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# Gutzwiller-correlated wave functions for degenerate bands: exact results in infinite dimensions

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**Abstract.** We introduce Gutzwiller-correlated wave functions for the variational investigation of general multi-band Hubbard models. We set up a diagrammatic formalism which allows us to evaluate analytically ground-state properties in the limit of infinite spatial dimensions. In this limit recent results obtained within the Gutzwiller approximation are seen to become exact for these wave functions. We further show that the slave-boson mean-field theory for degenerate bands becomes variationally controlled at zero temperature in infinite dimensions. Lastly, we briefly comment on the variational approach to the Anderson transition in strongly correlated electron systems.

## 1. Introduction

During the last few decades the theoretical investigation of strongly correlated electron systems concentrated on the one-band Hubbard model [1], which serves as the standard model for electrons with strong short-range interactions; for a recent review, see [2]. The Hubbard model was originally proposed for the description of 3d electrons in transition metals to explain ferromagnetism and antiferromagnetism in iron and nickel and their oxides [1, 3]. For these substances the band degeneracy and intra-atomic (Hund's rule) exchange couplings apparently play an important role and, consequently, multi-band Hubbard models need to be investigated.

Until recently, band degeneracies were considered mostly for immobile f electrons which hybridize with featureless conduction electrons. The corresponding single-impurity Anderson model [4] and its periodic generalization (the Varma–Yafet model [5]) apply, e.g. for the rare-earth materials. Since the Coulomb interaction between the f electrons is very large, one often encounters the situation where the  $N_f$ -fold degenerate levels are at most singly occupied. Hence, the issue of degenerate bands with finite electron density need not be addressed in these cases.

In the past few years the multi-band Hubbard model received new attention. The Gutzwiller approximation to Gutzwiller-correlated variational wave functions was generalized in [6–9], the slave-boson mean-field approach along the lines of Kotliar and Ruckenstein [10] was developed and used in [11–13], and dynamical mean-field methods were applied in [14, 15]. In this paper we extend the method in [16, 17] to evaluate general Gutzwiller-correlated wave functions in the limit of infinite space dimensions without further approximations. In this way we recover the results of [6–9] and thus show that these earlier results become exact in infinite dimensions within the variational approach. Furthermore, we

prove that the slave-boson mean-field results are variationally controlled at zero temperature in this limit. Similar results hold for the one-band Hubbard model; see [18] and chapters 3.4 and 3.5 of [2] for brief reviews.

Our paper is organized as follows. In section 2 we introduce a general class of Gutzwiller-correlated wave functions which allows for the variational study of Hubbard models with general spin-orbit structure. We set up a diagrammatic perturbation theory to calculate expectation values for the variational ground-state energy and other physical quantities of interest. In section 3 we use our formalism to derive exact analytical expressions for the ground-state energy in the limit of infinite spatial dimensions. In section 4 we compare them to the results of approximate treatments of Gutzwiller-correlated wave functions and those of the slave-boson mean-field theory. Since our treatment allows for the inclusion of site-diagonal energetic disorder in the Hamiltonian, we briefly discuss the consequences of strong correlations for the Anderson transition within our variational description. A summary in section 5 closes our presentation.

## 2. Gutzwiller-correlated wave functions

In this section we introduce the Hubbard Hamiltonian for degenerate bands and the class of Gutzwiller-correlated wave functions as our approximate ground states. The minimization of the ground-state energy fixes the variational parameters contained in these trial states. For the evaluation of the corresponding many-body expectation values we develop a diagrammatic formalism which allows for the complete solution of the problem in infinite space dimensions.

### 2.1. Definitions

In his first two papers on narrow-band electron systems Hubbard [1, 3] considered 3d electrons with a purely local interaction. To simplify our considerations we make the further assumption that the interaction depends only on the number densities of electrons in the  $d$  orbitals. Then we may write the Hamiltonian in the form

$$\hat{H} = \sum_{i \neq j; \sigma, \sigma'} t_{i,j}^{\sigma, \sigma'} \hat{c}_{i;\sigma}^+ \hat{c}_{j;\sigma'} + \sum_{i;\sigma} \epsilon_i^\sigma \hat{n}_{i;\sigma} + \sum_{i;\sigma, \sigma'} U_i^{\sigma, \sigma'} \hat{n}_{i;\sigma} \hat{n}_{i;\sigma'} \quad (1)$$

where  $\sigma, \sigma' = 1, \dots, 2N$  are combined spin-orbit indices ( $N = 5$  for  $d$  electrons),  $i$  and  $j$  denote lattice sites, and  $t_{i,j}^{\sigma, \sigma'}$  is the matrix element for the electron transfer between two sites  $i$  and  $j$  with spin-orbit indices  $\sigma$  and  $\sigma'$ , respectively. In the following we will use the term ‘orbital’ for spin-orbital states.

The local energies  $t_{i,i}^{\sigma, \sigma'} = \delta_{\sigma, \sigma'} \epsilon_i^\sigma$  can be arbitrarily chosen to describe different orbital energy levels, e.g. in compounds or to mimic the influence of impurities and other lattice defects. As we will show below, expectation values for Gutzwiller-correlated wave functions can be calculated analytically in infinite dimensions even in the presence of energetically random impurity potentials.

Finally,  $U_i^{\sigma, \sigma'}$  describes the local Coulomb interaction between two electrons in the orbitals  $\sigma$  and  $\sigma'$  on the same lattice site. The local interaction partly accounts for the atomic exchange coupling. For example, in the case where  $N = 2$  the ground state of an atom with two electrons should be a spin triplet according to Hund’s first rule. According to our Hamiltonian (1) the interaction energy of the local  $S^z = \pm 1$  states is different from that of the  $S^z = 0$  states. However, the two  $S^z = 0$  states are still energetically degenerate in (1), i.e. the interaction does not fully distinguish between triplet and singlet states, as required

by Hund's first rule. In this work we restrict ourselves to density-dependent terms only. This should be the generic case for  $C_{60}$  and other fullerenes for which exchange coupling is less important because of the large diameter of the molecules; see, e.g., [19]. For other materials it might be necessary to include local spin-flip terms both in the Hamiltonian and in the variational description. Since the evaluation of many-body wave functions is fairly complicated we restrict ourselves to Gutzwiller correlators which are solely dependent on the density operators (see (7) below), and also omit the spin-flip terms in the Hamiltonian for consistency.

We introduce the following notation for the  $2^{2N}$  possible configurations of a given lattice site.

(i) An atomic configuration  $I$  is characterized by the electron occupation of the orbitals,  $I \in \{\emptyset; (1), \dots, (2N); (1, 2), \dots, (2, 3), \dots, (2N-1, 2N); \dots; (1, \dots, 2N)\}$  (2)

where the order of the numbers in  $(abc\dots)$  is irrelevant. The symbol  $\emptyset$  in (2) means that the site is empty. In general, we interpret the indices  $I$  in (2) as sets in the usual sense. For example, in the atomic configuration  $I \setminus I'$  only those orbitals in  $I$  which are not in  $I'$  are occupied. The complement of  $I$  is  $\bar{I} = (1, 2, \dots, 2N) \setminus I$ , i.e. in the atomic configuration  $\bar{I}$  all orbitals but those in  $I$  are occupied.

(ii) The absolute value  $|I|$  of a configuration is the number of elements in it, i.e.

$$|\emptyset| = 0 \quad |(a)| = 1 \quad |(a, b)| = 2 \quad \dots \quad |(1, \dots, 2N)| = 2N. \quad (3)$$

(iii) The operator which projects onto a specific configuration  $I$  on site  $i$  is given by

$$\hat{m}_{i;I} = \prod_{\sigma \in I} \hat{n}_{i;\sigma} \prod_{\sigma \in \bar{I}} (1 - \hat{n}_{i;\sigma}) \quad m_{i;I} = \langle \hat{m}_{i;I} \rangle \quad (4a)$$

where  $\langle \dots \rangle$  denotes the expectation value in the Gutzwiller-correlated wave function; see below. The operators  $\hat{m}_{i;I}$  measure the 'net' occupancy. Besides these we define the operators for the 'gross' occupancy as

$$\hat{n}_{i;I} = \prod_{\sigma \in I} \hat{n}_{i;\sigma} \quad n_{i;I} = \langle \hat{n}_{i;I} \rangle \quad \hat{n}_{i;\emptyset} \equiv 1. \quad (4b)$$

The gross occupancy operator  $\hat{n}_{i;I}$  gives a non-zero result when applied to  $I'$  only if  $I$  contains electrons in the same orbitals as  $I'$ . However,  $I$  and  $I'$  need not be identical because  $I'$  could contain additional electrons in further orbitals, i.e. only  $I \subseteq I'$  is required.

Each gross (net) operator can be written as a sum of (net) gross operators:

$$\hat{n}_{i;I} = \sum_{I' \supseteq I} \hat{m}_{i;I'} \quad (5a)$$

$$\hat{m}_{i;I} = \sum_{I' \supseteq I} (-1)^{|I' \setminus I|} \hat{n}_{i;I'}. \quad (5b)$$

For practical calculations the net operators  $\hat{m}_{i;I}$  are more useful than the gross operators  $\hat{n}_{i;I}$  because the former are projection operators onto a given configuration  $I$  on site  $i$ , i.e.  $\hat{m}_{i;I} \hat{m}_{i;I'} = \delta_{I,I'} \hat{m}_{i;I}$ .

With these definitions we may rewrite the interaction part of the Hamiltonian (1) as

$$\sum_{i;\sigma,\sigma'} U_i^{\sigma,\sigma'} \hat{n}_{i;\sigma} \hat{n}_{i;\sigma'} = \sum_{i;I (|I| \geq 2)} U_{i;I} \hat{m}_{i;I} \quad (6a)$$

with

$$U_{i;I} = \sum_{\sigma,\sigma' \in I} U_i^{\sigma,\sigma'}. \quad (6b)$$

With the help of these definitions we may formulate the class of Gutzwiller-correlated wave functions for degenerate bands as

$$|\Psi_G\rangle = \hat{P}_G |\Psi_0\rangle \quad (7a)$$

$$\hat{P}_G = \prod_i \prod_{(|I| \geq 2)} g_{i;I}^{\hat{m}_{i;I}}. \quad (7b)$$

The trial states depend on  $K_N = 2^{2N} - (2N + 1)$  real numbers  $g_{i;I}$  for each lattice site and on further variational parameters in  $|\Psi_0\rangle$ . The generalized Gutzwiller correlator  $\hat{P}_G$  in (7) suppresses fluctuations in the multiple orbital occupancy for repulsive interactions. In a translationally invariant system the Gutzwiller wave functions for degenerate bands as proposed in [9] are recovered by setting  $g_{i;I} \equiv g_I$ . Similar but different expressions for the Gutzwiller wave function for degenerate bands can be found in the work by Gutzwiller [20], Chao and Gutzwiller [21], and Chao [22]. Note that, in general, the gross occupation densities  $n_{i;\sigma}$  in  $|\Psi_G\rangle$  are different from those in  $|\Psi_0\rangle$ .

## 2.2. Diagrammatic evaluation

To gain further insight into the physics of the variational wave functions we have to evaluate the expectation values

$$\langle \hat{O} \rangle = \frac{\langle \Psi_G | \hat{O} | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle}. \quad (8)$$

The variational parameters in  $|\Psi_G\rangle$  are obtained by the minimization of the expectation value of the Hamiltonian (1):

$$E_0^{\text{var}} = \min_{g_{i;I}; |\Psi_0\rangle} \langle \hat{H} \rangle \quad (9a)$$

$$\langle \hat{H} \rangle = \sum_{i,j;\sigma,\sigma'} t_{i,j}^{\sigma,\sigma'} \langle \hat{c}_{i;\sigma}^+ \hat{c}_{j;\sigma'} \rangle + \sum_{i;I (|I| \geq 2)} U_{i;I} \langle \hat{m}_{i;I} \rangle. \quad (9b)$$

The variational ground-state energy  $E_0^{\text{var}}$  is an upper bound for the exact ground-state energy. This upper-bound property applies only if we are able to evaluate the variational ground-state energy without further approximations.

The evaluation of expectation values with correlated wave functions is a many-particle problem that cannot be solved in general; see [18] and chapter 3.4 of [2] for a review. In this paper we will use the method introduced by Gebhard [16, 17], which allows the approximation-free evaluation of general Gutzwiller-correlated wave functions in the limit of infinite spatial dimensions. The formalism is based on a diagrammatic expansion of expectation values in such a way that the (variational) self-energy identically vanishes in infinite dimensions.

As shown in more detail in [16] we have to carry out the following programme: (i) choose the appropriate expansion parameters, (ii) apply Wick's theorem, and (iii) use the linked-cluster theorem. If the expansion parameters are properly chosen the lowest order in the expansion already gives the exact result in infinite dimensions.

**2.2.1. Choice of the expansion parameters.** As a first step we choose the appropriate expansion parameter(s) for our diagrammatic theory. In this respect the variational approach is more flexible than the standard perturbation theory for Green functions in interacting electron systems.

We express the one-particle product wave function  $|\Psi_0\rangle$  in the form

$$|\Psi_0\rangle = \prod_i \eta_{i;\emptyset} \eta_{i;1}^{\hat{n}_{i;1}} \cdots \eta_{i;2N}^{\hat{n}_{i;2N}} |\Phi_0\rangle \quad (10)$$

where  $|\Phi_0\rangle$  is another, normalized one-particle product wave function. The real numbers  $\eta_{i;\emptyset}, \dots, \eta_{i;2N}$  are chosen such that the square of the ‘modified’ (local) Gutzwiller correlator

$$\hat{P}_i \equiv \eta_{i;\emptyset} \prod_{\sigma=1}^{2N} \eta_{i;\sigma}^{\hat{n}_{i;\sigma}} \prod_{(|I|\geq 2)} g_{i;I}^{\hat{m}_{i;I}} = \eta_{i;\emptyset} \prod_{\sigma=1}^{2N} [1 + (\eta_{i;\sigma} - 1) \hat{n}_{i;\sigma}] \prod_{(|I|\geq 2)} [1 + (g_{i;I} - 1) \hat{m}_{i;I}] \quad (11)$$

can be written in the form

$$\hat{P}_i^2 = 1 + x_{i;1,2} \hat{n}_{i;1,2}^{\text{HF}} + x_{i;1,3} \hat{n}_{i;1,3}^{\text{HF}} + \cdots + x_{i;1,\dots,2N} \hat{n}_{i;1,\dots,2N}^{\text{HF}}. \quad (12)$$

Here, the parameters  $x_{i;I}$  are real numbers and the Hartree–Fock (HF) operators  $\hat{n}_{i;I}^{\text{HF}}$  are defined as

$$\hat{n}_{i;I}^{\text{HF}} = \prod_{\sigma \in I} (\hat{n}_{i;\sigma} - n_{i;\sigma}^0) \quad \text{for } |I| \geq 1 \quad (13)$$

and  $\hat{n}_{i;\emptyset}^{\text{HF}} \equiv 1$ . Note that the definition of the Gutzwiller correlator and the Hartree–Fock operators differs from the one given in [16, 17]. In (13) we introduced

$$n_{i;\sigma}^0 = \langle \Phi_0 | \hat{n}_{i;\sigma} | \Phi_0 \rangle \equiv \langle \hat{n}_{i;\sigma} \rangle_0 \quad (14)$$

as the local densities in orbital  $\sigma$  in the *new* single-particle product state  $|\Phi_0\rangle$ . Equation (12) poses  $2^{2N}$  conditions for the  $2^{2N} - (2N + 1)$  parameters  $x_{i;I}$  ( $|I| \geq 2$ ) and the  $2N + 1$  parameters  $\eta_{i;\emptyset}, \dots, \eta_{i;2N}$ . We will solve for them in terms of the original variational parameters  $g_{i;I}$  ( $|I| \geq 2$ ) in the next section.

The parameters  $x_{i;I}$  ( $|I| \geq 2$ ) go to zero for small interaction strengths since  $g_{i;I}(U_i^{\sigma,\sigma'} \rightarrow 0) \rightarrow 1$ . Hence, we may use them as the expansion parameters for a perturbative approach. In its diagrammatic formulation the  $x_{i;I}$  play the role of (internal) vertices at which (at least) four lines intersect. The crucial point in the expansion (12) is the fact that there will be no Hartree (‘bubble’) diagrams which are of order unity in all dimensions. Since we are interested in simple expressions in infinite dimensions, we included their contribution in the expansion parameters  $x_{i;I}$ . Note that we will make the necessary assumption that local ‘Fock terms’ do not occur, i.e. we demand

$$\langle \Phi_0 | \hat{c}_{i;\sigma}^+ \hat{c}_{i;\sigma'} | \Phi_0 \rangle = \delta_{\sigma,\sigma'} n_{i;\sigma}^0 \quad (15)$$

for the one-particle product wave function  $|\Phi_0\rangle$ .

**2.2.2. Application of Wick’s theorem.** As our second step we formally expand the expectation values that we need for the calculation of the variational ground-state energy (9). With the help of (12) we may write

$$\langle \Psi_G | \hat{m}_{f;I} | \Psi_G \rangle = \langle \Phi_0 | \hat{P}_f \hat{m}_{f;I} \hat{P}_f \prod_{i \neq f} \hat{P}_i^2 | \Phi_0 \rangle \quad (16a)$$

$$\langle \Psi_G | \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} | \Psi_G \rangle = \langle \Phi_0 | (\hat{P}_f \hat{c}_{f;\sigma_f}^+ \hat{P}_f) (\hat{P}_h \hat{c}_{h;\sigma_h} \hat{P}_h) \prod_{i \neq f} \hat{P}_i^2 | \Phi_0 \rangle \quad (16b)$$

$$\prod_{i \neq f (f,h)} \hat{P}_i^2 = 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \sum'_{i_1, \dots, i_k} \sum_{l_1, \dots, l_k} \prod_{j=1}^{i_k} (x_{j;l_j} \hat{n}_{j;l_j}^{\text{HF}}) \quad (16c)$$

( $|I| \geq 2$ )

where the prime on the summation indicates that all lattice sites are different,

$$f \neq h \neq i_1 \neq \dots \neq i_k. \quad (16d)$$

There are still some Hartree contributions contained in (16a) and (16b) which come from the ‘external’ sites  $f$  and  $h$ . With the help of (4) we can always find unique expansions of the form

$$\hat{P}_f \hat{m}_{f;I} \hat{P}_f = \sum_{I_f} o_{f;I_f}^I \hat{n}_{f;I_f}^{\text{HF}} \quad (17a)$$

$$\hat{P}_f \hat{c}_{f;\sigma_f}^+ \hat{P}_f = \hat{c}_{f;\sigma_f}^+ \sum_{I_f (\sigma_f \notin I_f)} z_{f;I_f}^{\sigma_f} \hat{n}_{f;I_f}^{\text{HF}} \quad (17b)$$

$$\hat{P}_h \hat{c}_{h;\sigma_h} \hat{P}_h = \hat{c}_{h;\sigma_h} \sum_{I_h (\sigma_h \notin I_h)} z_{h;I_h}^{\sigma_h} \hat{n}_{h;I_h}^{\text{HF}}. \quad (17c)$$

Later, in section 3.2, we will calculate explicitly the coefficients  $o_{f;I_f}^I$  and  $z_{f;I_f}^{\sigma_f}$  in terms of the variational parameters  $g_{i;I}$  and  $\eta_{i;\emptyset}$ ,  $\eta_{i;\sigma}$ . We introduce the abbreviations

$$T_{f,i_1,\dots,i_k}^{I_f,I_1,\dots,I_k} = \langle \Phi_0 | \hat{n}_{f;I_f}^{\text{HF}} \prod_{j=i_1}^{i_k} \hat{n}_{j;I_j}^{\text{HF}} | \Phi_0 \rangle \quad (18a)$$

$$S_{f,h,i_1,\dots,i_k}^{I_f,I_h,I_1,\dots,I_k}(\sigma_f, \sigma_h) = \langle \Phi_0 | \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} \hat{n}_{f;I_f}^{\text{HF}} \hat{n}_{h;I_h}^{\text{HF}} \prod_{j=i_1}^{i_k} \hat{n}_{j;I_j}^{\text{HF}} | \Phi_0 \rangle \quad (18b)$$

where the products are replaced by unity for  $k = 0$ . This notation allows us to rewrite (16) as

$$\langle \Psi_G | \hat{m}_{f;I} | \Psi_G \rangle = \sum_{I_f} o_{f;I_f}^I \left[ T_{f,i_1,\dots,i_k}^{I_f,I_1,\dots,I_k} + \sum_{k=1}^{\infty} \frac{1}{k!} \sum'_{i_1,\dots,i_k} \sum_{\substack{I_1,\dots,I_k \\ (|I_i| \geq 2)}} \left( \prod_{j=i_1}^{i_k} x_{j;I_j} \right) T_{f,i_1,\dots,i_k}^{I_f,I_1,\dots,I_k} \right] \quad (19a)$$

$$\begin{aligned} \langle \Psi_G | \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} | \Psi_G \rangle &= \sum_{I_f, I_h} z_{f;I_f}^{\sigma_f} z_{h;I_h}^{\sigma_h} \\ &\times \left[ S_{f,h,i_1,\dots,i_k}^{I_f,I_h,I_1,\dots,I_k}(\sigma_f, \sigma_h) + \sum_{k=1}^{\infty} \frac{1}{k!} \sum'_{i_1,\dots,i_k} \sum_{\substack{I_1,\dots,I_k \\ (|I_i| \geq 2)}} \left( \prod_{j=i_1}^{i_k} x_{j;I_j} \right) S_{f,h,i_1,\dots,i_k}^{I_f,I_h,I_1,\dots,I_k}(\sigma_f, \sigma_h) \right]. \end{aligned} \quad (19b)$$

The primes on the lattice sums indicate that all lattice indices are different from each other. Moreover, the definition (3) implies that a given orbital index occurs only once at each lattice site.

Now we are in the position to apply Wick’s theorem [23]. The expectation values (18) can then be written as determinants. Equation (18a) becomes

$$T_{f,i_1,\dots,i_k}^{I_f,I_1,\dots,I_k} = \begin{vmatrix} M_{f,f} & M_{f,i_1} & \dots & M_{f,i_k} \\ M_{i_1,f} & M_{i_1,i_1} & \dots & M_{i_1,i_k} \\ \vdots & \vdots & \ddots & \vdots \\ M_{i_k,f} & M_{i_k,i_1} & \dots & M_{i_k,i_k} \end{vmatrix} \quad (20)$$

where we introduced the submatrices

$$M_{i,j} = \begin{pmatrix} P_{i,j}^{\sigma_i, \sigma'_i} & \dots & P_{i,j}^{\sigma_i, \sigma'_{|I_j|}} \\ \vdots & & \vdots \\ P_{i,j}^{\sigma_{|I_i|}, \sigma'_i} & \dots & P_{i,j}^{\sigma_{|I_i|}, \sigma'_{|I_j|}} \end{pmatrix}. \quad (21)$$

Here, the orbital indices  $\sigma_1, \dots, \sigma_{|I_i|}$  ( $\sigma'_1, \dots, \sigma'_{|I_j|}$ ) are the elements of  $I_i$  ( $I_j$ ), and

$$P_{i,j}^{\sigma,\sigma'} = (1 - \delta_{i,j}) \langle \Phi_0 | \hat{c}_{i;\sigma}^+ \hat{c}_{j;\sigma'} | \Phi_0 \rangle \equiv (1 - \delta_{i,j}) \langle \hat{c}_{i;\sigma}^+ \hat{c}_{j;\sigma'} \rangle_0 \quad (22)$$

is the one-particle density matrix for the one-particle product wave function  $|\Phi_0\rangle$  for  $i \neq j$ . These objects play the role of ‘lines’ in our diagrammatic expansion. Note that we do not have to distinguish between ‘hole’ and ‘particle’ lines because all sites are different when we apply Wick’s theorem [16–18]. Furthermore, local terms did not arise because we subtracted the Hartree contributions and ruled out Fock terms according to (15). Similarly, equation (18b) becomes

$$S_{f,h,i_1,\dots,i_k}^{I_f,I_h,I_{i_1},\dots,I_{i_k}}(\sigma_f, \sigma_h) = (-1)^{|I_f||I_h|-|I_f|-|I_h|} \begin{vmatrix} M_{h,f} & M_{h,h} & M_{h,i_1} & \dots & M_{h,i_k} \\ M_{f,f} & M_{f,h} & M_{f,i_1} & \dots & M_{f,i_k} \\ M_{i_1,f} & M_{i_1,h} & M_{i_1,i_1} & \dots & M_{i_1,i_k} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ M_{i_k,f} & M_{i_k,h} & M_{i_k,i_1} & \dots & M_{i_k,i_k} \end{vmatrix}. \quad (23)$$

The matrices  $M_{i,j}$  in (23) are again given by (21). Here, the orbital indices belonging to the lattice sites  $f$  and  $h$  are elements of  $I_f$ ,  $I_f \cup \sigma_f$ ,  $I_h$ , and  $I_h \cup \sigma_h$ , respectively.

To calculate expectation values for  $|\Psi_G\rangle$  we have to divide the numerators, equation (19), by the norm

$$\langle \Psi_G | \Psi_G \rangle = \langle \Phi_0 | \Phi_0 \rangle + \sum_{k=1}^{\infty} \frac{1}{k!} \sum'_{i_1,\dots,i_k} \sum_{\substack{I_{i_1},\dots,I_{i_k} \\ (|I_l| \geq 2)}} \left( \prod_{j=i_1}^{i_k} x_{j;I_j} \right) T_{i_1,\dots,i_k}^{I_{i_1},\dots,I_{i_k}}. \quad (24)$$

In principle, we could derive diagram rules for the series expansion of the determinants in powers of the parameters  $x_{j;I_j}$ . In this paper we restrict ourselves to the limit of infinite dimensions where not a single diagram needs to be calculated.

**2.2.3. The linked-cluster theorem.** The summation restrictions prevent us from applying the linked-cluster theorem. In the case of a single band ( $N = 1$ ) the summation restrictions (16d) can simply be dropped because the determinants (20) and (23) vanish identically if two lattice indices coincide. Since we may then independently sum over all lattice sites the linked-cluster theorem applies [23] such that the disconnected diagrams in the numerator are cancelled by the norm [16].

The case where  $N \geq 2$  requires more care because, in general, the determinants  $T$  in (20) and  $S$  in (23) remain finite when we equate two lattice sites. To make progress we note that a summation restriction over the spin-orbit indices in  $I_{i_1}, \dots, I_{i_k}$  will not destroy the applicability of the linked-cluster theorem. To see this, we write a typical spin-orbit sum in (19) in the form [17]

$$\sum_I f(I) = \sum_{r=1}^{2N} \frac{1}{r!} \sum'_{\alpha_1,\dots,\alpha_r} f(\alpha_1, \dots, \alpha_r). \quad (25)$$

The ensuing summation restriction  $\alpha_1 \neq \alpha_2 \neq \dots \neq \alpha_r$  can be removed because the determinants in (20) and (23) vanish if two of these indices are identified.

Now we equate two lattice sites  $l$  and  $m$ , e.g. in the determinant (20). Two different cases have to be distinguished: (i) if  $I_l$  and  $I_m$  have at least two elements in common the determinant (20) vanishes since at least two rows or columns will be identical; (ii) otherwise, if  $I_l$  and  $I_m$  have no common element, the determinant (20) remains finite. When we equate two lattice sites in the determinant we effectively map two vertices onto each other in the

corresponding diagrammatic expansion, i.e. we generate a diagram that already appeared at some lower order in the expansion; see [17] for a simple example for this ‘vertex packing’. The original diagram with  $l$  and  $m$  put equal and the corresponding lower-order diagram have the same topology but different prefactors,  $x_{i;I_i \cup I_m}$  for the lower-order diagram and  $x_{l;I_l} x_{m;I_m}$  for the new contribution. If we relax all summation restrictions in the numerator and in the norm we must replace the vertices  $x_{i;I_i}$  and the coefficients  $o_{i;I_i}^l$  and  $z_{i;I}^\sigma$  by effective ones, i.e.  $x_{i;I} \rightarrow \tilde{x}_{i;I}$ ,  $o_{i;I_i}^l \rightarrow \tilde{o}_{i;I_i}^l$ , and  $z_{i;I}^\sigma \rightarrow \tilde{z}_{i;I}^\sigma$ . Fortunately, the lowest-order coefficients  $o_{i;\emptyset}^l$  and  $z_{i;\emptyset}^\sigma$  remain unchanged by this procedure because these coefficients correspond to diagrams without an internal vertex whereas the ‘vertex packing’ leaves behind at least one internal vertex [17]. In the next section we will show that  $o_{i;\emptyset}^l$  and  $z_{i;\emptyset}^\sigma$  alone give the exact result in infinite dimensions. Since the number of correction terms generated in a given order of the expansion remains finite, the calculation of systematic  $1/d$  corrections is still possible although very tedious.

Now that we have formally eliminated all summation restrictions we can apply the linked-cluster theorem. We thus find

$$\langle \hat{m}_{f;I} \rangle = o_{f;\emptyset}^I + \sum_{\substack{I_f \\ (|I_f| \geq 1)}} \tilde{o}_{f;I_f}^I \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{i_1, \dots, i_k} \sum_{\substack{I_{i_1}, \dots, I_{i_k} \\ (|I_i| \geq 2)}} \left\{ \hat{n}_{f;I_f} \prod_{j=i_1}^{i_k} \tilde{x}_{j;I_j} \hat{n}_{j;I_j}^{\text{HF}} \right\}_0^{\text{C}} \quad (26a)$$

$$\begin{aligned} \langle \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} \rangle &= z_{f;\emptyset}^{\sigma_f} z_{h;\emptyset}^{\sigma_h} \langle \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} \rangle_0 + \sum_{\substack{I_f, I_h \\ (|I_f| + |I_h| \geq 1)}} z_{f;I_f}^{\sigma_f} z_{h;I_h}^{\sigma_h} \\ &\times \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{i_1, \dots, i_k} \sum_{\substack{I_{i_1}, \dots, I_{i_k} \\ (|I_i| \geq 2)}} \left\{ \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} \hat{n}_{f;I_f}^{\text{HF}} \hat{n}_{h;I_h}^{\text{HF}} \prod_{j=i_1}^{i_k} \tilde{x}_{j;I_j} \hat{n}_{j;I_j}^{\text{HF}} \right\}_0^{\text{C}} \end{aligned} \quad (26b)$$

where, as usual,  $\{\dots\}_0^{\text{C}}$  indicates that only the connected diagrams need to be considered.

### 3. Exact results in infinite dimensions

In this section we briefly review the diagrammatic simplifications which occur in infinite dimensions. We find that in our approach not a single diagram needs to be calculated in this limit. Consequently, we derive explicit analytic expressions for the variational ground-state energy, the one-particle density matrices, and the average net occupation densities which are exact in infinite dimensions and valid for the whole class of Gutzwiller-correlated wave functions.

#### 3.1. Simplifications

Systematic studies of the limit of infinite dimensions for itinerant-electron systems started with the work of Metzner and Vollhardt [24]; for details and a recent review, see chapter 5 of [2].

To obtain a sensible limit  $d \rightarrow \infty$  on a hypercubic lattice the matrix elements between two sites  $i$  and  $j$  have to be scaled as

$$t_{i,j}^{\sigma,\sigma'} = \tilde{t}_{i,j}^{\sigma,\sigma'} d^{-|i-j|/2} \quad (27)$$

where  $\tilde{t}_{i,j}^{\sigma,\sigma'}$  is independent of the dimension and  $|i-j| = \sum_{l=1}^d |i_l - j_l|$  is the distance between the two sites in the New York metric.

One of the resulting simplifications is the following: if two vertices  $l$  and  $m$  are connected by three independent (Green function) lines, only the contribution for  $l = m$  survives in infinite dimensions. For example, in the one-band case the (proper) self-energy becomes purely local in this limit. In our variational theory the lines between two sites represent the one-particle density matrices  $P_{l,m}^{\sigma,\sigma'}$  (22). They *vanish* by construction, if we set  $l = m$ . Consequently, the variational (proper) self-energy is identically zero in the limit of infinite dimensions in the one-band case [16, 17]. Note that we guaranteed in our expansion that there are no Hartree contributions such that all (internal) vertices are connected by at least three lines. For the case where  $N \geq 2$ , vertices with more than four lines appear for which our arguments particularly apply, and any diagram with more than one line must vanish in infinite dimensions.

Consequently, not a single diagram needs to be calculated. Instead, we immediately find from (27)

$$\langle \hat{m}_{f;l} \rangle^{(d=\infty)} = o_{f;\emptyset}^I \quad (28a)$$

$$\langle \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} \rangle^{(d=\infty)} = z_{f;\emptyset}^{\sigma_f} z_{h;\emptyset}^{\sigma_h} \langle \hat{c}_{f;\sigma_f}^+ \hat{c}_{h;\sigma_h} \rangle_0 \quad (28b)$$

in infinite dimensions. Thus, the problem is formally solved since only the coefficients  $o_{f;\emptyset}^I$  and  $z_{f;\emptyset}^{\sigma_f}$  and the properties of the single-particle product wave function  $|\Phi_0\rangle$  enter the final expressions.

### 3.2. Explicit results for the ground-state energy

Thus far the variational ground-state energy for general Gutzwiller-correlated wave functions could only be accomplished for  $N = 1$  [16, 18]. Here we show that explicit expressions for the ground-state energy can be obtained for all interaction strengths and all  $N \geq 1$ . In the following considerations we suppress the spatial index.

The remaining problem is the calculation of the coefficients  $o_{i;\emptyset}^I$  and  $z_{i;\emptyset}^\sigma$ . We recast the modified Gutzwiller correlator (11) into the form

$$\hat{P} = \eta_\emptyset \left[ 1 + \sum_I (\tilde{\eta}_I g_I - 1) \hat{m}_I \right] \quad (29)$$

where we have introduced the notation

$$\begin{aligned} \tilde{\eta}_\emptyset &= 1 \\ \tilde{\eta}_I &= \prod_{\sigma \in I} \eta_\sigma \quad \text{for } |I| \geq 1 \\ g_I &= 1 \quad \text{for } |I| \leq 1. \end{aligned} \quad (30)$$

Then, the left-hand side of (17a) becomes

$$\hat{P} \hat{m}_I \hat{P} = \eta_\emptyset^2 \tilde{\eta}_I^2 g_I^2 \hat{m}_I. \quad (31)$$

Now we expand the net occupancy operators  $\hat{m}_I$  in terms of the Hartree–Fock operators  $\hat{n}_I^{\text{HF}}$  as

$$\hat{m}_I = \prod_{\sigma \in I} (n_\sigma^0 + \hat{n}_\sigma^{\text{HF}}) \prod_{\sigma \in \bar{I}} ((1 - n_\sigma^0) - \hat{n}_\sigma^{\text{HF}}) = \sum_{I'} \left[ (-1)^{|\bar{I} \cap I'|} \prod_{\sigma \in I \setminus I'} n_\sigma^0 \prod_{\sigma \in \bar{I} \setminus I'} (1 - n_\sigma^0) \right] \hat{n}_{I'}^{\text{HF}}. \quad (32)$$

We compare this expression with the right-hand side of (17a) and find the simple result

$$o_{I'}^I = (-1)^{|\bar{I} \cap I'|} \eta_\emptyset^2 \tilde{\eta}_I^2 g_I^2 \prod_{\sigma \in I \setminus I'} n_\sigma^0 \prod_{\sigma \in \bar{I} \setminus I'} (1 - n_\sigma^0). \quad (33)$$

The representation of the modified Gutzwiller correlator in (29) allows us to write

$$\hat{P}^2 = \eta_\emptyset^2 \left[ 1 + \sum_I (\tilde{\eta}_I^2 g_I^2 - 1) \hat{m}_I \right]. \quad (34)$$

Again, we expand the net occupancy operators  $\hat{m}_I$  in terms of the Hartree–Fock operators  $\hat{n}_I^{\text{HF}}$ , equation (32).

Now we are in the position to compare (34) with (12). The constant coefficient gives

$$\eta_\emptyset^2 \left[ 1 + \sum_I (\tilde{\eta}_I^2 g_I^2 - 1) m_I^0 \right] = 1 \quad (35a)$$

where

$$m_I^0 = \prod_{\sigma \in I} n_\sigma^0 \prod_{\sigma \in \bar{I}} (1 - n_\sigma^0) \quad (35b)$$

is the corresponding net occupation density in the uncorrelated wave function  $|\Phi_0\rangle$ . By construction, the coefficient to first order in  $\hat{n}_\sigma^{\text{HF}}$  is zero in (12). We thus find

$$\eta_\emptyset^2 \sum_{I(\sigma \in I)} (\tilde{\eta}_I^2 g_I^2 - 1) \frac{m_I^0}{n_\sigma^0} - \eta_\emptyset^2 \sum_{I(\sigma \notin I)} (\tilde{\eta}_I^2 g_I^2 - 1) \frac{m_I^0}{1 - n_\sigma^0} = 0. \quad (36)$$

Finally, the higher orders in the Hartree–Fock operators in (34) and (12) fix the coefficients  $x_I$ :

$$x_I = \sum_{I'} \frac{\tilde{\eta}_{I'}^2 g_{I'}^2 - 1}{\tilde{\eta}_{I'}^2 g_{I'}^2} o_{I'}^I \quad (37)$$

where we used (33). For  $N \geq 2$  one cannot explicitly solve (35), (36), and (37) for  $\eta_\emptyset$ ,  $\eta_\sigma$ , and  $x_I$  in terms of  $n_\sigma^0$  and  $g_I$ .

In the limit of infinite dimensions we can obtain explicit results for the ground-state energy. From (28a) we find

$$m_I = \langle \hat{m}_I \rangle = o_{I'}^I = \eta_\emptyset^2 \tilde{\eta}_I^2 g_I^2 m_I^0 \quad (38)$$

in infinite dimensions. Equation (38) implies that the  $\eta$ -terms can be expressed by the net occupancy densities as

$$\eta_\emptyset^2 = \frac{m_\emptyset}{m_\emptyset^0} \quad \eta_\sigma^2 = \frac{m_\sigma m_\emptyset^0}{m_\sigma^0 m_\emptyset}. \quad (39)$$

Note that these simple results do not hold in terms of the single-particle product wave function  $|\Psi_0\rangle$  in (7a) but only in terms of  $|\Phi_0\rangle$ ; compare equation (10). Furthermore, equation (38) allows us to replace the original variational parameters  $g_I$  by their physical counterparts, the net occupancy densities  $m_I$  ( $|I| \geq 2$ ), as

$$\begin{aligned} g_{a,b}^2 &= \frac{m_\emptyset m_{ab}}{m_a m_b} \\ &\vdots \\ g_{1,\dots,2N}^2 &= \frac{(m_\emptyset)^{2N-1} m_{1,\dots,2N}}{m_1 \cdots m_{2N}}. \end{aligned} \quad (40)$$

Equations (40) are well known from the Gutzwiller approximation for the one-band [26, 25] and the multi-band cases [9]. They show that the parameters  $g_I^2$  rule the law of mass action between single occupancies of a site on the one hand and its multiple occupancies and vacancies on the other hand.

In infinite dimensions equation (35) is trivially fulfilled since

$$\sum_I m_I = 1 \quad (41)$$

is true by definition. From the definition of net and gross operators (4) we know that the (gross) occupancy in the orbital  $\sigma$  is given by

$$n_\sigma = \sum_{I(\sigma \in I)} m_I. \quad (42a)$$

We further use

$$\sum_{\substack{I(\sigma \notin I) \\ |I| \geq 1}} m_I = 1 - m_\emptyset - n_\sigma \quad (42b)$$

in (36). With the help of (39) it is easy to show that

$$n_\sigma = n_\sigma^0 \quad (43)$$

holds in infinite dimensions. It is thus seen that the local densities in the Gutzwiller-correlated wave function  $|\Psi_G\rangle$  and in the one-particle product wave function  $|\Phi_0\rangle$  are the same. This would not have been so if we had worked with the one-particle product wave function  $|\Psi_0\rangle$ ; see (7a). For this reason we introduced the new one-particle state  $|\Phi_0\rangle$  in (10), where the single-particle  $\eta$ -terms could be interpreted as ‘chemical potentials’ which guarantee that the average single-orbital occupancies remain unchanged by the modified Gutzwiller correlator (11).

Thus far we have replaced the original variational parameters  $g_I$  by their physical counterparts, the average multiple occupancies  $m_I$ . As a last step we have to express the coefficients  $z_\emptyset^\sigma$  in terms of our new variational parameters. According to (9b) and (28b) they can be interpreted as site-dependent renormalization factors for the electron transfer between two sites. For their derivation we introduce the operators

$$\hat{m}_I^\sigma = \prod_{\sigma' \in I \setminus \sigma} \hat{n}_{\sigma'} \prod_{\sigma' \in \bar{I} \setminus \sigma} (1 - \hat{n}_{\sigma'}). \quad (44)$$

Thus we may write

$$\begin{aligned} \hat{P} \hat{c}_\sigma^+ \hat{P} &= \eta_\emptyset \left( 1 + \sum_{I(\sigma \in I)} (\tilde{\eta}_I g_I - 1) \hat{m}_I \right) \hat{c}_\sigma^+ \eta_\emptyset \left( 1 + \sum_{I(\sigma \notin I)} (\tilde{\eta}_I g_I - 1) \hat{m}_I \right) \\ &= \eta_\emptyset^2 \hat{c}_\sigma^+ \left( 1 + \sum_{I(\sigma \notin I)} (\tilde{\eta}_{I \cup \sigma} g_{I \cup \sigma} - 1) \hat{m}_I^\sigma \right) \left( 1 + \sum_{I(\sigma \in I)} (\tilde{\eta}_I g_I - 1) \hat{m}_I^\sigma \right) \\ &= \eta_\emptyset^2 \hat{c}_\sigma^+ \left( 1 + \sum_{I(\sigma \notin I)} (\tilde{\eta}_{I \cup \sigma} g_{I \cup \sigma} \tilde{\eta}_I g_I - 1) \hat{m}_I^\sigma \right). \end{aligned} \quad (45)$$

With the help of (32) we may again expand the projection operators  $\hat{m}_I^\sigma$  in terms of the Hartree–Fock operators  $\hat{n}_I^{\text{HF}}$ . A comparison with the definition (17b) then gives

$$z_I^\sigma = \eta_\emptyset^2 \delta_{I, \emptyset} + \eta_\emptyset^2 \sum_{I'(\sigma \notin I')} (-1)^{|I \cap \bar{I}'|} (\tilde{\eta}_{I' \cup \sigma} g_{I' \cup \sigma} \tilde{\eta}_{I'} g_{I'} - 1) \prod_{\sigma' \in I' \setminus I} n_{\sigma'}^0 \prod_{\sigma' \in \bar{I}' \setminus (I \cup \sigma)} (1 - n_{\sigma'}^0). \quad (46)$$

This includes the special case of  $I = \emptyset$  which we need for the calculation of the renormalization factors for the electron transfers:

$$z_{\emptyset}^{\sigma} = \eta_{\emptyset}^2 + \eta_{\emptyset}^2 \sum_{I(\sigma \notin I)} (\tilde{\eta}_{I \cup \sigma} g_{I \cup \sigma} \tilde{\eta}_I g_I - 1) \frac{m_I^0}{1 - n_{\sigma}^0}. \quad (47)$$

We use (38) and the identities

$$m_{I \cup \sigma}^0 = \frac{n_{\sigma}^0}{1 - n_{\sigma}^0} m_I^0 \quad (48a)$$

$$\sum_{I(\sigma \notin I)} m_I^0 = 1 - n_{\sigma}^0 \quad (48b)$$

(see (35b) and (42a)), and finally arrive at

$$\sqrt{q_{\sigma}} \equiv z_{\emptyset}^0 = \frac{1}{\sqrt{(1 - n_{\sigma}^0) n_{\sigma}^0}} \sum_{I(\sigma \notin I)} \sqrt{m_{I \cup \sigma} m_I}. \quad (49)$$

This leads to our final expression for the ground-state energy

$$E_0^{\text{var}}(m_{i;I}; |\Phi_0\rangle) = \sum_{i,j;\sigma,\sigma'} \sqrt{q_{i;\sigma}} \sqrt{q_{j;\sigma'}} t_{i,j}^{\sigma,\sigma'} \langle \hat{c}_{i;\sigma}^+ \hat{c}_{j;\sigma'} \rangle_0 + \sum_{i;I(|I| \geq 2)} U_{i;I} m_{i;I}. \quad (50)$$

To fix the variational parameters  $m_{i;I}$  ( $|I| \geq 2$ ) and those in  $|\Phi_0\rangle$ , the minimum of this expression has to be determined. We plan to publish applications of the formalism elsewhere.

#### 4. Comparison with other approaches

In this section we compare our results to those of related work, namely the Gutzwiller approximation and the slave-boson mean-field approach, which are seen to become variationally controlled in infinite dimensions. Finally, we briefly discuss the applicability of the variational approach to the Anderson transition in strongly correlated electron systems.

##### 4.1. Generalized Gutzwiller approximations

For the one-band case it is known that the results of the Gutzwiller approximation for the Gutzwiller wave function become exact in infinite dimensions [16, 24, 27]. In addition, the variational calculation of correlation functions is straightforward in infinite dimensions [16], whereas their consistent treatment is beyond the Gutzwiller approximation scheme.

Generalizations of the Gutzwiller approximation to other situations than the translationally invariant, paramagnetic one-band Gutzwiller wave function encounter two conceptual difficulties. (i) It is not clear from the beginning whether the generalized Gutzwiller approximations in [6–9] lead to physically acceptable results over the whole parameter space. For example, early extensions of the Gutzwiller approximation to the case of antiferromagnetism gave rise to negative occupation densities [28]. (ii) The Gutzwiller approximation may give the correct results in infinite dimensions but the corresponding wave function could not be identified properly. For example, in a recent treatment Okabe [7] found the correct expression for the ground-state energy (50) in infinite dimensions for a special case but he did not specify the corresponding Gutzwiller wave function. Therefore, his results could not be tested against numerical approaches. In contrast, the wave function (7) provides a solid starting point for variational Monte Carlo simulations. Hence, an assessment of the quality of the Gutzwiller approximation for finite dimensions can now be performed; see, e.g., [29, 30] for applications to the one-band case.

The proper choice of the wave function (7) was essential for its approximation-free evaluation in infinite dimensions. In our definition of generalized Gutzwiller-correlated wave functions *each* multiple occupancy of a lattice site is controlled by its own variational parameter. Equations (40) show that we may then replace these variational parameters by their physical counterparts, the net multiple occupancies  $m_I$ . In contrast, Chao and Gutzwiller [21] and Chao [22] considered a trial state for  $N = 2$ , which includes only variational parameters for the gross occupancies  $n_I$  for  $|I| = 2$ :

$$|\Psi'_G\rangle = \prod_i \prod_{(|I|=2)} g_I^{\hat{n}_{i,I}} |\Psi_0\rangle \quad (51)$$

where we have used our notation. In their evaluation the ‘maximum-term conditions’ of the Gutzwiller approximation [20] also lead to a set of  $2^{2N} - (2N + 1)$  equations similar to (40) but it cannot be solved explicitly because there are only  $N(2N - 1)$  variational parameters  $g_I$  ( $|I| = 2$ ) in (51). To make progress Chao set to zero all terms with multiple occupancies  $|I| \geq 3$ , an assumption not warranted by the wave function (51). If we (artificially) put  $m_{i,I} = 0$  for  $|I| \geq 3$  for our wave function (7) we recover Chao’s results. Hence, Chao’s results do apply to the Gutzwiller-correlated wave function (7) in a special limit.

Similarly, the results of Lu [6] are found to be correct if his further assumptions are adopted. He used site- and orbital-independent Coulomb interactions,  $U_i^{\sigma,\sigma'} = U$ , and assumed that some of the multiple occupancies vanish identically. In [9] it was shown that the latter assumption might not hold close to the Brinkman–Rice transition on the metallic side.

The proper form of the wave function for arbitrary band degeneracies (7) was first given by Bünemann and Weber [9] for translationally invariant systems ( $g_{i,I} \equiv g_I$ ). Using the Gutzwiller approximation they derived the equations (40), (49), and (50). Okabe, in a more recent treatment of the problem [8], also specified the proper Gutzwiller-correlated wave function for the translationally invariant case in the absence of inter-orbit hopping. In this work we showed that their results become exact in infinite dimensions. Furthermore, we explicitly covered all cases of symmetry breaking in the one-particle product wave functions  $|\Phi_0\rangle$ ; the cases of spin and orbital ordering in materials with degenerate bands can equally well be studied with the help of Gutzwiller-correlated wave functions.

#### 4.2. Slave-boson mean-field theory

For the one-band case the slave-boson mean-field theory [10, 32–34] yields the same results as Gutzwiller-correlated variational wave functions in infinite dimensions, including the cases of broken symmetry [16, 17]. Therefore, the slave-boson approach is variationally controlled at zero temperature in this limit. The slave-boson saddle-point free energy can be rederived from a ‘variational partition function’ [16, 17]. This construction shows that, at best, the slave-boson mean-field theory is applicable up to excitation energies for which Fermi-liquid theory is valid. Since Fermi-liquid parameters can be derived from the variational ground-state energy [25], the low-energy properties can equally well be described with the variational and the slave-boson mean-field approach.

Recently, the slave-boson mean-field theory for degenerate Hubbard models was worked out by Hasegawa [12] who used the extension of the Kotliar–Ruckenstein approach for the degenerate Anderson model given by Dorin and Schlottmann [11]. His results for  $N = 2$  completely agree with ours and, thus, the above statements on the virtues and limitations of the slave-boson mean-field approach also apply for the case of degenerate

bands. Independently, Frésard and Kotliar [13] derived a set of slave-boson mean-field equations and, as an application, reproduced Lu's results on the Mott transition [6].

#### 4.3. The Anderson transition in strongly correlated electron systems

Our approach also covers the case of local, energetically random impurity potentials  $\epsilon_i^\sigma$ . For illustrative purposes we restrict ourselves to  $N = 1$ ,  $U = \infty$ , and no spin-flip hopping. In this case the system is a Mott insulator at half-band-filling,  $\delta = 0$ , where  $\delta = 1 - (1/L) \sum_i n_i$  is the doping degree of the lower Hubbard band [2]. In this case the variational ground-state energy becomes

$$E_0^{\text{var}}(\Phi_0) = \sum_{i \neq j; \sigma} t_{i,j}^{\sigma,\sigma} \sqrt{q_{i;\sigma}} \sqrt{q_{j;\sigma}} \langle \Phi_0 | \hat{c}_{i;\sigma}^+ \hat{c}_{j;\sigma} | \Phi_0 \rangle + \sum_i \epsilon_i n_i \quad (52a)$$

$$q_{i;\sigma} = \frac{1 - n_i}{1 - n_{i;\sigma}}. \quad (52b)$$

Recall that the local occupation densities  $n_i = n_{i;\sigma} + n_{i;-\sigma} \leq 1$  are given by  $n_{i;\sigma} = \langle \hat{n}_{i;\sigma} \rangle = \langle \Phi_0 | \hat{n}_{i;\sigma} | \Phi_0 \rangle$ .

We may *interpret* our variational results (52) in terms of a two-fluid picture which naturally arises for strongly correlated disordered electron systems. A recent introduction and overview on the theory of the Anderson transition in interacting electron systems is given in [31]. (i) A certain fraction of electrons may localize, e.g. a  $\sigma$ -electron is localized on site  $l$  in  $|\Phi_0\rangle$ ,  $n_l = n_{l;\sigma} = 1$ . From the expectation value for the ground-state energy (52) it follows that the probability that the electron hops off the site  $l$  is zero. In addition, a  $-\sigma$ -electron will not hop onto this site because this is dynamically forbidden,  $q_{l;-\sigma} = 0$ . Within our variational description the occupation of site  $l$  does not change. The site  $l$  is equally likely occupied by a  $\sigma$ - or a  $-\sigma$ -electron and, therefore, the site contributes to a Curie-like susceptibility. (ii) The excluded sites represent an unretarded (random) hardcore potential for the remaining electrons besides the fluctuating local potentials  $\epsilon_i$  and the dynamical constraint of no double occupancy. The strength of the impurity potentials  $\epsilon_i$  and the degree of doping determine the fraction of 'localized' and 'mobile' electrons.

For a small degree of doping of the lower Hubbard band,  $\delta \ll 1$ , even the 'mobile' fraction of the electrons cannot carry DC current since their wave functions do not spread over macroscopic distances. The doping has to exceed some 'percolation threshold' to guarantee a finite DC conductivity. Above the critical doping for the Anderson transition  $\delta_c$  one should observe a metallic conductivity at zero temperature but the magnetic signatures of the localized fraction of the electrons ('local moments') should remain. It requires further doping beyond  $\delta_c$  to destroy the Curie behaviour of the magnetic susceptibility.

Qualitatively similar results are found by Dobrosavljević and Kotliar [35]. They used the dynamical mean-field theory approach and approximated the remaining local-impurity problem with the help of the slave-boson mean-field approach of Barnes, Coleman, and Read and Newns [32–34]. They also address the strong-coupling limit and find that local moments form in the metallic phase before the Anderson transition takes place. In their case the strength of the impurity potentials is varied for fixed doping. In both cases the position of the mobility edge is varied with respect to the Fermi energy, and the physics should qualitatively be the same. It should be clear, though, that our variational approach gives only a rather crude description for the local moment formation and the Anderson transition in the lower Hubbard band.

## 5. Summary

In this work we introduced a general class of Gutzwiller-correlated wave functions for multi-band Hubbard models. In contrast to earlier generalizations of the original Gutzwiller wave function [20] to the case of degenerate bands [17, 21, 22] we introduced independent variational parameters for each multiple occupancy of a lattice site. Only in this most general form can each of the original variational parameters  $g_{i,l}$  be expressed in terms of the net occupancy densities  $m_{i,l}$  which give the average probability that configuration  $l$  is present on site  $i$ .

We developed a diagrammatic formalism which allows the approximation-free evaluation of our general Gutzwiller-correlated wave functions in the limit of infinite spatial dimensions. Our analytical results reproduce recent results obtained within the Gutzwiller approximation [6–9] and extend these to the case of a broken symmetry. In addition, the slave-boson mean-field theory [11–13] becomes variationally controlled at zero temperature in the limit of infinite dimensions. As can be inferred from the single-band case, the slave-boson approach at finite temperatures is limited to the Fermi-liquid regime [16, 17]; see also chapter 3.5 of [2]. Lastly, we briefly discussed the results of the variational approach to the Anderson transition in strongly correlated one-band systems.

In principle, we could go beyond the limitations of the Gutzwiller approximation and systematically calculate ground-state correlation functions and  $1/d$  corrections. However, the diagrammatic evaluation would be very tedious, and we consider it unlikely that such an effort would lead to qualitative changes of our understanding of band-degenerate Hubbard models based on our variational approach. For the moment it appears to be more rewarding to elucidate the ground-state energy (50) in more detail. Thus far this expression has been investigated only for rather simple model systems [7–12]. These preliminary studies showed significant differences for the ground-state magnetization as a function of the interaction strength between the Hartree–Fock and the Gutzwiller-correlated wave functions, as expected from the one-band case. Furthermore, discontinuous metal–insulator transitions occur for  $N \geq 2$  for which the gap jumps to a finite value at the critical interaction strength [9, 12].

The investigation of the variational ground-state phase diagram for realistic models, e.g. for five  $d$  orbitals, is a numerically difficult task because the number of variational parameters increases exponentially with the number of orbitals. Nevertheless, one may use various symmetries of different multiple occupancies which considerably reduces the number of independent variational parameters such that the realistic case  $N = 5$  for transition metals and their compounds should become tractable.

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