\}_0^{\mathrm{FC}} \ , \tag{34c}$$

$$\tilde{Y}_\sigma^{(4)}(\mathbf{g},\mathbf{h}) = \{(n_{\mathbf{g}\sigma} - \langle \hat{n}_{\mathbf{g}\sigma} \rangle_0)(n_{\mathbf{h}-\sigma} - \langle \hat{n}_{\mathbf{h}-\sigma} \rangle_0)\tilde{\mathcal{D}}\}_0^{\mathrm{FC}} \ , \tag{34d}$$

$$\tilde{Y}^{(5)}(\mathbf{g},\mathbf{h}) = -\{c_{\mathbf{g}\uparrow}^\dagger c_{\mathbf{h}\uparrow} c_{\mathbf{h}\downarrow}^\dagger c_{\mathbf{g}\downarrow}\tilde{\mathcal{D}}\}_0^{\mathrm{FC}} \ . \tag{34e}$$

$\{\cdots\}_0^{\mathrm{FC}}$ means to take the sum over all graphs which arise from Wick's theorem where the external points $\mathbf{g}$ and $\mathbf{h}$ are connected via a path of continuous fermion lines (fully connected graphs, see Refs. 7 and 14). The graphs contributing to $\tilde{Y}_\sigma^{(1)}, \ldots, \tilde{Y}_\sigma^{(4)}$ up to third order in $x_{\mathbf{i}}$ can be found in Ref. 7, the graphs contributing to $\tilde{Y}^{(5)}$ can be derived from those of $\tilde{Y}_\sigma^{(1)}$ by changing a σ line running from $\mathbf{g}$ to $\mathbf{h}$ to a $(-\sigma)$ line while ensuring that there are two σ and two $(-\sigma)$ lines at each vertex.

Applying the formalism described in Secs. II B and II C we obtain the following results:

$$C^{S^zS^z}(\mathbf{j}) = \frac{1}{4}\frac{1}{L}\sum_{\mathbf{i}\sigma}[1 - x_{\mathbf{i}}(1 - \langle \hat{n}_{\mathbf{i}-\sigma} \rangle_0)\langle \hat{n}_{\mathbf{i}-\sigma} \rangle_0]\Big[\Big[\sum_{\sigma'}[1 - x_{\mathbf{i}+\mathbf{j}}(1 - \langle \hat{n}_{\mathbf{i}+\mathbf{j},-\sigma'} \rangle_0)\langle \hat{n}_{\mathbf{i}+\mathbf{j},-\sigma'} \rangle_0](\sigma\sigma')\tilde{Y}_{\sigma\sigma'}(\mathbf{i},\mathbf{i}+\mathbf{j})\Big] - 4\sigma m_{\mathbf{i}+\mathbf{j},0}\tilde{Y}_\sigma^{(2)}(\mathbf{i},\mathbf{i}+\mathbf{j})\Big] + \frac{1}{L}\sum_{\mathbf{i}} m_{\mathbf{i},0}m_{\mathbf{i}+\mathbf{j},0}\tilde{Y}^{(3)}(\mathbf{i},\mathbf{i}+\mathbf{j}) \ , \tag{35a}$$

$$C^{\mathrm{NN}}(\mathbf{j}) = \frac{1}{L}\sum_{\mathbf{i}\sigma}[1 + x_{\mathbf{i}}(1 - \langle \hat{n}_{\mathbf{i}-\sigma} \rangle_0)\langle \hat{n}_{\mathbf{i}-\sigma} \rangle_0]\Big[\Big[\sum_{\sigma'}[1 + x_{\mathbf{i}+\mathbf{j}}(1 - \langle \hat{n}_{\mathbf{i}+\mathbf{j},-\sigma'} \rangle_0)\langle \hat{n}_{\mathbf{i}+\mathbf{j},-\sigma'} \rangle_0]Y_{\sigma\sigma'}(\mathbf{i},\mathbf{i}+\mathbf{j})\Big] + 4(1 - n_{\mathbf{i}+\mathbf{j},0})\tilde{Y}_\sigma^{(2)}(\mathbf{i},\mathbf{i}+\mathbf{j})\Big] + 4\frac{1}{L}\sum_{\mathbf{i}}(1 - n_{\mathbf{i}},0)(1 - n_{\mathbf{i}+\mathbf{j}},0)\tilde{Y}^{(3)}(\mathbf{i},\mathbf{i}+\mathbf{j}) \ , \tag{35b}$$

$$C^{S^+S^-}(\mathbf{j}) = \frac{1}{L}\sum_{\mathbf{i}}\left[\frac{x_{\mathbf{i}}x_{\mathbf{i}+\mathbf{j}}}{(g^2-1)^2}\right]^{1/2}\tilde{Y}^{(5)}(\mathbf{i},\mathbf{i}+\mathbf{j}) \ , \tag{35c}$$

where

$$\tilde{Y}_{\sigma\sigma'} = \begin{cases} \tilde{Y}_\sigma^{(1)} & \text{for } \sigma' = \sigma \ , \\ \tilde{Y}_\sigma^{(4)} & \text{for } \sigma' = -\sigma \ . \end{cases} \tag{35d}$$

The expressions for correlation functions like C^{ND}, C^{DD}, etc., can be calculated analogously.

In $d=\infty$ considerable simplifications occur. Firstly, both in $\tilde{Y}_\sigma^{(2)}(\mathbf{g},\mathbf{h})$ and in $\tilde{Y}^{(3)}(\mathbf{g},\mathbf{h})$ there are always parts in the graphs where two vertices are connected by three or more separate paths. In $d=\infty$ we therefore have

$$\tilde{Y}_\sigma^{(2)}(\mathbf{g},\mathbf{h}) \equiv 0 \ , \tag{36a}$$

$$\tilde{Y}^{(3)}(\mathbf{g},\mathbf{h}) \equiv 0 \ . \tag{36b}$$

Secondly, in $d=\infty$ lines are given by the *noninteracting*

"propagator" $\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{j})$. Usually one has to work with dressed propagators, defined as

$$\bar{P}_{\sigma}(\mathbf{i},\mathbf{j})=\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{j})+\sum_{\mathbf{g},\mathbf{h}}\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{g})\tilde{S}_{\sigma}(\mathbf{g},\mathbf{h})\tilde{P}^{0}_{\sigma}(\mathbf{h},\mathbf{j}) .$$

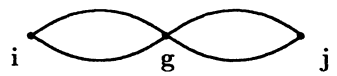
In the limit $d\rightarrow\infty$ such a renormalization does not occur [see Eq. (30)]. Thirdly, $\tilde{Y}_{\sigma\sigma'}(\mathbf{g},\mathbf{h})$ in (35d) *remains nontrivial* because it is possible to build up graphs only of RPA bubbles, i.e., of diagrams where two lines run from $\mathbf{g}$ to an internal vertex $\mathbf{l}_1$, from there to a second internal vertex $\mathbf{l}_2$ and so on up to the other external vertex $\mathbf{h}$ (internal lattice vectors are summed over). The first two graphs belonging to this series are shown in Figs. 1(a) and 1(b).

Hence, all CF's remain nontrivial in the limit $d=\infty$ but are only built up of RPA bubbles with $\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{j})$ lines. It is straightforward to show that Eqs. (35a)–(35c) completely agree with the formulas in Ref. 14 in the case of the translational and spin-invariant GWF. It was also shown there that it is sufficient for the CF's at *nearest-neighbors* (NN) to consider only the first bubble diagram to calculate the leading order contribution for $d\rightarrow\infty$ which is of order $(1/d)$. In general, one has to consider contributions to $1,\ldots,\nu$ RPA bubbles for neighbors which have a distance $|\mathbf{j}|=\nu$ from the origin. Therefore, the NN CF's are easy to obtain in high dimensions, but the calculation of the behavior for large distances $\nu\rightarrow\infty$ is not easy to extract even in $d=\infty$. For the GWF the asymptotic behavior is calculated in Ref. 14.

III. EXACT EVALUATIONS IN $d=\infty$

We give general results for the variational ground-state energy of the Hubbard model (Sec. III A) and the NN CF's (Sec. III B). As an *example* we consider the general Gutzwiller correlated antiferromagnetic spin-density wave function. For this wave function we rederive the results of MV (Refs. 13 and 19) in a compact form. Furthermore we give the NN spin-spin CF's for this wave function explicitly.

(a)



(b)

FIG. 1. RPA-like bubble diagrams for the CF's in $d=\infty$; (a) first-order bubble, (b) second-order bubble.

A. Ground-state energy

Using (33) for the double occupancy we have

$$x_{\mathrm{i}}=(\bar{d}_{\mathrm{i}}-\bar{d}_{\mathrm{i},0})/[\bar{d}_{\mathrm{i},0}(1-n_{\mathrm{i},0}+\bar{d}_{\mathrm{i},0})] .$$

Together with (14a) we find

$$g^2=\frac{\bar{d}_{\mathrm{i}}(1-n_{\mathrm{i},0}+\bar{d}_{\mathrm{i}})}{(\langle\hat{n}_{\mathrm{i}\uparrow}\rangle_0-\bar{d}_{\mathrm{i}})(\langle\hat{n}_{\mathrm{i}\downarrow}\rangle_0-\bar{d}_{\mathrm{i}})} . \tag{37}$$

This expression has the form from a law of mass action.[3] It is typical for a result obtained within the "quasichemical approximation" in the theory of mixtures.[25] Instead of a Boltzmann factor we have g^2 regulating the equilibrium between the local concentration of doubly occupied sites $(\bar{d}_{\mathrm{i}})$ and empty sites $(1-n_{\mathrm{i},0}+\bar{d}_{\mathrm{i}})$ relative to that of the singly occupied sites $[(\langle\hat{n}_{\mathrm{i}\uparrow}\rangle_0-\bar{d}_{\mathrm{i}})(\langle\hat{n}_{\mathrm{i}\downarrow}\rangle_0-\bar{d}_{\mathrm{i}})]$. For the GWF we have no site dependence ($\bar{d}_{\mathrm{i}}=\bar{d}$, etc.). In this special case Eq. (37) was proven to be exact in $d=\infty$ by MV.[13] Now we see that it indeed holds *locally* when we deal with a general wave function $|\Psi_g\rangle$ of the form in Eq. (12).

Equation (37) enables us to express all expectation values by the physical quantity $\bar{d}_{\mathrm{i}}$, the double occupancy in the interacting system. We have

$$q_{\mathrm{i}\sigma}=\frac{1}{\langle\hat{n}_{\mathrm{i}\sigma}\rangle_0(1-\langle\hat{n}_{\mathrm{i}\sigma}\rangle_0)}\times\left[\sqrt{(1-n_{\mathrm{i},0}+\bar{d}_{\mathrm{i}})(\langle\hat{n}_{\mathrm{i}\sigma}\rangle_0-\bar{d}_{\mathrm{i}})}+\sqrt{\bar{d}_{\mathrm{i}}(\langle\hat{n}_{\mathrm{i}-\sigma}\rangle_0-\bar{d}_{\mathrm{i}})}\right]^2 \tag{38}$$

and the expectation value of the Hubbard Hamiltonian reads

$$\langle\hat{H}\rangle=\sum_{\langle\mathrm{ij}\rangle}\sqrt{q_{\mathrm{i}\sigma}}\sqrt{q_{\mathrm{j}\sigma}}P^{0}_{\sigma}(\mathbf{i},\mathbf{j})+U\sum_{\mathrm{i}}\bar{d}_{\mathrm{i}} . \tag{39}$$

This form was first obtained by Kotliar and Ruckenstein[26] from a slave-boson approach to the Hubbard model. In the translationally invariant case $q_{\mathrm{i}\sigma}=q_{\sigma}$ is the renormalization factor for the kinetic energy in the GWF (Ref. 3) proven to be exact in $d=\infty$ by MV. For this wave function the correct q factors can be derived by counting possible hopping processes (see Ref. 5 for details). As in the case of the double occupancy $\bar{d}$ we can now generalize the results of this concept to arbitrary $|\Psi_g\rangle$ in (12) by introducing *local* renormalization factors $\sqrt{q_{\mathrm{i}\sigma}}$.

B. Nearest-neighbor correlation functions

We now give the exact results for the NN CF's. As outlined above, for the nearest-neighbor CF's ($\mathbf{j}\equiv\tau$) we only need the first bubble diagram in Fig. 1(a) to calculate this quantity up to $O(1/d)$. Hence, we find that

$$\tilde{Y}_{\sigma\sigma'}(\mathbf{i},\mathbf{i}+\tau)=-\delta_{\sigma\sigma'}[\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{i}+\tau)]^2$$

and

$$\tilde{Y}^{(5)}(\mathbf{i},\mathbf{i}+\tau)=-[\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{i}+\tau)][\tilde{P}^{0}_{-\sigma}(\mathbf{i},\mathbf{i}+\tau)] .$$

This shows that NN correlations can be calculated for *general* $|\Phi_0\rangle$ without much effort in high dimensions. This is important because these quantities determine the energy of Hamiltonians with NN interactions, e.g., the Heisenberg or the *t-J* model[20–22] proposed for high-T_c superconductivity. Defining

$$a_{\mathbf{i},\sigma}=(\bar{d}_{\mathbf{i}}-\bar{d}_{\mathbf{i},0})/[\langle\hat{n}_{\mathbf{i}\sigma}\rangle_0(1-\langle\hat{n}_{\mathbf{i}\sigma}\rangle_0)]$$

and

$$b_{\mathbf{i},\sigma}=(\langle\hat{n}_{\mathbf{i}\sigma}\rangle_0-\bar{d}_{\mathbf{i}})/(\langle\hat{n}_{\mathbf{i}\sigma}\rangle_0-\bar{d}_{\mathbf{i},0})$$

we find explicitly

$$C^{S^zS^z}(\tau)=-\frac{1}{4}\frac{1}{L}\sum_{\mathbf{i}\sigma}(1-a_{\mathbf{i},\sigma})(1-a_{\mathbf{i}+\tau,\sigma})\times[\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{i}+\tau)]^2 , \tag{40a}$$

$$C^{\mathrm{NN}}(\tau)=\frac{1}{L}\sum_{\mathbf{i}\sigma}(1+a_{\mathbf{i},\sigma})(1+a_{\mathbf{i}+\tau,\sigma})\times[\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{i}+\tau)]^2 , \tag{40b}$$

$$C^{S^+S^-}(\tau)=\frac{1}{L}\sum_{\mathbf{i}}\sqrt{b_{\mathbf{i},\sigma}b_{\mathbf{i},-\sigma}b_{\mathbf{i}+\tau,\sigma}b_{\mathbf{i}+\tau,-\sigma}}\times[\tilde{P}^{0}_{\sigma}(\mathbf{i},\mathbf{i}+\tau)][\tilde{P}^{0}_{-\sigma}(\mathbf{i},\mathbf{i}+\tau)] . \tag{40c}$$

In the case of the paramagnetic GWF we recover all results derived in Refs. 14 and 19 where it was shown that

$$C^{XY}(\tau,g,n)=g_{XY}C^{XY}(\tau,g=1,n) \tag{41}$$

with, e.g.,

$$g_{S^zS^z}=g_{S^+S^-}=[(n-2\bar{d})/(n-2\bar{d}_0)]^2$$

and

$$g_{\mathrm{NN}}=[(n-n^2+2\bar{d})/(n-n^2+2\bar{d}_0)]^2 .$$

C. Results for a general Gutzwiller correlated spin-density wave function

As an example we now analyze a general Gutzwiller correlated spin-density wave function. For less than a half-filled band ($n\leq 1$) it is given by

$$|\Phi_0\rangle=\prod_{\sigma}\prod_{\varepsilon(\mathbf{k})\leq\varepsilon_F}(\tilde{u}_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\sigma}+\sigma\tilde{v}_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma})|\mathrm{vac}\rangle . \tag{42a}$$

Here $\mathbf{Q}=(\pi,\pi,\ldots,\pi)$ is half of a reciprocal-lattice vector. The infinitely many variational parameters $\tilde{u}_{\mathbf{k}},\tilde{v}_{\mathbf{k}}$ can be written as

$$\tilde{u}_{\mathbf{k}}=\{\tfrac{1}{2}[1+(1-\tilde{\theta}^2_{\mathbf{k}})^{1/2}]\}^{1/2} ,$$
$$\tilde{v}_{\mathbf{k}}=-\mathrm{sgn}[\varepsilon(\mathbf{k})]\{\tfrac{1}{2}[1-(1-\tilde{\theta}^2_{\mathbf{k}})^{1/2}]\}^{1/2} , \tag{42b}$$

with $\tilde{\theta}_{\mathbf{k}+\mathbf{Q}}=\tilde{\theta}_{\mathbf{k}}$. The sublattice magnetization is given by

$$m=m_{\mathbf{i}}=|\langle\hat{n}_{\mathbf{i}\uparrow}\rangle-\langle\hat{n}_{\mathbf{i}\downarrow}\rangle| ,$$

where, in $d=\infty$, we have

$$m=m_0=(2/L)\sum_{\varepsilon(\mathbf{k})\leq\varepsilon_F}\tilde{\theta}_{\mathbf{k}}$$

and $n_{\mathbf{i},0}=n_0=n$. From (37) we have $\bar{d}_{\mathbf{i}}=\bar{d}$ and $q=\sqrt{q_{i\in A,\sigma}}\sqrt{q_{i\in B,\sigma}}$ is the σ independent renormalization factor for hopping from an A to a B site. The minimization problem for the Hubbard model (1) is then given by

$$\langle\hat{H}\rangle=2q(m,\bar{d})\sum_{\varepsilon(\mathbf{k})\leq\varepsilon_F}\varepsilon(\mathbf{k})(1-\tilde{\theta}^2_{\mathbf{k}})^{1/2}+U\bar{d} \tag{43a}$$

with

$$q(m,\bar{d})=\frac{2(1-n+2\bar{d})[(n-2\bar{d})^2-m^2]^{1/2}+4(n-2\bar{d})\sqrt{\bar{d}(1-n+\bar{d})}}{\{(n^2-m^2)[(2-n)^2-m^2]\}^{1/2}} , \tag{43b}$$

where we can use $\bar{d}$ instead of g as variational parameter. Variation with respect to $\tilde{\theta}_{\mathbf{k}}$ yields

$$\tilde{\theta}_{\mathbf{k}}=\frac{\Delta}{([\varepsilon(\mathbf{k})]^2+\Delta^2)^{1/2}} . \tag{44}$$

Equation (44) implies that we were able to reduce the infinite number of variational parameters in (42a) to just two parameters Δ and $\bar{d}$. Inserting this into Eq. (43a) we recover the result of MV (see Ref. 13 for a detailed discussion). Note that in the formulation of MV the optimum $|\Psi_g\rangle$, written as $|\Psi_g\rangle=g^{\hat{D}}|\Psi_0\rangle$, has a much more complicated form.

One can easily calculate the NN spin-spin CF for the GSDW as well. In this case we have

$$\frac{1}{L}\sum_{\mathbf{i}}\langle\hat{\mathbf{S}}_{\mathbf{i}}\cdot\hat{\mathbf{S}}_{\mathbf{i}+\tau}\rangle=-\frac{m^2}{4}+g_{S^zS^z}C^{S^zS^z}(\tau,g=1,n)+g_{S^+S^-}C^{S^+S^-}(\tau,g=1,n) , \tag{45}$$

with

$$g_{S^zS^z}=4\frac{(n-2\bar{d}-m^2)^2-(1-n)^2m^2}{(n^2-m^2)[(2-n)^2-m^2]} , \tag{46}$$

$$g_{S^+S^-}=4\frac{(n-2\bar{d})^2-m^2}{(n^2-m^2)[(2-n)^2-m^2]} , \tag{47}$$

for $n\neq m$. Due to the broken symmetry we have, in general, $g_{S^+S^-}\neq g_{S^zS^z}$. Note that these amplification factors are only defined for the CF's where the long-range-order part of the correlation is subtracted (in our example we have the term $\langle\hat{S}^z_{\mathbf{i}}\rangle\langle\hat{S}^z_{\mathbf{i}+\tau}\rangle=-m^2/4$ from the sublattice magnetization). Only for CF's as defined in Eq. (6) can there be application factors at all. This is not true for expectation values like $\langle\hat{S}^z_{\mathbf{i}}\hat{S}^z_{\mathbf{i}+\tau}\rangle$, with the obvious expectation of cases where $\langle\hat{S}^z_{\mathbf{i}}\rangle\equiv 0$. Furthermore, the term $-m^2/4$ in Eq. (45) is of order unity and has $(1/d)$ correction itself [see Eq. (28)]. Therefore, it is not a trivi-

al task to calculate the expectation value $(1/L)\sum_i \langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle$ up to order $(1/d)$. We perform this calculation in Sec. VII B.

IV. COMPARISON WITH APPROXIMATE METHODS

In this section we compare the exact results in high dimensions derived from the formalism in Sec. II with those of approximate methods. We are able to check whether the results of these approximate treatments give the correct results at least in the limit of high dimensions or not. We further comment on the validity of these methods themselves. The first techniques under investigation (Sec. IV A) are refined Gutzwiller-type approximations.[15–18,21,27–32] Secondly (Sec. IV B) we address the slave-boson approach to the Hubbard model of Kotliar and Ruckenstein (KR).[26]

A. Gutzwiller-type approximations

To calculate the variational energy for the Hubbard model, Gutzwiller[3] introduced an approximation ("Gutzwiller approximation"). The physical meaning of the GA was clarified later[5,27] but it was an open problem to generalize the GA for more complicated Gutzwiller projected VWF's. We mainly discuss two sets of generalized VWF's, firstly, variational ground states proposed for the periodic Anderson model, secondly antiferromagnetic ground states for the Hubbard model.

1. Gutzwiller-type approximations for the periodic Anderson model

To investigate ground-state properties of the periodic Anderson model a generalized Gutzwiller correlated VWF was investigated by several groups[15–18] using approximations in the spirit of the GA. Again this VWF is *translationally invariant* but the number of particles in the highly correlated f band is not a conserved quantity as in the case of the GWF. The results of these approximations[15,16,18] were shown to be correct in $d=\infty$ in Ref. 19 by a straightforward extension of the method of MV.

Recently, Oleś and Zaanen[32] analyzed the same VWF where they allowed for antiferromagnetism. It is a straightforward task to generalize the formalism in Sec. II to the present situation of hybridization between a conduction band and a highly correlated f band, because the total number of particles is still fixed.[33] As a consequence, one recovers the exact results in $d=\infty$ for the translationally invariant case.[19] Furthermore, one finds that the *results* for the ground-state energy of Oleś and Zaanen agree with ours in $d=\infty$ (Sec. II). The *wave function* is, however, substantially *different*, i.e., although they do find the exact result in $d=\infty$ their approximation does not allow them to identify the actual VWF producing these results. Making use of the formalism in Sec. II we cure this lack of consistency.

2. Gutzwiller-type approximations for the Hubbard model

To describe antiferromagnetism in terms of $|\Psi_g\rangle$ it was necessary to generalize the GA for the case of a broken translational symmetry. As first shown by MV,[13] *none* of the earlier attempts[21,27,29,31] gave the exact results in $d=\infty$ for the optimal Gutzwiller correlated spin-density wave function [see Eqs. (43a) and (43b)]. In all approximate treatments there is an *ad hoc* assumption for the structure of $\tilde{u}_k, \tilde{v}_k$ in Eq. (42a). Consequently, they did not obtain the optimal VWF and only calculated within a restricted subclass. Ogawa, Kanda, and Matsubara[27] (OKM) found an expression similar to Eq. (43a). They obtained a factor q_{OKM} with, e.g.,

$$q_{\mathrm{OKM}}(m,\bar{d}=0)=[2n(1-n)]/(2n-n^2+m^2)\ .$$

However, q_{OKM} differs from the exact q factor for all values of $m\neq 0$. Furthermore, MV (Ref. 13) showed that an expression as in Eq. (43a) cannot be obtained within the restricted subclass of VWF's analyzed by Ogawa *et al.* Hence, their approximate treatment is not systematic.

In the Gutzwiller-type "renormalized mean-field approach"[21] Zhang *et al. assume* the validity of (43a) and then derive q_{OKM} by counting arguments (see Ref. 5 for details of the counting method in the case of the GWF). Because q_{OKM} does not agree with the exact q in (43b) one cannot be sure to get the correct q factors in $d=\infty$ from the counting method in general. Besides, the validity of (43a) had to be *assumed.* The method shares the same shortcoming as mentioned above in the case of the VWF analyzed by Oleś and Zaanen:[32] even if one obtains q correctly, one cannot assign the correct VWF to this result. In fact, counting methods derive results which are valid in $d=\infty$ for $|\Psi_g\rangle$ written as $|\Psi_g\rangle=g^{\hat{K}}|\Phi_0\rangle$, Eq. (12). On the other hand, these methods suggest that they analyze $|\Psi_g\rangle=g^{\hat{D}}|\Phi_0\rangle$. Hence, the comparison of numerical data with the results of the "renormalized mean-field approach"[21] is questionable because one indeed compares *different* wave functions. We will come back to this problem in Sec. VII where we derive new VWF's which are optimized in high dimensions and can be tested numerically in low dimensions.

The approach in Ref. 21 was also applied to the evaluation of the nearest-neighbor spin-spin CF's including the possibility of antiferromagnetism. Applying the counting method Zhang *et al.* obtained

$$\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle = c \langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle_0 \ , \tag{48a}$$

$$c = \left[\frac{2n}{2n-n^2+m^2} \right]^2 , \tag{48b}$$

in the limit of localized electrons ($\bar{d}=0$). In the case of the GWF we have $m=0$ and $\langle \hat{\mathbf{S}}_i \rangle = 0$ so that Eqs. (46) and (47) and Eq. (48b) agree. Hence, the result (48a) is correct for the GWF up to order $(1/d)$. As is shown in Ref. 21 it compares very well to numerical data for the GWF.

On the other hand, Eq. (48a) cannot become exact in high dimensions in the case of $m\neq 0$. This can be seen from Eq. (45) where the left-hand side (lhs) of (48a) is given by

$$\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle = (-m^2/4) + g_{S^z S^z} C^{S^z S^z}(\tau, g=1, n) + g_{S^+ S^-} C^{S^+ S^-}(\tau, g=1, n) \ . \quad (49)$$

Thus, Eqs. (48a) and (48b) cannot be correct in high dimensions for several reasons.

(i) There are different amplification factors $g_{S^z S^z} \neq g_{S^+ S^-}$ due to the broken spin symmetry [both of them are different from c in (48b)].

(ii) There is no amplification factor for the term $(-m^2/4)$ which results from the antiferromagnetic long-range order.

(iii) The term $(-m^2/4)$ is of order unity and has a nontrivial $(1/d)$ correction. Such a correction cannot be obtained by counting, it will be calculated in Sec. VII.

To sum up, Gutzwiller-type approximations yield the exact results in $d=\infty$ for translationally invariant VWF's. However, they appear to be insufficient for more complicated, e.g., antiferromagnetic, VWF's. Furthermore, they do not allow for a systematic improvement.

B. Slave-boson method of Kotliar and Ruckenstein

Kotliar and Ruckenstein[26] (KR) treat the Hubbard model by a slave-boson approach. They replaced the slave-boson operators by their *static, local* expectation values. This treatment corresponds to a saddle-point approximation applied to a properly defined path-integral representation of the Hubbard Hamiltonian. In general, they obtain an effective Hamiltonian

$$\hat{H}_{\text{eff}} = \sum_{i,j\sigma} t_{ij} \sqrt{q_{i\sigma}} \sqrt{q_{j\sigma}} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \bar{d}_i \ . \quad (50)$$

Here we used the notation of this work [Eqs. (38) and (39)]. $\langle \hat{H}_{\text{eff}} \rangle_0$ has then to be optimized with respect to $\bar{d}_i$ and $\langle \hat{n}_{i\sigma} \rangle_0$. Hence, the static saddle-point approximation of KR for a path-integral representation of the Hubbard model yields results which we now recover from a variational treatment of this model in $d=\infty$. This has already been shown by MV for the case of the translationally invariant GWF and the case of the antiferromagnetic GSDW discussed above. We are now able to demonstrate this correspondence in general. Therefore, we can gain new insight into the slave-boson–path-integral technique of KR.

(i) We can give the explicit wave function which belongs to a certain solution of the saddle-point equations [e.g., for the antiferromagnetic case, see (42a), (42b), and (44)]. Wave functions offer a direct insight into the physics behind them.

(ii) There are no ambiguities in the method itself because all expectation values are calculated exactly in $d=\infty$. Furthermore, this opens up the possibility of a systematic improvement via a $(1/d)$ expansion.

(iii) From the variational principle in $d=\infty$ it follows that one obtains upper bounds for the ground-state energy of the Hubbard-model in this limit.

(iv) One can show that the "partition function" Z_{KR} and the "free energy" f_{KR} of KR are mathematically ill-defined quantities. Nevertheless, f_{KR} can be used to describe low-temperature properties of correlated Fermi systems. This point is discussed in more detail in Appendix A.

The KR approach has a natural extension ("fluctuations around the saddle point"), by which the boson fields are no longer treated as static, but dynamic quantities.[34–36] It is an open question of how to incorporate such dynamics into a VWF approach.

V. CALCULATION OF $(1/d)$-CORRECTIONS FOR THE GWF

In this section we calculate the mean double occupancy $\bar{d}$, the momentum distribution $\langle \hat{n}_{k\sigma} \rangle$, and the kinetic energy $\langle \hat{T} \rangle$ for the GWF in a $(1/d)$ expansion. In the first subsection we derive explicit expressions up to order $(1/d)$ for arbitrary band filling n and variational parameter g (i.e., interaction strength U in the Hubbard model). Due to particle-hole symmetry we can restrict our discussion to $n \leq 1$. In Sec. V B we calculate up to order $(1/d)^2$ for the case of the half-filled band $(n=1)$.

A. First-order correction for arbitrary band filling

In the GWF $|\Phi_0\rangle$ is given by the paramagnetic Fermi sea. Due to translational invariance we have $\langle \hat{n}_{i\sigma} \rangle = \langle \hat{n}_{i\sigma} \rangle_0 = n/2$ and

$$x_i = x = [4(G-1)]/[(G+1)n(2-n)] \ .$$

Here G is given by

$$G = [1 + n(2-n)(g^2-1)]^{1/2} \ . \quad (51)$$

The factors q and α in Eqs. (16b) and (16c) are given by

$$\sqrt{q_{i\sigma}} \equiv \sqrt{q} = \frac{1}{G+1} [\sqrt{(2-n)(G+1-n)} + \sqrt{n(G-1+n)}] \ , \quad (52a)$$

$$\alpha_{i\sigma} \equiv \alpha = -\frac{n}{2} \frac{G+1}{G-1} + \frac{1}{G-1} \left[\frac{n(G-1+n)}{q} \right]^{1/2} \ . \quad (52b)$$

In $d=\infty$ we have

$$\bar{d}(g,n,d=\infty) = \bar{d}_{\text{GA}}(g,n) = (n/2)(G+n-1)/(G+1)$$

and

$$\langle \hat{n}_{k\sigma} \rangle (g,n,d=\infty) = \langle \hat{n}_{k\sigma} \rangle_{\text{GA}}(g,n) = (n/2)(1-q) + q \langle \hat{n}_{k\sigma} \rangle_0 \ .$$

We denote the Fourier transform of the self-energy $\tilde{S}_\sigma(i,j)$ by

$$\tilde{S}_\sigma(\mathbf{k}) = (1/L) \sum_{i,j} \exp[i\mathbf{k}(\mathbf{i}-\mathbf{j})] \tilde{S}_\sigma(\mathbf{i},\mathbf{j}) \ .$$

Then we can write

$$\bar{d}(g,n) = \bar{d}_{\text{GA}}(g,n) - \frac{(G+n-1)(G+1-n)}{G(G^2-1)} \times \frac{1}{L} \sum_{\mathbf{k}} \left[\langle \hat{n}_{k\sigma} \rangle_0 - \frac{n}{2} \right] \tilde{S}_\sigma(\mathbf{k}) \ , \quad (53a)$$

$$\langle \hat{n}_{\mathbf{k}\sigma}\rangle(g,n)=\langle \hat{n}_{\mathbf{k}\sigma}\rangle_{\mathrm{GA}}(g,n) +q\left[\left[\langle \hat{n}_{\mathbf{k}\sigma}\rangle_0-\frac{n}{2}-\alpha\right]^2\tilde{S}_\sigma(\mathbf{k}) -\frac{1}{L}\sum_{\mathbf{k}}\left[\langle \hat{n}_{\mathbf{k}\sigma}\rangle_0-\frac{n}{2}-\alpha\right]^2\tilde{S}_\sigma(\mathbf{k})\right] . \tag{53b}$$

From particle conservation, Eq. (32), we obtain

$$\tilde{S}_\sigma(\mathbf{i},\mathbf{i})=\frac{2(n-1)(G-1)}{n(2-n)G}\sum_{\mathbf{f}}\tilde{P}^0_\sigma(\mathbf{i},\mathbf{f})\tilde{S}_\sigma(\mathbf{f},\mathbf{i}) . \tag{54}$$

Equation (54) shows that we only have to consider the off-diagonal part of the self-energy. In general, however, one has to calculate this quantity by itself (see Sec. VII).

The only graph contributing to the off-diagonal part of the self-energy in order $O(1/d)$ is shown in Fig. 2(a). This graph gives the contribution on the NN cluster of a site $\mathbf{i}$ (i.e., $\mathbf{j}=\mathbf{i}+\tau$) to the self-energy $\tilde{S}_\sigma(\mathbf{i},\mathbf{j})$. Higher-order graphs, as those in Fig. 2(b), which are of order x^3, would also incorporate information about the correlation between $\mathbf{j}=\mathbf{i}+\tau$ and $\mathbf{l}=\mathbf{i}+\tau'$ ($\tau\neq\tau'$) and are therefore of higher order in $(1/d)$. The analytic expression is given by

$$\tilde{S}_\sigma(\mathbf{i},\mathbf{j})=-\left[\frac{G-1}{G+1}\frac{4}{n(2-n)}\right]^2[\tilde{P}^0_\sigma(\tau)]^3 \quad \text{for } \tau=\mathbf{i}-\mathbf{j} , \tag{55a}$$

$$\tilde{P}^0_\sigma(\tau)=\frac{1}{2d}\sum_{\tau}\sum_{\varepsilon(\mathbf{k})\le\varepsilon_F}e^{i\mathbf{k}\cdot\tau}=-\frac{1}{2\sqrt{2d}}\bar{\varepsilon}_0 , \tag{55b}$$

where $\bar{\varepsilon}_0$ is the mean kinetic energy in the noninteracting ground state, ε_F is the Fermi energy. Thus, we obtain

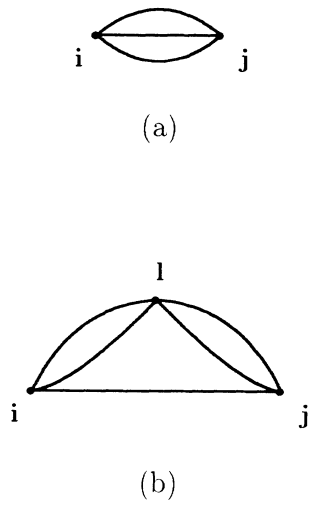


FIG. 2. Lowest-order graphs contributing to the self-energy $\tilde{S}_\sigma(\mathbf{i},\mathbf{j})$; (a) graph to second order in x, (b) graph to third order in x.

$$\tilde{S}^{(1)}_\sigma(\mathbf{i},\mathbf{i})=-\frac{(n-1)(G-1)^3}{[n(2-n)]^3(G+1)^2G}(\bar{\varepsilon}_0)^4 . \tag{56}$$

Here we introduced

$$\mathcal{O}(g,n,d)=\mathcal{O}_{\mathrm{GA}}(g,n)+\sum_{r=1}^{\infty}(1/d)^r\mathcal{O}^{(r)}(g,n)$$

to denote the $(1/d)$ expansion for an expectation value $\mathcal{O}(g,n)$. Recall that $\tilde{S}_{\sigma,\mathrm{GA}}(\mathbf{i},\mathbf{j})=0$. $\tilde{S}_\sigma(\mathbf{k})$ is continuous in $\mathbf{k}$ because $\tilde{S}_\sigma(\mathbf{k})$ is given by the skeleton graph in this order. From (53a) and (53b) we finally obtain

$$\bar{d}^{(1)}(g,n)=\frac{(G+1-n)(G+n-1)(G-1)}{2G(G+1)^3n^2(2-n)^2}(\bar{\varepsilon}_0)^4 , \tag{57a}$$

$$\langle \hat{n}_{\mathbf{k}\sigma}\rangle^{(1)}(g,n)=\left[\frac{1}{1+g}\right]^2\left[\frac{G-1}{G+1}\right]^2[n(G+1-n)+2(1-n)(G-1)\langle \hat{n}_{\mathbf{k}\sigma}\rangle_0] \times\left[\frac{|\bar{\varepsilon}_0|}{n(2-n)}\right]^3\left[\frac{(n-1)(G-1)}{n(2-n)G}\bar{\varepsilon}_0+\varepsilon(\mathbf{k})\right] , \tag{57b}$$

and the $(1/d)$ correction to the discontinuity at the Fermi surface is given by

$$q^{(1)}(g,n)=\left[\frac{1}{1+g}\right]^2\left[\frac{|\bar{\varepsilon}_0|}{n(2-n)}\right]^3\left[\frac{G-1}{G+1}\right]^2 2(1-n)(G-1)\left[\frac{(n-1)(G-1)}{n(2-n)G}\bar{\varepsilon}_0+\varepsilon_F\right] . \tag{57c}$$

Equation (57c) shows that $q^{(1)}(g,n)\ge 0$, in general. In $d=\infty$ we find that the mean kinetic energy per site as

$$(1/L)\langle \hat{T}\rangle(g,n,d=\infty)=(1/L)\langle \hat{T}\rangle_{\mathrm{GA}}(g,n)=q\bar{\varepsilon}_0 .$$

The first-order correction reads

$$\frac{1}{L}\langle \hat{T}\rangle^{(1)}(g,n)=2\left[\frac{1}{1+g}\right]^2\left[\frac{|\bar{\varepsilon}_0|}{n(2-n)}\right]^3\left[\frac{G-1}{G+1}\right]^2\left[-\frac{(1-n)^2(G-1)^2}{n(2-n)G}(\bar{\varepsilon}_0)^2+n(G+1-n)+(1-n)(G-1)\bar{\varepsilon}_0^2\right] , \tag{57d}$$

where we used $(1/L)\sum_{\mathbf{k}}[\varepsilon(\mathbf{k})]^2=1$ in all dimensions.

In Eqs. (57a)–(57d) $\bar{\varepsilon}_0$ and higher moments like $\bar{\varepsilon}_0^2$ occur. These quantities are defined as

$$\overline{\varepsilon_0^m}=2\int_{-\infty}^{\varepsilon_F} d\varepsilon\,\rho(\varepsilon)\varepsilon^m ,$$

where $\rho(\varepsilon)$ is the density of states (DOS). They depend on the dimension themselves (e.g., $|\bar{\varepsilon}_0|=2\sqrt{2}/\pi=0.900$, $8/\pi^2=0.811$, $\sqrt{2}/\sqrt{\pi}=0.798$ in $d=1,2,\infty$, respectively). To be consistent in $O(1/d)$ in each step we would have to expand the DOS $\rho(\varepsilon)$ in powers of $(1/d)$ (for details, see Ref. 37), determine ε_F from $n=2\int_{-\infty}^{\varepsilon_F}\rho(\varepsilon)d\varepsilon$ and insert the expressions up to the given order in Eqs. (57a)–(57d). This is not only tedious and lengthy but also the physical features of such a DOS never coincide with that of any realistic DOS (e.g., finite band width, Van Hove singularities). Therefore, we will always use the *exact* DOS for a given dimension when we compare with results for finite d. Hence, one can argue that the calculations do not represent a systematic expansion in $(1/d)$ any longer. But the errors introduced in this way are of order $(1/d)^{m+1}$ for an expression to order $(1/d)^m$. As we will see in Sec. VI, this kind of approximation fits exact ($d=1$) and numerical results ($d=2,3$) very well.

The formalism in Sec. II also serves to identify that parameter region for g and n where the GA for the GWF is already a good approximation. The reason is that $\tilde{S}_\sigma(\mathbf{k})$ is given by a series expansion in $(n/2)^2x$ where $x=x_{\mathbf{i}}$ is given in Eq. (14a) [in each order in x there are two new lines in the graphs which result in an extra factor $(n/2)^2$]. Hence, the GA for the GWF is a good approximation for small x. This is the case for $g\to 1$ ($G\to 1$), i.e., for small interaction strength U in (1), and/or for small densities n ($n\to 0$). Furthermore, the series in x is convergent for all (g,n) where the radius of convergence is reached at $(g=0,n=1)$.[6] This implies that the $(1/d)$ series converges for all (g,n) with the exception $g=0,n=1$. As will be shown below, the $(1/d)$ series is indeed only an asymptotic series for these values of g and n.

B. Second-order correction for half-filled band

For the half-filled band ($n=1$) we have particle-hole symmetry which allows to calculate up to order $(1/d)^2$ without too much effort. In this case we have $x=4(g-1)/(g+1)$, $q=(4g)/(1+g)^2$, $\alpha=0$, and $\tilde{S}_\sigma(\mathbf{i},\mathbf{i})=0$. This yields

$$\bar{d}(g,n=1)=\frac{g}{2(1+g)}\left[1+\frac{2}{1-g}\frac{1}{L}\sum_{\varepsilon(\mathbf{k})\le 0}\tilde{S}_\sigma(\mathbf{k})\right], \quad (58a)$$

$$\langle\hat{n}_{\mathbf{k}\sigma}\rangle(g,n=1)=\frac{1}{2}\left[\frac{1-g}{1+g}\right]^2+\frac{4g}{(1+g)^2}\langle\hat{n}_{\mathbf{k}\sigma}\rangle_0 + \frac{g}{(1+g)^2}\tilde{S}_\sigma(\mathbf{k}) . \quad (58b)$$

p-h symmetry also implies that $\tilde{P}_\sigma^0(\mathbf{i},\mathbf{j})=0$ for $\mathbf{i},\mathbf{j}$ on the same sublattice, i.e., if two lattice points in a graph are connected by a line, they have to be on different sublattices. Hence, for the case of half-filled band the graph in Fig. 2(b) *vanishes* ($\mathbf{i}$ and $\mathbf{l}$, $\mathbf{l}$ and $\mathbf{j}$, $\mathbf{i}$ and $\mathbf{j}$ cannot be at different lattices at the same time). Furthermore, the graph in Fig. 2(a) has no $(1/d)^2$ correction because for such a term $\mathbf{j}$ must be NNN to $\mathbf{i}$, i.e., $\mathbf{j}$ is on the same sublattice as $\mathbf{i}$. All graphs that contribute in $O((1/d)^2)$ are shown in Fig. 3. Their values in $\mathbf{k}$ space are listed in Table I. This table also contains the sign and the multiplicity ("weight") of a graph which results from Wick's theorem. To obtain the second-order contribution one has to multiply the values of the graphs by their signs and weights and has to add up these terms afterwards. Note that the graph in Fig. 3(c) strongly depends on dimensionality. One finds the main contributions if all lattice vectors are NN to each other. For high dimensions ($d\ge 2$) these contributions give the value of graph (c) in Table I but are considerably smaller in $d=1$. Therefore, the $(1/d)^2$ expressions below lead to a good approximation for $d\ge 2$. Then the self-energy corrections are given by

$$\tilde{S}_\sigma^{(1)}(\mathbf{k})=-\left[\frac{1-g}{1+g}\right]^2(\bar{\varepsilon}_0)^3\varepsilon(\mathbf{k}) , \quad (59a)$$

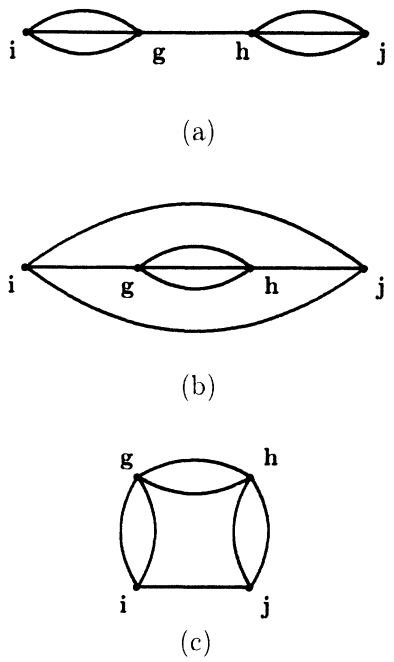


FIG. 3. All graphs contributing to second order in $(1/d)$ for the half-filled GWF.

TABLE I. Spins, weights, and values of the graphs in Fig. 3 to order $O((1/d)^2)$.

Graph	Sign	Weight	Value
a	+	1	$(\langle\hat{n}_{\mathbf{k}\sigma}\rangle_0-\frac{1}{2})\left[\frac{(\bar{\varepsilon}_0)^3\varepsilon(\mathbf{k})}{16d}\right]^2$
b	+	3	$\frac{(\bar{\varepsilon}_0)^5\varepsilon(\mathbf{k})}{512d^2}$
c	−	3	$\frac{3}{512d^2}(\bar{\varepsilon}_0)^7\varepsilon(\mathbf{k})$

$$\tilde{S}_\sigma^{(2)}(\mathbf{k})=\tilde{S}_\sigma^{(1)}(\mathbf{k})\left[\frac{1-g}{1+g}\right]^2(\bar{\varepsilon}_0)^2$$
$$\times[\tfrac{3}{2}-\tfrac{9}{2}(\bar{\varepsilon}_0)^2+\bar{\varepsilon}_0\varepsilon(\mathbf{k})(\langle\hat{n}_{\mathbf{k}\sigma}\rangle_0-\tfrac{1}{2})]\ . \quad (59b)$$

The corrections to the mean double occupancy finally read

$$\bar{d}^{(1)}(g)=-\bar{d}_{\mathrm{GA}}(g)\frac{1-g}{(1+g)^2}(\bar{\varepsilon}_0)^4\ , \quad (60a)$$

$$\bar{d}^{(2)}(g)=\bar{d}^{(1)}(g)\left[\frac{1-g}{1+g}\right]^2(\bar{\varepsilon}_0)^2[\tfrac{9}{2}(\bar{\varepsilon}_0)^2-2]\ , \quad (60b)$$

where $\bar{d}_{\mathrm{GA}}=g/[2(1+g)]$. The corrections to the mean kinetic energy are given by

$$\langle\hat{T}\rangle^{(1)}(g)=-\langle\hat{T}\rangle_{\mathrm{GA}}(g)\frac{(\bar{\varepsilon}_0)^2}{2}\left[\frac{1-g}{1+g}\right]^2 \quad (61a)$$

$$\langle\hat{T}\rangle^{(2)}(g)=\langle\hat{T}\rangle^{(1)}(g)\frac{(\bar{\varepsilon}_0)^2}{2}\left[\frac{1-g}{1+g}\right]^2$$
$$\times[-3+9(\bar{\varepsilon}_0)^2-\bar{\varepsilon}_0(\bar{\varepsilon}_0^3)]\ , \quad (61b)$$

where

$$(1/L)\langle\hat{T}\rangle_{\mathrm{GA}}(g)=4g\bar{\varepsilon}_0/[(1+g)^2]\ .$$

Note that there are no corrections to the discontinuity for $n=1$, i.e., $q(g)=(4g)/[(1+g)^2]+\mathcal{O}((1/d)^3)$. Because $q(g,n=1)$ is the same in $d=1,2,\infty$ due to the p-h symmetry[6] and there are no $(1/d)$ corrections to this quantity up to order $(1/d)^2$, we support the conjecture in Ref. 6 that $q(g,n=1)$ is the same in *all* dimensions d.

VI. COMPARISON WITH EXACT AND NUMERICAL RESULTS FOR THE GWF IN $d=1,2,3$

In this section we show that we obtain an excellent agreement between the analytic expressions of the first few orders in the $(1/d)$ expansion and all numerical results in $d=2,3$ for the GWF. We obtain surprisingly good results even in $d=1$, where we can compare with an exact solution.[6] The only shortcoming of any finite-order $(1/d)$ expansion is the prediction of a Brinkman-Rice localization transition[4] which does not occur in any finite dimension but only in $d=\infty$.[14] On the other hand, the absolute values of $(1/d)$ corrections to the GA for the

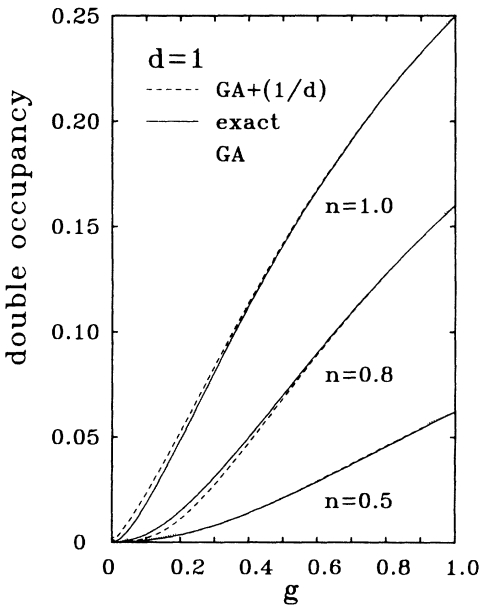


FIG. 4. Mean double occupancy $\bar{d}(g,n)$ in the GWF for different band fillings in $d=1$. The exact result (Ref. 6) and the result of the $(1/d)$ expansion up to $(1/d)$ are compared.

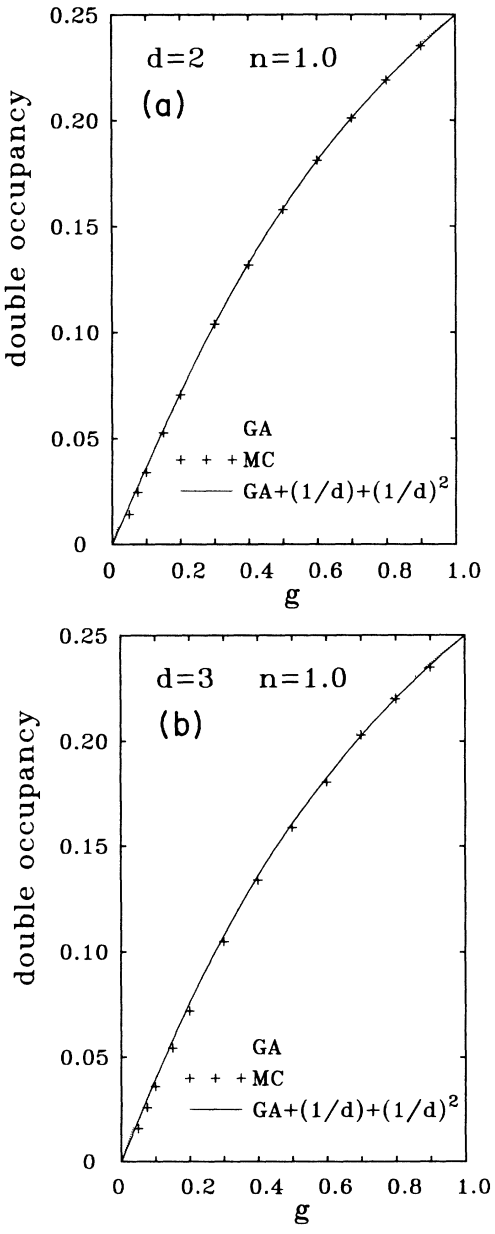


FIG. 5. Mean double occupancy $\bar{d}(g,n=1)$ in the GWF. Numerical results (Ref. 8) and the result of the $(1/d)$ expansion up to $(1/d)^2$ are compared. (a) in $d=2$, (b) in $d=3$.

GWF are very small in $d=3$. Therefore, the physics derived from the GA for the GWF is qualitatively *contained* in the GWF in $d=3$ and is *not* an artifact of the GA.

A. Double occupancy $\bar{d}$

In principle, we cannot *expect* a $(1/d)$ expansion to yield reasonable results for $d=1$. Nevertheless, since there is an analytic solution for $\bar{d}(g,n)$ in $d=1$,[6]

$$\bar{d}(g,n,d=1)=\frac{g^2}{2(1-g^2)^2}\{-\ln[1-n(1-g^2)] -n(1-g^2)\}\ , \tag{62}$$

we can compare the results to order $(1/d)$ in (57a) with an *exact* expression. This is done in Fig. 4 for $n=0.5$, 0.8, and 1. We see that for small densities n the agreement is excellent for all g. The same is true for all $g \geq 0.2$ where the error is smaller than 10% for all densities n. A reason for these surprisingly good results is the smallness of x in the parameter region where n is small and/or g is close to unity. On the other hand, the GA for the GWF deviates considerably from the exact result in $d=1$.

The quality of the $(1/d)$ results is even better in $d=2,3$ where we compare the results to order $(1/d)^2$ for $\bar{d}(g,n=1)$ with numerical results.[8] This is done in Fig. 5(a) for $d=2$ and Fig. 5(b) for $d=3$. In $d=2$ all numerical points lie on the analytical curve. For $d=3$ the analytical result is even more reliable than in $d=2$. Because the numerical results deviate from the analytical curve we conclude that the numerical result ($6\times6\times6=216$ lattice points) is slightly too low due to finite-size effects. From the comparison we deduce that the analytic expression for $\bar{d}(g,n=1)$ to order $(1/d)^2$ is very accurate up to very low values of g ($g \geq 0.02$ in $d=3$).

The only problematic region in the parameter space (g,n) is $g \to 0$, $n \to 1$. Equation (58a) explicitly shows that *any* finite $(1/d)$ expansion yields[14]

$$\bar{d}(g,n=1)=c_2 g \quad \text{for } g \to 0\ . \tag{63a}$$

In the $(1/d)$ expansion we have from (60a) and (60b)

$$c_2=\frac{1}{2}\left[1-\frac{(\bar{\varepsilon}_0)^4}{d}-\frac{(\bar{\varepsilon}_0)^6}{d^2}\left[\tfrac{9}{2}(\bar{\varepsilon}_0)^2-2\right]\right]\ . \tag{63b}$$

So c_2 is seen to be diminished in finite dimensions but never equals zero for any finite order of the $(1/d)$ expansion. There is both strong analytical[14] and numerical[8] evidence that $c_2=0$, i.e., $\bar{d}(g,n=1)$ vanishes more rapidly than linear in g for $g \to 0$. We therefore conclude that the $(1/d)$ series (63b) for c_2 is only asymptotic so that (63a) gives the *wrong* small g behavior for $\bar{d}(g,n=1)$. The linear behavior of $\bar{d}(g,n)$ for small g has drastic implications for the variational ground-state energy[14] (see below).

B. Mean kinetic energy and variational ground-state energy

The behavior of the mean kinetic energy $\langle \hat{T} \rangle(g,n)$ is reproduced by the $(1/d)$ expansion for all (g,n). This can be seen from Figs. 6(a) and 6(b) where we compare the exact ($d=1$) (Ref. 6) and the numerical ($d=2$) (Ref. 8) results for $g=0$ for different values of n. Even in this extreme case (low dimensions d, highly correlated regime $g=0$) the exact and numerical data are fitted very well by the first-order $(1/d)$ expression. For $n=1$, $g \to 0$ we have

$$\frac{1}{L}\langle \hat{T} \rangle = c_1 \bar{\varepsilon}_0 g \quad \text{for } g \to 0\ . \tag{64a}$$

To order $(1/d)^2$ we have [see (61a) and (61b)]

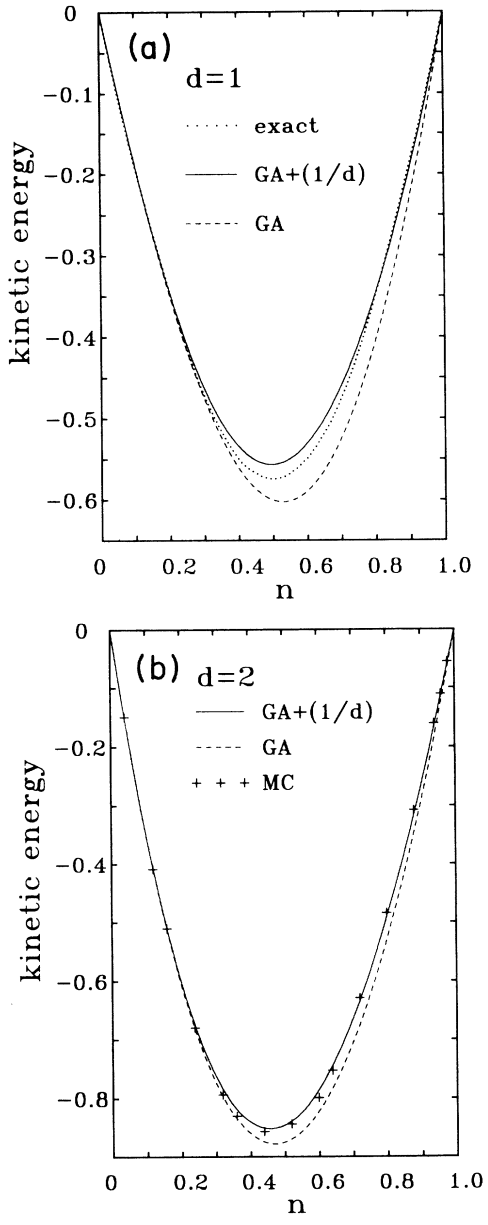


FIG. 6. Mean kinetic energy $(1/L)\langle \hat{T} \rangle(g=0,n)$ in the GWF for different band fillings (hole kinetic energy); (a) result of the $(1/d)$ expansion to order $(1/d)$ compared with the exact result in $d=1$ (Ref. 6); (b) the result of the $(1/d)$ expansion to order $(1/d)$ compared with numerical results in $d=2$ (Ref. 8).

$$c_1=4\left[1-\frac{(\bar{\varepsilon}_0)^2}{2d}-\left[\frac{1}{2d}\right]^2(\bar{\varepsilon}_0)^4[-3+9(\bar{\varepsilon}_0)^2-\bar{\varepsilon}_0(\bar{\varepsilon}_0^3)]\right] . \tag{64b}$$

Knowing both $\bar{d}(g,n)$ and $\langle\hat{T}\rangle(g,n)$ we can now minimize

$$(\langle\hat{H}\rangle/L)(g,n)=(\langle\hat{T}\rangle/L)(g,n)+U\bar{d}(g,n)$$

w.r.t. g for given parameter U. This yields the variational ground-state energy

$$E(U,n)=(\langle\hat{H}\rangle/L)(g^{\rm opt},n) .$$

Note that $U=U/t^*=U/(\sqrt{2d}\,t)$ in our notation. In Fig. 7(a) we show the analytical result for $E(U/t,n=1)$ together with the numerical result in $d=2$ from Ref. 8. In Fig. 7(b) we show the result for $E(U/t,n=1)$ in $d=3$ together with the GA. As a consequence of the linear dependence of both $\bar{d}(g,n=1)$ and $\langle\hat{T}\rangle(g,n=1)$ on g we find an unphysical transition to $E(U/t,n=1)=0$ for $U\geq U_c$ with[14]

$$U_c/t^*=\frac{c_1}{c_2}|\bar{\varepsilon}_0| . \tag{65}$$

This transition is the well-known Brinkman-Rice transition[4] which indeed *only* occurs in $d=\infty$ but should *never* occur in any finite dimension.[8,14] Any finite order expansion in $(1/d)$ merely shifts U_c to a larger value. Up to order $(1/d)^2$ we have

$$U_c^d=U_c^\infty\left[1+\frac{1}{d}(\bar{\varepsilon}_0)^2[(\bar{\varepsilon}_0)^2-\tfrac{1}{2}]+\left[\frac{1}{2d}\right]^2(\bar{\varepsilon}_0)^4[3+\bar{\varepsilon}_0(\bar{\varepsilon}_0^3)-19(\bar{\varepsilon}_0)^2+22(\bar{\varepsilon}_0)^4]\right] , \tag{66a}$$

$$U_c^\infty=8|\bar{\varepsilon}_0| . \tag{66b}$$

The corrections to U_c^∞ are indeed very small, i.e., of order 8% in $d=2$ and 4% in $d=3$. This implies that one can rely on the results of the $(1/d)$ expansion up to values of U which are very close to U_c^d. Furthermore, as seen in Fig. 7(b), the GA for the GWF is a good approximation in $d=3$ for all values of U. Hence, the GA for the GWF is a reasonable approximation for all U which are not too close to U_c^∞.

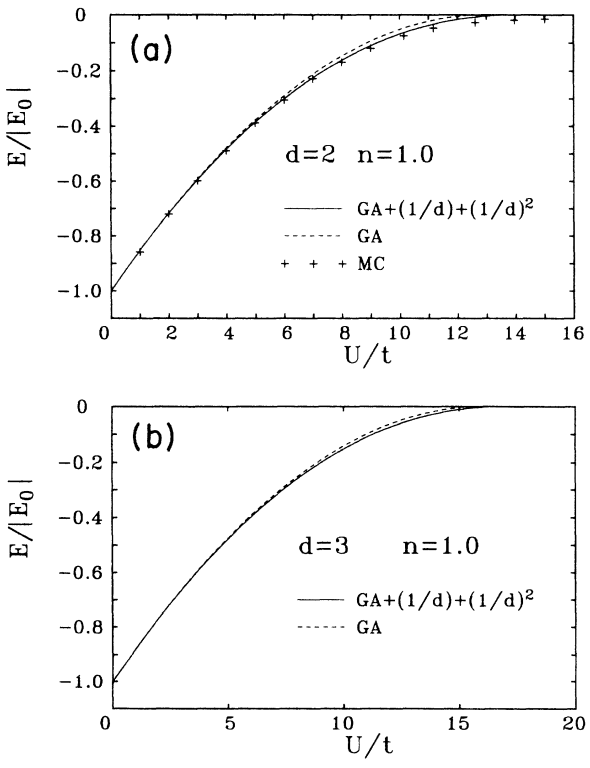


FIG. 7. Variational ground-state energy $E(U/t,n=1)$ for the GWF in the $(1/d)$ expansion to order $(1/d)^2$; (a) in $d=2$ compared with numerical results (Ref. 8), (b) in $d=3$ compared with the Gutzwiller approximation (GA) which is the result in $d=\infty$ (Ref. 6).

C. Momentum distribution and discontinuity

As a last example for the applicability of the $(1/d)$ expansion we analyze the momentum distribution. We

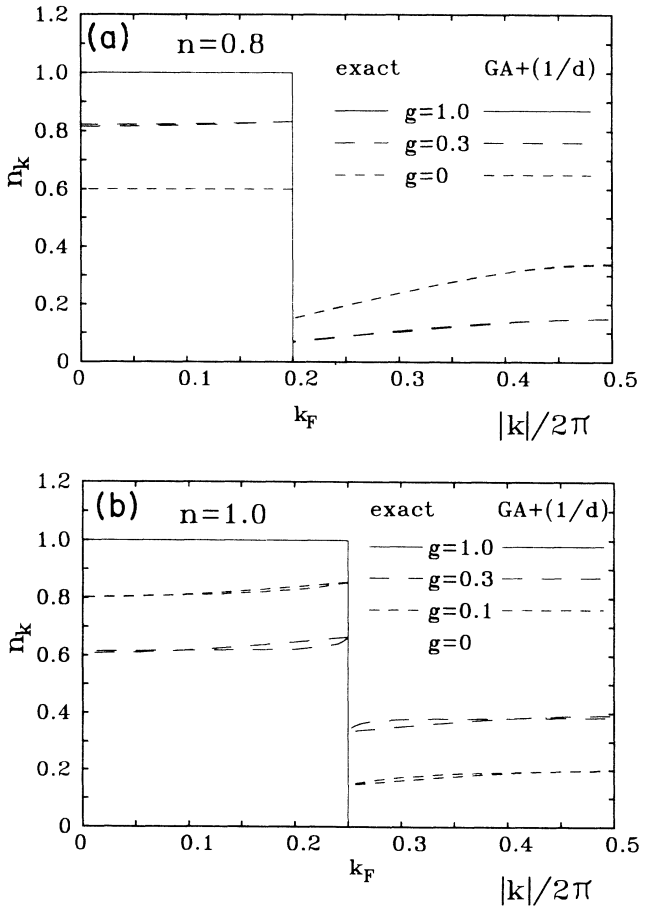


FIG. 8. Momentum distribution $\langle\hat{n}_{k\sigma}\rangle(g,n)$ for the GWF in the $(1/d)$ expansion to order $(1/d)$ compared with the exact result in $d=1$ (Ref. 6) for (a) $n=0.8$, (b) $n=1.0$.

compare $\langle \hat{n}_{k\sigma} \rangle$ in Eq. (57b) with the exact result in $d=1$. Figure 8(a) shows the case $n=0.8$, Fig. 8(b) shows the case $n=1.0$ for different values of g. The curves agree very well—not only qualitatively, but even quantitatively. The agreement still improves for $d=2,3$. Note that our expansion reproduces the unexpected curvature of $\langle \hat{n}_{k\sigma} \rangle$ in the GWF correctly while other methods failed.[28]

One of the physically most interesting quantities is the discontinuity at the Fermi surface where $\varepsilon(\mathbf{k})=\varepsilon_F$. This is because in the Fermi-liquid theory[5] the effective mass enhancement m^*/m is proportional to q^{-1}, i.e., the effective mass diverges for $q \to 0$ (localization transition). Because $q^{-1} \propto (1/g)$ we find a divergent effective mass for $g \to 0$ and the discussion above shows that g drops to very small values within a small range of $U \to U_c$, i.e., m^* rises quickly and the fermions seem to become localized ("nearly localized Fermi liquid"[5]). As argued in Ref. 38 and confirmed now, this picture and its implications are still correct even if the transition does not actually occur.

When one applies this concept to a metal-insulator transition,[4] it implies that the conductivity does *not* drop to zero discontinuously in the GWF in any finite dimension. It stays small but finite for all $U_c \le U < \infty$ and a metal-insulator transition in the Mott-Hubbard sense does not occur.

VII. NEW VARIATIONAL WAVE FUNCTIONS

In this last section we have shown that properties of the GWF in finite dimensions are well described by a $(1/d)$ expansion. We therefore conclude that the concept of high dimensions is also fruitful in low dimensions for more complicated Gutzwiller correlated VWF's. In this section we consider the general class of Gutzwiller correlated antiferromagnetic spin-density wave functions as possible ground states for the Hubbard, t-J, and antiferromagnetic Heisenberg models. In Sec. VII A we propose a new VWF for the Hubbard and t-J model based on the optical GSDW in $d=\infty$. In Sec. VII B we propose yet another new VWF for the Heisenberg model. For this purpose we calculate the optimal GSDW up to order $(1/d)$.

A. VWF for the Hubbard and t-J models

For a numerical analysis[8] the following Gutzwiller correlated spin-density wave function $|\Psi_g\rangle$ has been used:

$$|\Psi_g\rangle = g^{\hat{D}}|\Psi_0\rangle = g^{\hat{D}} \prod_{\varepsilon(\mathbf{k}) \le \varepsilon_F} \prod_{\sigma} (u_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma})|\mathrm{vac}\rangle \ , \tag{67}$$

where a Hartree-Fock form for $u_{\mathbf{k}}, v_{\mathbf{k}}$ was *assumed*. This is not the optimal parametrization in high dimensions, as can be seen from the results in Sec. III where we determined the optimal of infinitely many GSDW in $d=\infty$. It is possible to rewrite the GSDW in Sec. III in the form of Eq. (67). The parameters $\tilde{u}_{\mathbf{k}}, \tilde{v}_{\mathbf{k}}$ in Eqs. (42b) and (44) and $u_{\mathbf{k}}, v_{\mathbf{k}}$ are related by a simple linear transformation

$$u_{\mathbf{k}} = \frac{1}{2}\left[1+\frac{1}{\gamma}\right]\tilde{u}_{\mathbf{k}} + \frac{1}{2}\left[1-\frac{1}{\gamma}\right]\tilde{v}_{\mathbf{k}} \ , \tag{68a}$$

$$v_{\mathbf{k}} = \frac{1}{2}\left[1-\frac{1}{\gamma}\right]\tilde{u}_{\mathbf{k}} + \frac{1}{2}\left[1+\frac{1}{\gamma}\right]\tilde{v}_{\mathbf{k}} \ , \tag{68b}$$

where

$$\gamma = \left[\frac{4-x(n+m)(2-n+m)}{4-x(n-m)(2-n-m)}\right]^{1/2} , \tag{69a}$$

$$x = x_i = \frac{4(4\bar{d}-n^2+m^2)}{(n^2-m^2)[(2-n)^2-m^2]} \ . \tag{69b}$$

The latter equation follows from Eq. (14a). Here, $n=n_0$ is the particle density in the system and the sublattice magnetization $m=m_0$ in $|\Phi_0\rangle$ is given by

$$m = m_0 = (2/L) \sum_{\varepsilon(\mathbf{k}) \le \varepsilon_F} \frac{\Delta}{\{\Delta^2 + [\varepsilon(\mathbf{k})]^2\}^{1/2}} \ . \tag{70}$$

Equation (67), together with the parametrization in Eqs. (68a) and (68b), defines a new VWF which only depends on two variational parameters (Δ, g), since $\tilde{u}_{\mathbf{k}}$ and $\tilde{v}_{\mathbf{k}}$ follow from Eqs. (42b) and (44) as

$$\tilde{u}_{\mathbf{k}} = \left[\frac{1}{2}\left[1+\frac{|\varepsilon(\mathbf{k})|}{\{[\varepsilon(\mathbf{k})]^2+\Delta^2\}^{1/2}}\right]\right]^{1/2} ,$$
$$\tilde{v}_{\mathbf{k}} = -\mathrm{sgn}[\varepsilon(\mathbf{k})]\left[\frac{1}{2}\left[1-\frac{|\varepsilon(\mathbf{k})|}{\{[\varepsilon(\mathbf{k})]^2+\Delta^2\}^{1/2}}\right]\right]^{1/2} . \tag{71}$$

Such a VWF can be analyzed numerically in low dimensions. We believe that it is possible to *improve* on the results of earlier numerical work[8] when a wave function is used which has the analytic form of the *optimal* GSDW in $d=\infty$.

The formalism also applies to the t-J model.[20–22] This model can be deduced from the Hubbard Hamiltonian by an effective Hamiltonian approach starting from the limit $t/U \to 0$. Using the general GSDW one finally finds the same Hartree-Fock form for $\tilde{u}_{\mathbf{k}}, \tilde{v}_{\mathbf{k}}$ in $d=\infty$ as in the case of the Hubbard model. Hence, the proposal for a new wave function in (67), specified by Eqs. (68a), (68b), (69a), (69b), (70), and (71), applies also to the t-J model. Its quality can be tested numerically in low dimensions.

B. VWF for the spin-$\frac{1}{2}$ Heisenberg model

We now derive the optimal GSDW up to order $(1/d)$ for the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg model. The t-J model reduces to this Hamiltonian in the case of half-filling. The Hamilton operator is given by

$$\hat{H}_{\mathrm{Heis}} = \frac{J^*}{2d} \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j, \quad J^* = \frac{4(t^*)^2}{U} \ , \tag{72}$$

where we omitted a trivial constant. On the AB lattices *under consideration* the exact ground state of this Hamiltonian in $d=\infty$ is the Néel state,[39,40] which is obtained from the GSDW for $\tilde{u}_{\mathbf{k}}=\tilde{v}_{\mathbf{k}}=1/\sqrt{2}$. In this case there are no doubly occupied sites in $|\Phi_0\rangle$ and the Gutzwiller projector $P_{\bar{d}=0}=\prod_i (1-\hat{D}_i)$ is irrelevant.

1. Derivation of the optimal GSDW to order (1/d) for the Heisenberg model

The calculation of the optimal $u_{\mathbf{k}}, v_{\mathbf{k}}$ up to order $(1/d)$ for $|\Psi_{g=0}\rangle$ in Eq. (67) is performed in Appendices B and C. From (B9a)–(B9c) we obtain

$$m = 1 - \frac{1}{d}\langle\varepsilon^2\rangle^2 , \tag{73a}$$

$$\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle = (-\tfrac{1}{4})\left[1+\frac{2}{d}\langle\varepsilon^2\rangle(1-\langle\varepsilon^2\rangle)\right] , \tag{73b}$$

$$\langle\varepsilon^2\rangle = 2\int_{-\varepsilon_{\rm cut}}^{0} d\varepsilon\,\rho(\varepsilon)\varepsilon^2 , \tag{73c}$$

where $\varepsilon_{\rm cut}$ is the only variational parameter left. The analytical structure of $u_{\mathbf{k}} = u(\varepsilon(\mathbf{k})) = u(\varepsilon)$, $v_{\mathbf{k}} = (\varepsilon(\mathbf{k})) = v(\varepsilon)$, in (67) is given by

$$u(\varepsilon), v(\varepsilon) = \begin{cases} \sqrt{1/2} & \text{for } -\varepsilon_B \le \varepsilon \le -\varepsilon_{\rm cut} , \\ \sqrt{1/2}\left[1 \pm \dfrac{|\varepsilon|}{(\langle\varepsilon^2\rangle)^{1/2}}\right] & \text{for } -\varepsilon_{\rm cut} \le \varepsilon \le 0 , \end{cases} \tag{74}$$

where $-\varepsilon_B = -\sqrt{2d}$ is the lower-band edge. The contribution to the variational ground-state energy of states which belong to the energy shell $-\varepsilon_{\rm cut} \le \varepsilon \le 0$ becomes irrelevant for $d \to \infty$. The *existence* of that shell, however, is an intrinsic effect of finite dimensions.

The prediction for the ground-state energy readily follows from Eq. (73b), which is easily optimized by $\langle\varepsilon^2\rangle = \frac{1}{2}$. Hence, one finds to order $(1/d)$

$$m_{\rm opt} = 1 - \frac{1}{4d} , \tag{75a}$$

$$\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle_{\rm opt} = (-\tfrac{1}{4})\left[1+\frac{1}{2d}\right] . \tag{75b}$$

We can apply these formulas in $d=2$ and find $m_{\rm opt} = 0.875$, and $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle_{\rm opt} = -0.3125$.

2. Comparison with other treatments of the Heisenberg model

There are several attempts to determine $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle$ exactly or to derive bounds on that quantity. Table II lists some of the Monte Carlo (MC) results for the exact Hamiltonian (finite-size diagonalization, finite- and zero-temperature MC) and variational MC results. From these investigations one can conclude that the exact value lies in the range $-0.335 \le \langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle \le -0.334$. A rigorous lower bound was obtained by Anderson[39] as $-(\frac{1}{4})[1+(1/d)]$, i.e., -0.375 in $d=2$. Analytical upper bounds are shown in Table III, which also contains results of analytical (perturbative) methods. The optimal variational upper bound is -0.3344 given by Liang *et al.*[52] who analyzed a three-parameter VWF on a 180×180 lattice with variational MC. Sachdev[50] obtained the analytical upper bound -0.3317 with a one-parameter VWF.

TABLE II. Comparison of finite-size diagonalization Monte Carlo versus variational Monte Carlo results for $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle$. The numbers in parentheses are reference numbers.

Finite-size diagonalization, Monte Carlo	Variational Monte Carlo
−0.336 (41)	−0.328 (41)
−0.3364 (42)	−0.3319 (46)
−0.3336 (43)	−0.321 (8)
−0.3350 (44)	
−0.334 59 (45)	

TABLE III. Comparison of variational and perturbative results for $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle$. The numbers in parentheses are reference numbers.

Variational	Perturbative
−0.324 (47)	−0.358 (52)
−0.322 (48)	−0.332 (53)
−0.3221 (49)	−0.3336 (54)
−0.3317 (50)	−0.3337 (55)
−0.3344 (51)	−0.3348 (56)

The GSDW $|\Psi_{g=0}\rangle$ given in Eq. (67) with $u_{\mathbf{k}} = u[\varepsilon(\mathbf{k})] = u(\varepsilon)$, $v_{\mathbf{k}} = v[\varepsilon(\mathbf{k})] = v(\varepsilon)$ from Eq. (74) can be expected to yield a result for $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle$ which is very close to these bounds when it is evaluated numerically in $d=2$. This *conjecture* is supported by a comparison of the GSDW with the VWF analyzed numerically by Yokoyama and Shiba (YS) in Ref. 8. They used

$$u_{\rm YS}, v_{\rm YS} = \sqrt{1/2}\left[1 \pm \frac{2|\varepsilon|}{(4\varepsilon^2+\Delta_{\rm YS}^2)^{1/2}}\right]^{1/2} , \tag{76}$$

where $\Delta_{\rm YS}$ is their variational parameter. If we identify $\Delta_{\rm YS} \equiv (\langle\varepsilon^2\rangle)^{1/2} \le 1$ one can see that the VWF's *agree* for $|\varepsilon| \ll \Delta_{\rm YS}$, i.e., in the vicinity of $\varepsilon = 0$. But they essentially *disagree* for $|\varepsilon| \gg \Delta_{\rm YS}$. In the latter region (near the band edge) YS have $u_{\rm YS} \simeq 1$, $v_{\rm YS} \simeq 0$, i.e., the YS-VWF describes a projected Fermi sea of *free*-electron states. For the GSDW, we find instead $u(\varepsilon), v(\varepsilon) = 1/\sqrt{2}$ near the band edge, i.e., we described projected *antiferromagnetically ordered* states. This difference may allow to improve on the already very good results of Yokoyama and Shiba[8] who obtained $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle = -0.321$ for their VWF.

We further compare the results for the GSDW with linear spin-wave theory. This is an expansion approach to the Heisenberg model where $(1/Sz)$ serves as a small parameter, and $z = 2d$ is the number of NN. This technique is based on a bosonic representation of the Heisenberg model whereas we use a fermionic description. The

TABLE IV. Results of spin-wave theory for $\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle$ in $d=2$ for $S=1/2$. The numbers in parentheses are reference numbers.

Parameter and order of expansion	$\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+\tau}\rangle$
$(1/d)$	−0.3125 (57,58)
$(1/Sz)$	−0.329 (57,58)
$(1/d)^2$	−0.3340 (57,59)
$(1/Sz)^2$	−0.3352 (57,59)

analytical expression for $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle$ up to order $(1/Sz)^2$ can for $S=\frac{1}{2}$ be written as[57-59]

$$\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle = (-\tfrac{1}{4})(1+2c_0+c_0^2) , \tag{77a}$$

$$c_0 = \int_{-\varepsilon_B}^{\varepsilon_B} d\varepsilon \, \rho(\varepsilon) \left[1 - \left[1 - \frac{\varepsilon^2}{2d} \right]^{1/2} \right] . \tag{77b}$$

Clearly, the results of a $(1/Sz)$ expansion differ from those of a $(1/d)$ expansion. Up to order $(1/d)^2$ we have

$$c_0 = [1/(4d)] + [1/(16d^2)] \int_{-\varepsilon_B}^{\varepsilon_B} d\varepsilon \, \rho(\varepsilon) \varepsilon^4 .$$

Hence, the results for $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle$ and m of the GSDW completely agree with linear spin-wave theory up to order $(1/d)$. In Table IV we list the results of this theory according to (77a) in $d=2$. The $(1/d)^2$ result in linear spin-wave theory is very close to the expected exact value in $d=2$. This supports the conjecture that the same is true for the GSDW derived above.

3. *Interpretation of the new VWF*

We now *interpret* the physics described by the GSDW. In $d=\infty$ all states are "frozen" in the Néel ordering ($\uparrow$ spins on the A, $\downarrow$ spins on the B sublattice). In finite dimensions there will be spin flips or—in a fermionic picture—$\uparrow$ and $\downarrow$ electrons will move around due to (virtual) hopping processes. The issue is *how* the rigid correlation between the electrons $\hat{c}^\dagger_{\mathbf{k}}$ and $\hat{c}^\dagger_{\mathbf{k}+\mathbf{Q}}$ has to be broken up to obtain the wave function with lowest energy. Consider the half-filled Hubbard model at large U in the antiferromagnetic Hartree-Fock approximation. This theory describes two subbands in the magnetic Brillouin zone whose boundary is given by $\varepsilon(\mathbf{k})=0$. The Hartree-Fock ground state is given by a completely filled lower band (Fermi energy $\varepsilon_F=0$) and an empty upper band. For $U=\infty$ it describes the Néel state which is the exact ground state of the Heisenberg model in $d=\infty$. For $d<\infty$ the Néel state is not the exact ground state so that we expect excitations of states in the lower subband, especially near the Fermi energy. Hence, we argue that electron pairs $\hat{c}^\dagger_{\mathbf{k}}, \hat{c}^\dagger_{\mathbf{k}+\mathbf{Q}}$ near the magnetic Brillouin zone $[\varepsilon(\mathbf{k}) \simeq 0]$ should weaken their correlation while electron pairs in the vicinity of the lower band edge $[\varepsilon(\mathbf{k}) \simeq |\varepsilon_B|]$ stay rigidly Néel correlated. On the other hand, this means to create doubly occupied sites. These have to be projected out afterwards by the Gutzwiller projector. Thus, the advantage of breaking up the Néel correlation is diminished and there is also a mixing of all $\mathbf{k}$ states. But one may argue that the Gutzwiller projector affects all electron pairs in $\hat{c}^\dagger_{\mathbf{k}}, \hat{c}^\dagger_{\mathbf{k}+\mathbf{Q}}$ in the *same* manner. Hence, the dispersion relation $\varepsilon(\mathbf{k})$ of the *noninteracting* Fermi system selects which of the $\hat{c}^\dagger_{\mathbf{k}}, \hat{c}^\dagger_{\mathbf{k}+\mathbf{Q}}$ pair has to be broken up. This allows for an intuitive understanding why there appears a sharp cutoff energy ε_{cut} in the parameters $u(\varepsilon), v(\varepsilon)$ which determine the GSDW.

Because the GSDW is based on a fermionic description of the spin-$\frac{1}{2}$ Heisenberg model one is tempted to interpret ε_{cut} as a Fermi energy of spin-$\frac{1}{2}$ quasiparticles ("spinons"[22,60]). On the one hand, the cutoff energy ε_{cut} results from an analytic calculation of the optimal of infinitely many variational wave functions and is not put in by hand. Furthermore, the results to order $(1/d)$ for this wave function are very satisfactory. On the other hand, the GSDW is merely a trial state so it gives only an approximate description of the true ground state of the model. Furthermore, the notion of a Fermi energy is closely related to the kind of excitations in the system. The description of excitations is out of the scope of ground-state VWF's. Lastly, we deal with a highly correlated VWF $|\Psi_{g=0}\rangle = \prod_i (1-\hat{D}_i)|\Psi_0\rangle$ which not only contains the one-particle product wave function $|\Psi_0\rangle$ but also the Gutzwiller projector. Hence, the physics $|\Psi_{g=0}\rangle$ is not only determined by the physics in $|\Psi_0\rangle$ but also by the effects introduced by the Gutzwiller correlator. Therefore, one should not overinterpret the one-particle properties in $|\Psi_0\rangle$.

VIII. SUMMARY

In this paper we presented a formalism to study general Gutzwiller correlated variational wave functions in finite dimensions d via a $(1/d)$ expansion. The concept of high dimensions was introduced by Metzner and Vollhardt.[13] For the special case of the Gutzwiller wave function they showed[6,13] that the Gutzwiller approximation becomes exact in $d=\infty$. This opened up the possibility to extend the GA *systematically* to more general Gutzwiller correlated VWF's. Using a graph formalism MV obtained a closed but infinite set of equations which determines the variational ground-state energy in $d=\infty$ for such wave functions. However, these equations cannot be solved in practice for arbitrary VWF's.

To utilize the limit of high dimensions more economically we use the same graphs as MV but with new interpretations of vertices and lines. As a consequence, the self-energy vanishes in $d=\infty$. This allows for an exact evaluation of the variational ground-state energy in this limit for general Gutzwiller correlated variational wave functions without calculating a single graph. Furthermore, for all the VWF's we calculate the lowest-order term in $(1/d)$ for all nearest-neighbor correlation functions.

We compared these systematically derived results with other attempts to extend the GA. Recall that the GA becomes exact for the GWF in $d=\infty$. In this paper we found that the approximate treatment of the Gutzwiller correlated VWF's used in the context of the periodic Anderson model[15-18] *also* becomes exact in $d=\infty$.[15,16,18] However, the same is not true, in general, for other, more complicated (e.g., antiferromagnetic) VWF's (Refs. 21, 27-29, 31, and 32). For example, in certain methods[21,32] one does not calculate expectation values for a specified VWF but one makes an ansatz for the analytic form of $\langle \hat{H} \rangle (q_{i\sigma}, \bar{d}_i)$, where $q_{i\sigma}$ and $\bar{d}_i$ are determined approximately. This type of approximations does *not* become exact in $d=\infty$: the factors $q_{i\sigma}$ cannot be determined unambiguously[21,27,32] and often do not agree with the exact ones in $d=\infty$.[21,27] Furthermore, using these techniques one only *argues* with VWF's but one does not really *calculate* with them. As a consequence, the VWF's used for these argumentations are *not* the same as the VWF's we use for our exact calculations in $d=\infty$.

We can further compare with the results of Kotliar and Ruckenstein who attacked the Hubbard model with a slave-boson–path-integral technique. The $d=\infty$ results for the general Gutzwiller correlated VWF's reproduce the full set of static saddle-point equations. This allows for new insight into the meaning of such an approximation to a path integral.

Going beyond the Gutzwiller approximation for the Gutzwiller wave function, we derive analytic expressions for the one-particle density matrix, the mean double occupancy and the variational ground-state energy in the GWF up to order $(1/d)$ for arbitrary correlation strength and electron densities; for half-filling we calculate up to order $(1/d)^2$. None of the cluster expansions[28–30] to improve on the GA for the GWF agrees with the systematic $(1/d)$ expansion. We showed that the first-order terms in the $(1/d)$ expansion are sufficient to describe numerical results[8] in $d=2,3$ quantitatively. Furthermore, the conclusions derived from the GA for the GWF ("almost localized Fermi liquid"[27,38]) are supported by the results of the $(1/d)$ expansion.

Based on the latter results we provide a number of explicit examples which give further support to the observation that the limit of *high* dimensions allows for qualitatively correct results in *low* dimensions. We proposed new VWF's for the Hubbard, *t-J*, and antiferromagnetic spin-$\frac{1}{2}$ Heisenberg model. These VWF's have the analytic form of the *optimal* of infinitely many Gutzwiller correlated antiferromagnetic spin-density wave functions to order $(1/d)^0$ (Hubbard and *t-J* models) and to order $(1/d)$ (Heisenberg model). In the case of the Heisenberg model one finds very reasonable results when the expressions to $(1/d)$ are applied to $d=2$. Furthermore, the GSDW only depends on a cutoff energy which may be interpreted as a Fermi energy of spin-$\frac{1}{2}$ quasiparticles ("spinons"[22,60]).

The formalism in this paper is restricted to VWF's with a fixed total number of particles. However, a generalization to projected Bardeen-Cooper-Schrieffer (BCS) type wave functions is straightforward. These wave functions are closely related to Anderson's original resonating-valence-band (RVB) wave function proposed for high-T_c superconductivity.[61] The results for the RVB wave function are planned to be presented elsewhere.[23]

ACKNOWLEDGMENTS

I wish to thank Professor Dr. D. Vollhardt, Dr. P. G. J. van Dongen, and Dr. W. Metzner for stimulating and valuable discussions and for a careful reading of the manuscript. Support from the Konrad-Adenauer-Stiftung is gratefully acknowledged.

APPENIDX A: DERIVATION OF THE KOTLIAR-RUCKENSTEIN FREE ENERGY

To be definite we consider the case of translational and spin-flip invariance. The eigenstates of the kinetic part of (1) span the whole Hilbert space. We denote them by $|\Phi_n\rangle$. We can assign an energy $E_n(g)$ to each of these states which we define as

$$E_n(g)=\langle\Phi_n|g^{\hat{D}}\hat{H}g^{\hat{D}}|\Phi_n\rangle/\langle\Phi_n|g^{2\hat{D}}|\Phi_n\rangle\ . \tag{A1}$$

In $d=\infty$ we have

$$E_n(g)=q\sum_{\mathbf{k}\sigma}\varepsilon(\mathbf{k})\langle\hat{n}_{\mathbf{k}\sigma}\rangle_{\{\Phi_n\}}+UL\bar{d} \tag{A2}$$

because our formula (39) is valid for arbitrary states $|\Phi_n\rangle$. We then *define* the objects

$$Z_{\mathrm{KR}}=\sum_{\Phi_n}e^{-\beta E_n}\ , \tag{A3a}$$

$$f_{\mathrm{KR}}=-\frac{1}{\beta}\ln Z_{\mathrm{KR}}\ , \tag{A3b}$$

where $\beta=1/k_BT$. f_{KR} is then exactly the KR "free energy," Z_{KR} the KR "partition function."[26] As the states $|\Phi_n(g)\rangle=g^{\hat{D}}|\Phi_n\rangle$ are not mutually orthogonal it is obvious that Z_{KR} is not a well-defined partition function. For large U, minimization with respect to d will yield small $\bar{d}$ (or even $\bar{d}=0$) so that starting with a number of

$$\begin{pmatrix}L\\N_\uparrow\end{pmatrix}\begin{pmatrix}L\\N_\downarrow\end{pmatrix}$$

states $|\Phi_n\rangle$, one ends up with states $[\prod_{\mathbf{f}}(1-\hat{D}_{\mathbf{f}})]|\Phi_n\rangle$ without double occupied sites, i.e., in a space of dimension

$$\begin{pmatrix}L\\N_\uparrow\end{pmatrix}\begin{pmatrix}L-N_\uparrow\\N_\downarrow\end{pmatrix}\ .$$

This overcounting of states or entropy problem occurs due to the *mathematically* ill-defined partition function Z_{KR} and ends up in a physically unreasonable localization transition for $UT\gg1$.[26] Nevertheless, f_{KR} or Z_{KR} are useful for the study of low-temperature properties of correlated Fermi systems as in Refs. 34 and 36; "low" means that the number of relevant states in (A3a) does not exceed the number

$$\begin{pmatrix}L\\N_\uparrow\end{pmatrix}\begin{pmatrix}L-N_\uparrow\\N_\downarrow\end{pmatrix}$$

of states without double occupied sites. This is a minimum requirement to circumvent the entropy problem. However, phenomenological extensions of the Gutzwiller results to finite temperatures as done by Seiler *et al.* in Ref. 62 cannot be rejected by the KR method.

APPENDIX B: CALCULATION OF THE $(1/d)$ CORRECTION FOR THE GSDW

We expand around the Néel state where deviations should be small. Therefore, we expect $\tilde{\theta}_{\mathbf{k}}$ in (44) to be close to unity, i.e., $\tilde{\theta}_{\mathbf{k}}=1-\delta_{\mathbf{k}}/d$, $0\le\delta_{\mathbf{k}}\ll d$. Thereby we generate doubly occupied sites in $|\Phi_0\rangle$. Hence, we have to set $g=0$ *from the beginning*. This implies

$$\tilde{u}_{\mathbf{k}},\tilde{v}_{\mathbf{k}}=\sqrt{1/2}\left[1\pm\frac{1}{2}\left[\frac{2\delta_{\mathbf{k}}}{d}\right]^{1/2}+O\left[\frac{\delta_{\mathbf{k}}}{d}\right]\right]\ , \tag{B1a}$$

$$m_0=1-\frac{(\Delta m)_0}{d}=1-\frac{1}{d}\frac{2}{L}\sum_{\varepsilon(\mathbf{k})\le0}\delta_{\mathbf{k}}\ , \tag{B1b}$$

$$\bar{\varepsilon}_0=\left[\frac{2}{d}\right]^{1/2}(\Delta\varepsilon)_0$$

$$=\left[\frac{2}{d}\right]^{1/2}\frac{2}{L}\sum_{\varepsilon(\mathbf{k})\le0}\varepsilon(\mathbf{k})\sqrt{\delta_{\mathbf{k}}}+O(d^{-3/2})\ . \tag{B1c}$$

For $u_{\mathbf{k}}, v_{\mathbf{k}}$ in (68a) and (68b) one finds

$$u_{\mathbf{k}}, v_{\mathbf{k}} = \sqrt{1/2}\left[1 \pm \left[\frac{\delta_{\mathbf{k}}}{(\Delta m)_0}\right]^{1/2} + O\left[\frac{\delta_{\mathbf{k}}}{d}\right]\right] . \tag{B1d}$$

Note, that we can set $\delta_{\mathbf{k}} = \lambda f_{\mathbf{k}}$ and let λ go to zero while $u_{\mathbf{k}}, v_{\mathbf{k}}$ in (B1d) and $|\Psi_{g=0}\rangle$ defined in (67) stay nontrivial. This will be important later.

Now we calculate $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle$. From (46) and (47) we find $g_{S^z S^z} = 4$ and $g_{S^+ S^-} = 4/(1-m_0^2)$. Using $\tilde{P}_\tau = -[1/(2\sqrt{2d})]\bar{\varepsilon}_0$ it follows from Eq. (45) that we have

$$\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle = (-\tfrac{1}{4})\left[m^2 + \frac{1}{d}(\bar{\varepsilon}_0)^2\left[1 + \frac{2}{1-m_0^2}\right]\right] . \tag{B2}$$

Note that m is the sublattice magnetization in $|\Psi_{g=0}\rangle$ and has a $(1/d)$ correction via Eq. (28) itself. We define S as the on-site part of the self-energy. Due to p-h symmetry we have

$$S \equiv \tilde{S}_\uparrow(i \in A \text{ sublattice}) = -\tilde{S}_\uparrow(i \in B \text{ sublattice}) ,$$

with $\uparrow$ and $\downarrow$ interchanged for $A \leftrightarrow B$. The off-site contribution in (28) can easily be calculated. Using (B1b) and (B1c) we find

$$m = 1 - \frac{1}{d}\left[\frac{[(\Delta\varepsilon)_0]^4}{[(\Delta m)_0]^2} + (S+1)(\Delta m)_0\right] \tag{B3}$$

up to order $(1/d)$. To this order (B2) yields

$$\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle = (-\tfrac{1}{4})\left[1 + \frac{2}{d}\frac{[(\Delta\varepsilon)_0]^2}{(\Delta m)_0}\left[1 - \frac{[(\Delta\varepsilon)_0]^2}{(\Delta m)_0}\right] - \frac{2}{d}(\Delta m)_0(1+S)\right] . \tag{B4}$$

The on-site part of the self-energy S is calculated in Appendix C. We find that S is of order unity and, especially, $S > -1$. Furthermore, S is a function of the quantities $(\Delta\varepsilon)_0$, $(\Delta m)_0$, and

$$(\Delta\varepsilon_1)_0 = \frac{2}{L}\sum_{\varepsilon(\mathbf{k}) \le 0} \varepsilon(\mathbf{k})(\delta_{\mathbf{k}})^{3/2} , \tag{B5a}$$

$$(\Delta m_1)_0 = \frac{2}{L}\sum_{\varepsilon(\mathbf{k}) \le 0} (\delta_{\mathbf{k}})^2 . \tag{B5b}$$

Minimizing the variational energy (B4) w.r.t. $\delta_{\mathbf{k}}$ we obtain the following equation for $\delta_{\mathbf{k}} = \delta[\varepsilon(\mathbf{k})] \equiv \delta(\varepsilon)$:

$$[\delta(\varepsilon)]^{3/2} + \beta_2 \varepsilon \delta(\varepsilon) - \beta_1[\delta(\varepsilon)]^{1/2} - \beta_0 \varepsilon = 0 , \tag{B6}$$

with $\beta_0, \beta_1, \beta_2 \ge 0$ as three remaining variational parameters. They are chosen positive to give reasonable results for $\delta(\varepsilon)$ at the boundaries (the upper-band edge is $\varepsilon = 0$, the lower-band edge is $\varepsilon = -\varepsilon_B = -\sqrt{2d}$). To optimize (B4) we have to set

$$\delta(-\varepsilon_B) = \frac{\beta_0}{\beta_2} , \tag{B7a}$$

$$\delta(0) = 0 . \tag{B7b}$$

The second $(1/d)$ term in (B4) is always smaller than or equal to zero since $(\Delta m)_0 \ge 0$ and $S > -1$. Hence, we have to let $(\Delta m)_0 \to 0$. This implies $\delta(\varepsilon) \to 0$ which does not yield a trivial VWF as discussed above. It follows from (B7b) that $\beta_2 \to \infty$ ($\beta_0 \to 0$ yields trivial results). In this case (B6) is a quadratic equation for $\sqrt{\delta(\varepsilon)}$. Defining $\lambda \equiv (\beta_0/\beta_1)^2$ we can let $\beta_2 \to \infty$ with the result

$$\delta(\varepsilon) = \begin{cases} 0 & \text{for } -\varepsilon_B \le \varepsilon < -\varepsilon_{\text{cut}} , \\ \lambda\varepsilon^2 & \text{for } -\varepsilon_{\text{cut}} \le \varepsilon \le 0 . \end{cases} \tag{B8}$$

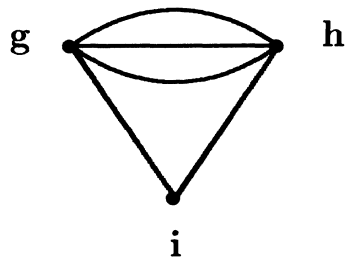
λ and ε_{cut} are the two remaining parameters. The quantity $[(\Delta\varepsilon)_0]^2/(\Delta m)_0$ is λ independent. We now let $\lambda \to 0$ to ensure that $(\Delta m)_0 \to 0$. We finally arrive at

$$m = 1 - \frac{1}{d}\langle\varepsilon^2\rangle^2 , \tag{B9a}$$

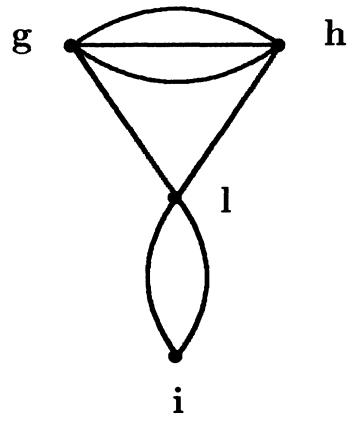
$$\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\tau} \rangle = (-\tfrac{1}{4})\left[1 + \frac{2}{d}\langle\varepsilon^2\rangle(1 - \langle\varepsilon^2\rangle)\right] , \tag{B9b}$$

$$\langle\varepsilon^2\rangle = 2\int_{-\varepsilon_{\text{cut}}}^{0} d\varepsilon\, \rho(\varepsilon)\varepsilon^2 . \tag{B9c}$$

Hence, only *one* variational parameter is left.



(a)



(b)

FIG. 9. First two graphs of a series for the local part $\tilde{S}_\sigma(i,i)$ in the self-energy up to order $(1/d)$; (a) graph to order x^3, (b) graph to order x^4.

APPENDIX C: CALCULATION OF THE ON-SITE PART OF THE SELF-ENERGY FOR THE GSDW

The on-site part of the self-energy is defined in Eq. (26) by

$$\tilde{S}_\sigma(\mathbf{i},\mathbf{i}) = -x_{\mathbf{i}}\{(n_{\mathbf{i},-\sigma} - \langle \hat{n}_{\mathbf{i}-\sigma}\rangle_0)\mathcal{D}\}_0^c \ . \tag{C1}$$

There is a whole class of graphs which contribute to S in order $(1/d)$. The graphs belonging to this class are easily identified. The first two graphs of this infinite series are shown in Figs. 9(a) and 9(b). Both of them are of order $(1/d)$ because the triple line from $\mathbf{g}$ to $\mathbf{h}$ requires these two lattice points to be NN to each other. But one can attach an infinite series of "RPA bubbles" to the graph in Fig. 9(a) without changing its order in $(1/d)$. Such an infinite series must be treated carefully in the limit $g=0$, $m_0 \to 1$. As we shall see below, the summed series is of order unity, instead of order $(1/d)$. To show this we introduce "dressed lines"

$$\overline{P_\sigma}(\mathbf{i},\mathbf{j}) = \tilde{P}^0_\sigma(\mathbf{i},\mathbf{j}) + \sum_{\mathbf{g}} \tilde{P}^0_\sigma(\mathbf{i},\mathbf{g})\tilde{S}_\sigma(\mathbf{g},\mathbf{g})\tilde{P}^0_\sigma(\mathbf{g},\mathbf{j}) \tag{C2}$$

for each of the lines occurring in the graphs. It is convenient to introduce the Fourier representation[13]

$$\overline{P_\sigma}(\mathbf{i},\mathbf{j}) = \frac{2}{L}\sum_{\varepsilon(\mathbf{k})\le 0} e^{-i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}\bar{P}_\sigma{}^{XY}(\mathbf{k}) \ , \tag{C3}$$

where $\mathbf{i}$ is on the X sublattice and $\mathbf{j}$ is on the Y sublattice. The inverse transformation reads

$$\bar{P}_\sigma^{XY}(\mathbf{k}) = \frac{2}{L}\sum_{\mathbf{i}\in X}\sum_{\mathbf{j}\in Y} e^{i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}\overline{P_\sigma}(\mathbf{i},\mathbf{j}) \ . \tag{C4}$$

It is convenient to arrange the quantities $\bar{P}_\sigma^{XY}(\mathbf{k})$ in a matrix, with $\bar{P}_\sigma^{AA}(\mathbf{k})$ as (1,1) element, etc. The advantage is that the convolution theorem holds for these matrices,[13] i.e., if

$$C(\mathbf{f},\mathbf{h}) = \sum_{\mathbf{j}} A(\mathbf{f},\mathbf{j})B(\mathbf{j},\mathbf{h})$$

then $C(\mathbf{k}) = A(\mathbf{k}) \circ B(\mathbf{k})$, where $\circ$ indicates the matrix product of A and B. From (C1) and (C4) we obtain $(n=1)$

$$\bar{P}_\sigma^{AA}(\mathbf{k}) = \frac{\sigma}{2}\left[\tilde{\theta}_{\mathbf{k}} - m_0 + \frac{S}{2}\left[(\tilde{\theta}_{\mathbf{k}} - m_0)^2 - (1-\tilde{\theta}_{\mathbf{k}}^2)\right]\right] , \tag{C5a}$$

$$\bar{P}_\sigma^{BB}(\mathbf{k}) = -\bar{P}_\sigma^{AA}(\mathbf{k}) \ , \tag{C5b}$$

$$\bar{P}_\sigma^{AB}(\mathbf{k}) = \bar{P}_\sigma^{BA}(\mathbf{k}) = \tfrac{1}{2}(1-\tilde{\theta}_{\mathbf{k}}^2)^{1/2}[1+S(\tilde{\theta}_{\mathbf{k}} - m_0)^2] \ , \tag{C5c}$$

Equation (C5c) shows that the hopping from A to B sites is spin independent. Because $(\tilde{\theta}_{\mathbf{k}} - m_0)$ is of order $(1/d)$ [see (B1a) and (B1b)] there is no correction of order unity for nearest neighbors. This justifies the use of $\bar{P}^0_\sigma$ instead of $\bar{P}_\sigma$ when we derived Eqs. (B3) and (B4). The equation for S now explicitly reads

$$\sigma S\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = x^3\sum_{\mathbf{f},\mathbf{g}} \overline{P_{-\sigma}}(\mathbf{i},\mathbf{f})(\overline{P_\tau})^3\delta_{\mathbf{f}-\mathbf{g},\tau}\overline{P_{-\sigma}}(\mathbf{g},\mathbf{i}) + (-x)(-\sigma)S\sum_{\mathbf{g}}[\overline{P_{-\sigma}}(\mathbf{i},\mathbf{g})]^2\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} , \tag{C6}$$

where

$$(\overline{P_\tau}) = -(1/\sqrt{2d})(2/L)\sum_{\varepsilon(\mathbf{k})\le 0}\varepsilon(\mathbf{k})\bar{P}^{AB}(\mathbf{k}) \ .$$

Using (C4) and (C5a)–(C5c) one can solve (C6). We find

$$S = \frac{2\sqrt{2d}\,x^3(\overline{P_\tau})^3\left[(2/L)\sum_{\varepsilon(\mathbf{k})\le 0}\varepsilon(\mathbf{k})\sigma\bar{P}_\sigma^{AA}(\mathbf{k})\bar{P}_\sigma^{AB}(\mathbf{k})\right]}{1-x\left[(2/L)\sum_{\varepsilon(\mathbf{k})\le 0}[\bar{P}_\sigma^{AA}(\mathbf{k})]^2 - [\bar{P}_\sigma^{AB}(\mathbf{k})]^2\right]} \ . \tag{C7}$$

We now perform the limit $g \to 0$ with

$$\tilde{\theta}_{\mathbf{k}} = 1 - \delta_{\mathbf{k}}/d + \kappa_{\mathbf{k}}/d^2$$

in (C7). We have to take into account a formal $(1/d)^2$ correction, $\kappa_{\mathbf{k}}$, which drops out at the end of the calculations for S. We use $x=(-4)/(1-m_0^2)$, $m_0 = (2/L)\sum_{\varepsilon(\mathbf{k})\le 0}\tilde{\theta}_{\mathbf{k}}$, and the definitions (B1b), (B1c), (B5a), and (B5b). After some algebra we arrive at

$$S = \frac{2[(\Delta\varepsilon)_0]^3[(\Delta\varepsilon)_0(\Delta m)_0 - (1+S)(\Delta\varepsilon_1)_0]}{[(\Delta m)_0]^2[(\Delta m_1)_0(1+S)^2 - (1+2S)[(\Delta m)_0]^2]} \ . \tag{C8}$$

Equation (C8) is a third-order equation for S dependent on known quantities. Since for $S \le -1$ both the denominator and the numerator are positive $[(\Delta\varepsilon)_0 \le 0$, $(\Delta\varepsilon_1)_0 \le 0]$, the right-hand side of Eq. (C8) is positive and there is no solution for $S \le -1$.

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