Properties of Gutzwiller wave functions for multiband models

Claudio Attaccalite[1] and Michele Fabrizio[1,2]
[1]*International School for Advanced Studies, SISSA, Via Beirut 2, I-34014 Trieste, Italy*
[2]*International Center for Theoretical Physics, ICTP, Strada Costiera 11, I-34100, Trieste, Italy*
(Received 31 March 2003; revised manuscript received 6 June 2003; published 24 October 2003)

We analyze the Mott transition in multiband Hubbard models with the inclusion of multiplet exchange splittings as it arises in infinite dimensions by using the generalized Gutzwiller wave function introduced by Bünemann, Weber, and Gebhard [Phys. Rev. B **57**, 6896 (1998)]. We also present an extension of that variational wave function to account for broken-symmetry solutions, which still allows an exact analytical treatment. Our analysis reveals some drawbacks of the variational wave function, which, in our opinion, imply that Gutzwiller-type wave functions do not properly characterize quasiparticles close to a Mott transition even in the limit of infinite dimensions.

DOI: 10.1103/PhysRevB.68.155117 PACS number(s): 71.30.+h, 71.10.−w

I. INTRODUCTION

After so many years since its proposal,[1] the Mott transition maintains intact its scientific interest, continually kept alive by the growing number of materials which, on the track of becoming Mott insulators, show rich and fascinating physical properties, among which high-T_c superconductivity is likely the most spectacular example.

Much of the theoretical effort till now has been devoted towards cuprate-inspired mainly single-band models, like the standard Hubbard model or its strongly correlated counterpart, the t-J model. Although unsolved questions still remain, a lot has been unveiled about the Mott transition in the single-band Hubbard model, especially after the development of the so-called dynamical mean-field theory (DMFT).[2] DMFT, which is exact in the limit of infinite coordination lattices, represents a quite reliable approach to investigate the on-site dynamical behavior across the Mott transition. Yet, in its original version, DMFT is not able to yield accurate results concerning intersite correlations, which are treated in a mean-field-like fashion, although several extensions have been proposed.[3] For that reason, other approaches have been often adopted to investigate the possible occurrence of d-wave superconductivity in proximity to the Mott insulating phase of single-band Hubbard and t-J models, most of which are more or less explicitly related to the Gutzwiller variational technique.[4] That amounts to studying a variational wave function consisting of a simple Slater determinant where doubly occupied sites are partially or completely projected out. The Gutzwiller wave function can be rigorously handled only numerically in finite dimensions, although an approximate analytical scheme to evaluate average values was proposed by Gutzwiller himself,[4] thereafter called the Gutzwiller approximation formula (GAF). Later on, it was realized that the GAF gives an exact account of the Gutzwiller wave function in the case of infinite coordination lattices,[5] and that it provides similar results to the slave-boson method within the saddle-point approximation.[5,6] Moreover, the GAF seems to be accurate enough whenever the Gutzwiller wave function yields a faithful description of the ground state,[6,7] which usually happens when already the unprojected trial wave function gives qualitatively correct ground state properties. In spite of the interesting developments achieved by means of the Gutzwiller variational wave function in single-band Hamiltonians, especially for what it concerns d-wave superconductivity in the t-J model,[8–10] there have been not many attempts to apply the same technique to multiband models, even though there are many interesting strongly correlated materials where orbital degrees of freedom play an important role. Indeed there exist several analyses based on multiband extensions of the GAF (Refs. 11–13) and of slave-boson technique,[14] but a direct comparison with more exact results to test the quality of the Gutzwiller wave function is still missing, even though DMFT results for multiband Hubbard models are by now available.[15–19]

In this paper, we review the multiband extension of the Gutzwiller wave function (GWF) proposed in Ref. 11 which has the big advantage of being analytically treatable in the limit of infinite dimensions. Moreover, we propose a further extension to broken-symmetry phases, which maintains the same property of being analytically accessible in infinite dimensions without losing any variational freedom. In this limit, we single out some peculiar properties of the GWF close to the Mott transition. The comparison with exact DMFT results reveals some drawbacks of the GWF which may lead to even qualitatively incorrect results. This may not come as quite a surprise. In fact, it is well known that the simplest Gutzwiller wave function, obtained by partly projecting out double occupancies from a paramagnetic Fermi sea, does not provide a very accurate description of the single-band Hubbard model at half-filling in finite dimensions because it does not properly account for relevant spatial correlations.[20–23] Just for that reason, the paramagnetic Gutzwiller wave function does not show any Mott transition in finite dimensions, while it does in infinite dimensions, where spatial correlations are not so crucial. Indeed, a comparison with exact DMFT results for the single-band Hubbard model seems to show that, at least in infinite dimensions, the Gutzwiller wave function does properly capture quasiparticle behavior across the Mott transition.[2] Moreover, since the driving mechanism leading to the Mott transition is local correlations, it is reasonable to assume that the gross quasiparticle features across the metal-to-insulator transition

are not very dependent upon dimensionality, one dimension being a rather exceptional case. All together, this may lead to the conclusion that the infinite-dimensional picture of the Mott transition provided by the Gutzwiller wave function is also qualitatively correct in finite dimensions. Our results show that this belief is not justified, even when spatial correlations are negligible as in infinite dimensions.

The plan of the paper is as follows. In Sec. II we present the generalized GWF introduced in Ref. 11 for multiband models and calculate the general expression of the variational energy in infinite dimensions. In Sec. III we study the infinite-dimension Mott transition both in the absence and in the presence of multiplet exchange splittings, which we discuss more in detail in Sec. IV. In Sec. V we present an extension of the GWF to symmetry broken phases which we use for a specific two-band model in Sec. VI. Finally, in Sec. VII we draw some conclusions.

II. MODEL

We consider a multiband lattice model where, on each lattice site, N valence orbitals are available for being occupied by the conduction electrons. Since our purpose is to discuss some general features of the Gutzwiller wave function, we will assume the most simple form of tight-binding energy with nearest neighbor hopping matrix elements diagonal in the orbital index, namely,

$$\hat{H}_0 = -\frac{t}{\sqrt{z}} \sum_{\langle ij \rangle} \sum_{a=1}^{N} \sum_{\sigma} c^{\dagger}_{i,a\sigma} c_{j,a\sigma} + \text{H.c.}, \tag{1}$$

where z is the lattice coordination, $c_{i,a\sigma}$ and $c^{\dagger}_{i,a\sigma}$ are, respectively, the annihilation and creation operators for an electron at site i with orbital index $a=1,\ldots,N$ and spin $\sigma=\uparrow,\downarrow$. The correlation among the electrons is introduced via two local interaction terms: an on-site Hubbard repulsion

$$\hat{H}_U = \frac{U}{2} \sum_i n_i^2, \tag{2}$$

where $n_i = \Sigma_{a=1}^{N} \Sigma_{\sigma} c^{\dagger}_{i,a\sigma} c_{i,a\sigma}$ is the electron occupation number at site i, as well as an exchange splitting term

$$\hat{H}_J = \sum_i \sum_{n=0}^{2N} \sum_{\Gamma_n} J_{\Gamma_n} |i,n,\Gamma_n\rangle\langle i,n,\Gamma_n|. \tag{3}$$

Here $|i,n,\Gamma_n\rangle$ denotes a multiplet of n-electron states at site i. Γ_n has a multiplicity g_{Γ_n}[24] such that

$$\sum_{\Gamma_n} g_{\Gamma_n} \equiv g_n = \binom{2N}{n},$$

the binomial on the right hand side being the total number g_n of available on-site n-electron states. Without loss of generality, we assume that $\hat{H}_J$ only splits multiplets at fixed n without affecting their center-of-gravity energy, implying $\Sigma_{\Gamma_n} g_{\Gamma_n} J_{\Gamma_n} = 0$.

In the absence of interaction, the ground state $|\Phi_0\rangle$ of Eq. (1) with an average electron number per site n_0 consists of N degenerate bands each one at filling $n_0/2N$, namely,

$$|\Phi_0\rangle = \prod_{a=1}^{N} \prod_{|\vec{k}|<k_F} c^{\dagger}_{k,a\uparrow} c^{\dagger}_{-k,a\downarrow} |0\rangle, \tag{4}$$

where

$$\frac{2}{V} \sum_{|\vec{k}|<k_F} = \frac{n_0}{N}.$$

If $0<n_0<2N$ is an integer, we expect that, for sufficiently large U, the correlated ground state of $\hat{H}=\hat{H}_0+\hat{H}_U+\hat{H}_J$ describes a Mott insulator. Analogously to what has been done for the single-band Hubbard model, we would like to have a system which allows us to study a metal-to-insulator (MIT) transition to an ideal *paramagnetic* Mott insulator, in contrast to a more conventional metal-to-band-insulator transition. For that reason, we further assume that the multiplet exchange splitting (3) is such that, within a perturbation expansion upon the uncorrelated ground state $|\Phi_0\rangle$, all self-energy diagrams are diagonal in spin and orbital indices and independent of them. Formally this assumption implies that the projection on any given multiplet of the local single-particle density matrix is simply

$$|i,n,\Gamma_n\rangle\langle i,n,\Gamma_n| c^{\dagger}_{i,a\sigma} c_{i,b\sigma'} |i,n,\Gamma_n\rangle\langle i,n,\Gamma_n| = \frac{n}{2N} \delta_{ab} \delta_{\sigma\sigma'} |i,n,\Gamma_n\rangle\langle i,n,\Gamma_n|. \tag{5}$$

This does not exclude that spin and/or orbital symmetry may be spontaneously broken especially close to the Mott transition, as it is known to occur for the half-filled single band Hubbard model on a bipartite hypercubic lattice in dimensions greater than 1. Rigorously speaking in that case there is not even a MIT, since, due to nesting, the ground state describes an antiferromagnetic insulator for any $U\neq 0$ (see, e.g., Ref. 25 for two dimensions). In most general cases with un-nested noninteracting Fermi surfaces, e.g., for nonbipartite lattices, longer range hopping matrix elements or non-half-filled bands, $n_0 \neq N$, we do expect a finite U MIT, although it might be accompanied by some spin and/or orbital ordering. Yet, in what follows, we will discard such a possibility and just discuss an idealized MIT at finite U, where neither the metal nor the Mott insulator break any of the symmetries of the Hamiltonian. We postpone the analysis of spontaneous symmetry breaking nearby the Mott transition to Sec. V.

Having this in mind, we start analyzing the role of the interaction by a Gutzwiller variational approach. That is, we search for the best variational wave function of the form

$$|\Psi_G\rangle = \prod_i \hat{P}_{i,G} |\Phi_0\rangle, \tag{6}$$

where the uncorrelated wave-function is the Slater determinant of Eq. (4) and the on-site Gutzwiller correlator,[11,13]

$$\hat{P}_{i,G}=\sum_n \sum_{\Gamma_n} \lambda_{n\Gamma_n}|i,n,\Gamma_n\rangle\langle i,n,\Gamma_n|, \tag{7}$$

tends to go along with the local interaction terms $\hat{H}_U$ and $\hat{H}_J$ in modifying the relative weights of on-site electronic configurations. As shown in Refs. 6 and 11, there is a certain arbitrariness in the choice of the variational parameters λ's, related to the fact that any transformation acting on $|\Phi_0\rangle$ and involving operators of which $|\Phi_0\rangle$ is an eigenstate amounts simply to a multiplicative factor. In our case, that arbitrariness allows one to impose, without losing generality, the normalization condition

$$\langle\Phi_0|\hat{P}^2_{i,G}|\Phi_0\rangle, \tag{8}$$

as well as an additional constraint on the single-particle density matrix,

$$\langle\Phi_0|\hat{P}_{i,G}c^\dagger_{i,a\sigma}c_{i,b\sigma'}\hat{P}_{i,G}|\Phi_0\rangle=\langle\Phi_0|c^\dagger_{i,a\sigma}c_{i,b\sigma'}|\Phi_0\rangle = \frac{n_0}{2N}\delta_{ab}\delta_{\sigma\sigma'}, \tag{9}$$

where the last equality derives from our choice of $|\Phi_0\rangle$ [Eq. (4)].

A formal solution of Eqs. (8) and (9) is obtained[11] by writing

$$\lambda^2_{n\Gamma_n}=\frac{P(n,\Gamma_n)}{P^{(0)}(n,\Gamma_n)}, \tag{10}$$

where $P^{(0)}(n,\Gamma_n)$ and $P(n,\Gamma_n)$ represent the occupation probabilities of the n-electron multiplet Γ_n in the uncorrelated, $|\Phi_0\rangle$, and correlated, $|\Psi_G\rangle$, wave functions. Upon inserting Eq. (10) into Eqs. (8) and (9), one obtains

$$\sum_n \sum_{\Gamma_n} P(n,\Gamma_n)=1, \tag{11}$$

the correct normalization for $P(n,\Gamma_n)$, as well as

$$\sum_n \sum_{\Gamma_n} nP(n,\Gamma_n)=n_0, \tag{12}$$

namely, the condition that the average number of electrons per site coincides with the uncorrelated value n_0. In this representation, the correlated probability distribution is the variational quantity which has to be optimized.

Equations (8) and (9) imply that, within a perturbation expansion in the parameters $(1-\lambda_{n\Gamma_n})$'s, only more than two fermionic lines can exit from any vertex $\hat{P}^2_{i,G}$ at site i, see Ref. 11. This property simplifies considerably the calculations in the limit of infinite coordination lattices, $z\to\infty$ in Eq. (1), where one can show the average variational energy per site:[11]

$$E_G=\frac{1}{V}\langle\Psi_G|\hat{H}_0+\hat{H}_U+\hat{H}_J|\Psi_G\rangle = ZT_0+\frac{U}{2}\sum_n\sum_{\Gamma_n}(n-n_0)^2P(n,\Gamma_n) + \sum_n\sum_{\Gamma_n}J_{\Gamma_n}P(n,\Gamma_n). \tag{13}$$

T_0 is the average value per site of the noninteracting tight-binding Hamiltonian

$$T_0=\lim_{z\to\infty}\frac{1}{V}\langle\Phi_0|\hat{H}_0|\Phi_0\rangle,$$

which is reduced by a factor Z through the Gutzwiller projection, and we have introduced a chemical potential term which makes the Hubbard interaction minimum at the average $n=n_0$. Our choice of $\hat{H}_J$ leads to the following expression:

$$\sqrt{Z}=\sum_{n=1}^{2N}\sum_{\Gamma_n,\Gamma_{n-1}}\frac{n}{2N}\frac{g_{\Gamma_n}g_{\Gamma_{n-1}}}{g_{n-1}}\left(\frac{n_0}{2N}\right)^{n-1}\left(1-\frac{n_0}{2N}\right)^{2N-n} \times\lambda_{n\Gamma_n}\lambda_{n-1\Gamma_{n-1}}=\sum_{n=1}^{2N}\sum_{\Gamma_n,\Gamma_{n-1}}\frac{n}{g_{n-1}}\sqrt{\frac{g_{\Gamma_n}g_{\Gamma_{n-1}}}{n_0(2N-n_0)}} \times\sqrt{P(n,\Gamma_n)P(n-1,\Gamma_{n-1})}. \tag{14}$$

When $\hat{H}_J=0$, namely, if nothing in the Hamiltonian splits the degeneracy among states at fixed n, there should exist a variational solution in which all configurations at fixed n are equally probable, a property owned by the Slater determinant $|\Phi_0\rangle$. In that case, a multiplet with degeneracy g_{Γ_n} occurs with probability

$$P(n,\Gamma_n)=\frac{g_{\Gamma_n}}{g_n}P(n), \tag{15}$$

$P(n)$ being the probability of a site to be occupied by n electrons irrespective of the configuration. Equation (15) inserted into Eq. (14) leads to the following simple expression of Z valid for $\hat{H}_J=0$:

$$\sqrt{Z}=\sum_{n=1}^{2N}\frac{n}{\sqrt{n_0(2N-n_0)}}\sqrt{\frac{g_n}{g_{n-1}}}\sqrt{P(n)P(n-1)}. \tag{16}$$

III. MOTT TRANSITION WITHIN THE GUTZWILLER APPROACH

The search for the optimal $P(n,\Gamma)$'s with arbitrary values of the interaction parameters is not straightforward. However, it is still possible to obtain simple analytical results close to the Mott transition, which is signaled by a vanishing hopping energy reduction factor Z, which is also the *quasiparticle residue* as obtained by the Fermi surface jump of the momentum distribution. Indeed, when $Z\ll 1$, one realizes,[12,26] by inspection of Eq. (13), that

$$P(n,\Gamma_n)\sim Z^{|n-n_0|}. \tag{17}$$

It is therefore justified to assume $P(n,\Gamma_n)=0$ for all n's but $n=n_0$ and $n=n_0\pm1$, which simplifies all calculations remarkably.

In the simple case $\hat{H}_J=0$, which we denote hereafter as $J=0$, this approximation leads through Eq. (16) to

$$\sqrt{Z}\simeq\frac{n_0}{\sqrt{n_0(2N-n_0)}}\sqrt{\frac{g_{n_0}}{g_{n_0-1}}}\sqrt{P(n_0)P(n_0-1)}+\frac{n_0+1}{\sqrt{n_0(2N-n_0)}}\sqrt{\frac{g_{n_0+1}}{g_{n_0}}}\sqrt{P(n_0+1)P(n_0)}. \tag{18}$$

The distribution probabilities have to satisfy

$$P(n_0-1)=P(n_0+1)\equiv d,$$

and consequently

$$P(n_0)=1-2d.$$

By inserting those expressions into Eq. (18), one obtains

$$Z=\frac{d(1-2d)}{n_0(2N-n_0)}[\sqrt{n_0(2N-n_0+1)}+\sqrt{(n_0+1)(2N-n_0)}]^2\equiv\gamma(N,n_0)d(1-2d); \tag{19}$$

hence

$$E_G=\gamma(N,n_0)d(1-2d)T_0+Ud. \tag{20}$$

The optimal d which minimizes Eq. (20) is readily found:

$$d=\frac{T_0\gamma(N,n_0)+U}{4T_0\gamma(N,n_0)}\equiv\frac{U_c(J=0)-U}{4U_c(J=0)}, \tag{21}$$

where

$$U_c(J=0)=-\gamma(N,n_0)T_0=-\frac{1}{2N-n_0}[\sqrt{n_0(2N-n_0+1)}+\sqrt{(n_0+1)(2N-n_0)}]^2\frac{T_0}{n_0} \tag{22}$$

is the value of the interaction at the Mott transition,[12] when the optimal $d=0$. The variational energy is therefore

$$E_G(J=0)=2T_0\gamma(N,n_0)d^2=-\frac{1}{8}\frac{[U_c(J=0)-U]^2}{U_c(J=0)}. \tag{23}$$

Let us now consider the case $H_J\neq0$. We assume that the exchange splitting favors at any given n a particular multiplet of states, which we denote as Γ_n^*. The Mott insulator described by the Gutzwiller wave function is therefore characterized by $P(n_0,\Gamma_{n_0}^*)=1$ and has energy $E_{ins}=J_{\Gamma_{n_0}^*}<0$. In order to better understand how the Mott transition occurs when $J\neq0$, it is convenient to consider separately two extreme cases which do not require any numerical calculation.

Let us start by considering an hypothetical metallic solution able to smoothly transform into the Mott insulator, in which therefore only the multiplets Γ_n^* favored by H_J are occupied close to the MIT. Since only $n_0\pm1$ and n_0 are relevant, one obtains an expression of Z similar to Eq. (19), with the only difference that

$$\gamma(N,n_0)\to\gamma_{eff}(N,n_0)\equiv\frac{1}{n_0(2N-n_0)}\left[\sqrt{n_0(2N-n_0+1)}\sqrt{\frac{g_{\Gamma^*_{n_0-1}}}{g_{n_0-1}}\frac{g_{\Gamma^*_{n_0}}}{g_{n_0}}}+\sqrt{(n_0+1)(2N-n_0)}\sqrt{\frac{g_{\Gamma^*_{n_0+1}}}{g_{n_0+1}}\frac{g_{\Gamma^*_{n_0}}}{g_{n_0}}}\right]^2<\gamma(N,n_0).$$

The variational energy now reads

$$E_G(J\neq0)=\gamma_{eff}(N,n_0)d(1-2d)T_0+Ud+(J_{\Gamma^*_{n_0-1}}+J_{\Gamma^*_{n_0+1}}-2J_{\Gamma^*_{n_0}})d+J_{\Gamma^*_{n_0-1}}.$$

Provided we substitute $\gamma\to\gamma_{eff}$ and

$$U\to U_{eff}\equiv U+(J_{\Gamma^*_{n_0-1}}+J_{\Gamma^*_{n_0+1}}-2J_{\Gamma^*_{n_0}}),$$

which is the actual Hubbard repulsion measured with respect to the energies of the lowest multiplets and not from the centers of gravity, the formal solution has the same expression as before. In particular the critical interaction at which that metallic phase becomes unstable is now

$$U_c(J\neq0)=-\gamma_{eff}(N,n_0)T_0-(J_{\Gamma^*_{n_0-1}}+J_{\Gamma^*_{n_0+1}}-2J_{\Gamma^*_{n_0}})=\frac{\gamma_{eff}(N,n_0)}{\gamma(N,n_0)}U_c(J=0)-(J_{\Gamma^*_{n_0-1}}+J_{\Gamma^*_{n_0+1}}-2J_{\Gamma^*_{n_0}}). \tag{24}$$

For very small J's, $U_c(J\neq0)$ is shifted down with respect to $U_c(J=0)$ by terms of order $|T_0|$, which already suggests that the above solution is not the most energetically favorable, although it has the merit to merge smoothly into the insulator.

Indeed, the best variational solution is actually different from the above one. If the J's are very small compared with T_0, we rather expect in the metallic phase that the probability distributions of the multiplets at any n are only slightly modified with respect to the $J=0$ case. If this were true, we could still search for a variational solution of the same form as for $J=0$, which has an energy given by Eq. (21) with d as in Eq. (23). This solution, however, does not converge into the insulating one, which has an energy $E_{ins}=J_{\Gamma^*_{n_0}}$. The two energies indeed cross when

$$-\frac{1}{8}\frac{[U_c(J=0)-U]^2}{U_c(J=0)}=J_{\Gamma^*_{n_0}},$$

namely, when $U=U_*$,

$$U_* = U_c(J=0) - \sqrt{-8U_c(J=0)J_{\Gamma^*_{n_0}}}. \tag{25}$$

For small J, U_* is larger than $U_c(J\neq 0)$ given in Eq. (24), which suggests not only that the $J=0$ metallic solution has lower energy but also that the Mott transition is first order. The explicit solution of the variational equations shows that, in the optimal metal at small J, the probability distributions are indeed only slightly modified with respect to the $J=0$ case by terms of order $\sqrt{|J/T_0|}$; hence that the Mott transition becomes first order as soon as a finite J is introduced.

In conclusion, if the multiplet exchange splitting term $|J|$ is much smaller than the uncorrelated bandwidth W, then the Gutzwiller variational approach leads to a first order phase transition from a metal, slightly modified with respect to the $J=0$ case, into a Mott insulator instead dominated by J. This transition is predicted to occur when the quasiparticle residue is

$$Z \sim \sqrt{\gamma(N,n_0)\left|\frac{J}{T_0}\right|}, \tag{26}$$

and arises because the metallic solution has to pay too much hopping energy to modify the relative weights of the multiplets, a cost which overcomes the exchange splitting energy gain.

A first order phase transition has indeed been found in Ref. 11 by an explicit numerical minimization of the variational energy in a two-band model, and agrees with linearized-DMFT results obtained in Ref. 16 on a similar model. Moreover, in the same Ref. 16 it is shown that the first order character reinforces with increasing exchange splitting strength J from $J=0$, while it weakens with further increasing J above some intermediate value. This also agrees with our above results. Indeed, when J gets so large to make $U_c(J\neq 0)$ [Eq. (24)] greater than U_* [Eq. (25)] we expect the Mott transition to turn again into a second order one. That requires a substantial $|J|\sim|T_0|$.

IV. DRAWBACKS OF THE GUTZWILLER WAVE FUNCTION

It is known that the simplest Gutzwiller wave function is not very accurate for the single band Hubbard model at half-filling in finite dimensions. The main reason is the inability to properly account for spatial correlations, either among the spins of singly occupied sites and among empty and doubly occupied sites.[20,21,23] Indeed, one expects physically that empty and doubly occupied sites should bind in the Mott insulator, otherwise the system would remain metallic all the way up to $U=\infty$, where only single occupancy is allowed. Since the simplest GWF does not include such correlations, it is unable to represent a Mott insulator in any finite dimension, unless the uncorrelated wave function is itself insulating, as it happens for an antiferromagnetic Slater determinant. Several attempts have been done to improve the GWF (Refs. 20, 27, and 28) by including spatial correlations among empty and doubly occupied sites, yet there are no numerical evidences of a MIT in finite dimensions when the uncorrelated wave function is metallic, e.g., the paramagnetic Fermi sea.

This problem should not be so severe in infinite dimensions, where the GWF does indeed show a MIT. In fact the GWF reproduces quite accurately exact DMFT results concerning quasiparticle properties across the MIT,[2] which moreover one expects do not strongly depend upon dimensionality, one dimension being an exception. This suggests that the infinite-dimensional Landau-Fermi liquid picture provided by the GWF is qualitatively correct even in finite dimensions, thus justifying the use of the Gutzwiller approximation even in cases where a rigorous numerical treatment of the GWF would yield completely different results. In Sec. III we identified the qualitative behavior across the Mott transition of the GWF for multiband Hubbard models in infinite dimensions. In the same limit, exact results can be obtained by DMFT,[2] which allows a direct comparison hence a test on the accuracy of the GWF in infinite dimensions.

Let us start by comparing the probabilities of a site to be occupied by n electrons, $P(n)$. This probability distribution has been calculated within DMFT for a three band model in Ref. 15. It was also conjectured that, before the MIT,

$$P(n) = (1-Z)P_{ins}(n) + ZP_{qp}(n), \tag{27}$$

where the quasiparticle residue Z can be evaluated independently from the single-particle Green's function, and $P_{ins}(n)$ is the occupation probability in the insulating phase just after the MIT, which is also accessible by DMFT. Thus Eq. (27) defines the unknown $P_{qp}(n)$, which was claimed to represent the quasiparticle occupation probability. This claim was confirmed by comparing $P_{qp}(n)$ with the noninteracting Fermi gas distribution, giving excellent agreement; see Figs. 3A''–3C'' compared with Fig. 3D'' in Ref. 15. The agreement was the more remarkable since the quasiparticle contribution is only a small fraction $\propto Z$ of the full $P(n)$ and Eq. (27) has no free parameter. Within the GWF, the Mott insulator is characterized by $P_{ins}(n)=\delta_{nn_0}$, so that, through Eqs. (17) and (27), one concludes that, for $n\neq n_0$,

$$P_{qp}(n) \sim \frac{Z^{|n-n_0|}}{Z}. \tag{28}$$

The above result contradicts the finding of Ref. 15, which rather supports a $P_{qp}(n)\sim O(1)$, namely a quasiparticle contribution to $P(n)$ of order Z; see Eq. (27). The origin of this disagreement can be easily traced back.

In fact, spatial correlations among unfavorable charge configurations are not fully suppressed even in infinite dimensions, and are responsible for the finite average value of the double occupancy $\langle n_\uparrow n_\downarrow\rangle$ in the insulating phase found by DMFT.[2] In particular $\langle n_\uparrow n_\downarrow\rangle$ as function of U displays a discontinuity in the slope across the Mott transition in infinite dimensions.[2] The singular part, which vanishes at the MIT, is attributed to the quasiparticles, and is qualitatively reproduced by the behavior of the double occupancy as obtained through the Gutzwiller wave function: a support to the belief that this wave function does correctly capture quasiparticle properties.

In a multiband Hubbard model the situation is different. If we just consider the occupation probability $P(n_0 \pm 1)$ of $(n_0 \pm 1)$ charge configurations, across the MIT we expect a behavior similar to the double occupancy in the single-band Hubbard model, still compatible with the GWF. Let us instead consider the occupation probability $P(n_0 \pm 2)$. In the GWF close to the Mott transition, those configurations get suppressed like Z^2. In reality, virtual processes from the more advantageous n_0 and $(n_0 \pm 1)$ charge configurations imply, first of all, that $P(n_0 \pm 2)$ is finite in the insulating phase too, and, second, that the singular $(n_0 \pm 2)$ quasiparticle contribution still linearly vanishes across the MIT, unlike what is found by the GWF. That disagreement is more profound than what it would seem to be. A quasiparticle probability distribution of the Gutzwiller type, namely $P_{qp}(n) \sim Z^{|n-n_0|}/Z$ [see Eqs. (27) and (28)] suggests that quasiparticles remain more strongly interacting than implied by the true behavior $P_{qp}(n) \sim O(1)$, even after the Hubbard side bands are well formed. This indicates that, unlike what happens in the single-band Hubbard model, the multiband GWF is not fully adequate to capture quasiparticle properties.

The second failure of the Gutzwiller variational approach regards the onset of the first order phase transition, which is predicted to occur when $Z \sim \sqrt{|J|}$, for $|J| \ll |T_0|$. It also originates from the lack of spatial correlations. If $J=0$, the Gutzwiller wave function leads to a Mott insulator with a finite entropy, related to the finite number of degenerate on-site electronic configurations with n_0 electrons. This state has an infinite susceptibility to a term $\hat{H}_J$ which splits that degeneracy, with an energy gain linear in J. This result is obviously wrong. The superexchange terms generated by virtual processes into unfavorable charge configurations lead to finite susceptibilities even in the Mott insulator. This implies that the actual energy gain is quadratic in J so that the Mott transition is either second order or weakly first order, in this case occurring when $Z \sim |J|$.

Indeed, this aspect is not peculiar to a multiband model but also occurs in a single band model in the presence of a magnetic field B which splits spin-up singly occupied sites from spin-down ones. Also in that case the Gutzwiller approach would predict a first order transition when $Z \sim \sqrt{B}$, while in reality, being the magnetic susceptibility finite,[2] the transition occurs at smaller Z (see Ref. 29), likely when $Z \sim B$.

Yet those defects of the Gutzwiller wave function might not qualitatively affect the physical behavior in the most common situations where the multiplet exchange splitting term leads to the conventional Hund's rules, i.e., favors high spin and angular momentum configurations. When magnetic ordering occurs, so that the on-site magnetic moments gets oriented along some easy axis, the ground state is usually well described by a Slater determinant, and hence is accessible by a mean-field approach which can be improved by the Gutzwiller correlator. However, there may be less conventional but still interesting cases where the multiplet exchange splitting favors low degeneracy states, which are not Slater determinants and hence unaccessible to mean field theories. Here the Gutzwiller wave function might be inadequate to describe the Mott transition mainly because it is unable to access the interesting region where the metallic kinetic energy gain $\sim Z|T_0|$ competes with the exchange splitting $\sim J$. In conclusion, we believe by the above discussion that an improvement of the GWF towards including spatial correlations is necessary, even in infinite dimensions.[30]

V. GUTZWILLER WAVE FUNCTIONS FOR SYMMETRY-BROKEN PHASES

In spite of its appealing features, an *ideal* Mott insulator at zero temperature is unlikely to exist, especially if it has huge degeneracy. Commonly one expects a symmetry-broken phase to occur at low temperature, at least in more than one dimension. For instance, in a single-band model at half-filling, the ideal Mott insulator has an infinite spin degeneracy which is likely reduced at low temperature by some magnetic ordering. Therefore, even though any mean field type of approach (including more sophisticated ones based on density functional theory) can only stabilize correlated insulators in broken-symmetry phases, namely can only describe band-insulators thus hiding the basic phenomena leading to a Mott insulator, yet they often provide a faithful description of the low temperature physics.

In this situation, the Gutzwiller variational approach should still be useful to improve the Hartree-Fock approximation. That would amount to searching for the best wave function of the form

$$|\Psi_G(\Delta)\rangle = \hat{P}_G |\Phi(\Delta_0)\rangle = \prod_i \hat{P}_{i,G} |\Phi(\Delta_0)\rangle, \qquad (29)$$

with $\hat{P}_{i,G}$ still given by Eq. (7), and where $|\Phi(\Delta_0)\rangle$ is a symmetry-broken uncorrelated trial wave function with a single-particle order parameter Δ_0. In general, after Gutzwiller projection, the correlated wave function will have a different order parameter Δ. This implies that the average values of the single-particle density matrix over $|\Psi_G(\Delta)\rangle$ and $|\Phi(\Delta_0)\rangle$ do not coincide. This does not obviously represent a problem for a numerical treatment, whereas it would seem to prevent the use of the method developed in Ref. 11 for analytically evaluating the average values in infinite dimensions. In fact that method relies on the possibility of constructing a GWF with the same average value of the single-particle density matrix as the uncorrelated wave function. We could still impose that condition for the wave function defined by Eq. (29), but that would reduce the variational freedom.

In this section we present a simple extension of the GWF to account for symmetry-broken phases while leaving the property of being analytically treatable in infinite dimensions without any variational loss. We start by noticing that there always exists a nonunitary operator $\hat{U} = \Pi_i \hat{U}_i$ such that its action

$$\hat{U}^{-1} |\Phi(\Delta_0)\rangle = |\Phi(\Delta)\rangle \qquad (30)$$

leads to a trial wave function $|\Phi(\Delta)\rangle$ of the same form as $|\Phi(\Delta_0)\rangle$ but with the same average value of the single-

particle density matrix as the Gutzwiller projected $|\Psi_G(\Delta)\rangle$, and hence the same order parameter Δ. Therefore,

$$|\Psi_G(\Delta)\rangle = \hat{P}_G|\Phi(\Delta_0)\rangle = \hat{P}_G\hat{U}|\Phi(\Delta)\rangle \equiv \hat{\mathrm{P}}_G|\Phi(\Delta)\rangle, \qquad (31)$$

which implies that, provided we substitute

$$\hat{P}_G \rightarrow \hat{\mathrm{P}}_G = \hat{P}_G\hat{U}, \qquad (32)$$

we can still search without loss of generality for a variational wave function

$$|\Psi_G(\Delta)\rangle = \hat{\mathrm{P}}_G|\Phi(\Delta)\rangle,$$

where the average single-particle density matrix stays unchanged after Gutzwiller projection. The cost is that we must work with a Gutzwiller correlator as given by Eq. (32), which is in general neither diagonal in the multiplets which appears in $\hat{H}_J$ [Eq. (3)], nor Hermitian.

Actually we can identify two distinct situations which may occur, one of them being already included in the formalism developed by Ref. 11. If the exchange splitting J favors a degenerate atomic configuration, then we reasonably expect that in the true ground state of the lattice only one of the degenerate states will be occupied on a given site, eventually changing from site to site. There the order parameter corresponds locally to a conserved quantity of the atomic Hamiltonian, for instance the z component of the on-site spin, which leads to a generalized $\hat{\mathrm{P}}_G$ still Hermitian and diagonal. Let us consider as a simple example a one-band model. The local Gutzwiller correlator is, in general,

$$\hat{P}_{i,G} = \lambda_0|i,0\rangle\langle i,0| + \lambda_2|i,2\rangle\langle i,2| + \lambda_1[|i,\uparrow\rangle\langle i,\uparrow| + |i,\downarrow\rangle \times \langle i,\downarrow|],$$

where $|i,0(2)\rangle$ denote the empty or doubly occupied site i, while $|i,\sigma\rangle$ the singly occupied site with spin σ. We assume that the uncorrelated wave function is magnetically ordered. Then Eq. (30) may be constructed by local operators

$$\hat{U}_i = \mathrm{e}^{2\alpha_i\hat{S}_i^z},$$

where $\hat{S}_i^z$ is the z component of the spin operator at site i. We find that

$$\hat{\mathrm{P}}_{i,G} = \hat{P}_{i,G}\hat{U}_i = \lambda_0|i,0\rangle\langle i,0| + \lambda_2|i,2\rangle\langle i,2| + \lambda_1\mathrm{e}^{\alpha_i}|i,\uparrow\rangle\langle i,\uparrow| + \lambda_1\mathrm{e}^{-\alpha_i}|i,\downarrow\rangle\langle i,\downarrow|.$$

Indeed, the modified Gutzwiller correlator is still diagonal and Hermitian, although there appear different variational parameters for spin-up and -down components. This additional degree of freedom gets fixed once we require that the order parameters of the correlated and uncorrelated wavefunctions coincide. The above type of GWF is actually a particular case of the generalized GWFs introduced in Ref. 11.

We can, however, envisage a different situation where the uncorrelated wave function $|\Phi_0\rangle$ has an order parameter which does not correspond locally to a conserved quantity. There a modified $\hat{\mathrm{P}}_G$ is unavoidably off-diagonal and non-Hermitian. Let us discuss an oversimplified example. We assume that the exchange term leads to a local Gutzwiller correlator of the form (we drop the site label)

$$\hat{P}_G = \lambda_a|a\rangle\langle a| + \lambda_b|b\rangle\langle b|,$$

and moreover that the uncorrelated wave-function has an order parameter identified by nonzero matrix elements

$$\langle\Phi_0|a\rangle\langle b|\Phi_0\rangle = \langle\Phi_0|b\rangle\langle a|\Phi_0\rangle.$$

The transformation $\hat{U}$ can be now taken of the form

$$\hat{U} = \alpha(|a\rangle\langle a| + |b\rangle\langle b|) + \beta(|a\rangle\langle b| + |b\rangle\langle a|).$$

We readily find that

$$\hat{\mathrm{P}}_G = \hat{P}_G\hat{U} = \alpha\lambda_a|a\rangle\langle a| + \alpha\lambda_b|b\rangle\langle b| + \beta\lambda_a|a\rangle\langle b| + \beta\lambda_b|b\rangle\langle a|,$$

indeed containing off-diagonal terms and evidently non-Hermitian. This is a novel situation which we are going to discuss more in detail in a particular example.

We conclude this section by pointing out that the non-Hermitian character plays a crucial role only if the ordering involves just the quasiparticles, while it is essentially irrelevant when both the quasiparticles and the Mott-Hubbard side bands contribute to the order parameter. In Sec. VI we analyze a two-band model where both cases may appear.

VI. A TWO-BAND MODEL STUDY

We consider a two-band Hubbard model described by Hamiltonians (1) and (2) where the orbital index $a=1,2$. Besides the local spin-density operators

$$\vec{S}_i = \frac{1}{2}\sum_{a=1}^{2}\sum_{\alpha\beta} c_{i,a\alpha}^{\dagger}\vec{\sigma}_{\alpha\beta}c_{i,a\beta},$$

where $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are the Pauli matrices, we introduce orbital pseudospin operators

$$\vec{T}_i = \frac{1}{2}\sum_{a,b=1}^{2}\sum_{\sigma} c_{i,a\sigma}^{\dagger}\vec{\tau}_{ab}c_{i,b\sigma}, \qquad (33)$$

where the Pauli matrices $\hat{\tau}$'s act on the orbital indices. The hopping and Hubbard terms [Eqs. (1) and (2)] have a very large SU(4) symmetry. Having in mind common physical realizations, like, e.g., d orbitals of e_g symmetry, we assume that SU(4) is lowered down to a spin SU(2) times an orbital O(2) by the exchange term, which can therefore be written as

$$\hat{H}_J = \sum_i J_S\vec{S}_i\cdot\vec{S}_i + J_T\vec{T}_i\cdot\vec{T}_i - 3(J_S+J_T)(T_i^z)^2. \qquad (34)$$

The above $\hat{H}_J$ just splits the on-site configurations with two electrons. There are six of those states on a given site i, a spin triplet orbital singlet $|i,n=2;S=1,S_z;T=0\rangle$, which we denote hereafter as $|i,2,t\rangle$, and a spin-singlet orbital triplet, for which we use the short notations $|i,n=2;S=0;T=1,T_z=0\rangle \equiv |i,2,0\rangle$ and $|i,n=2;S=0;T=1,T_z=\pm 1\rangle \equiv |i,2,\pm\rangle$. In this subspace, $\hat{H}_J$ has the form

$$\hat{H}_J = \sum_i 2J_S |i,2,t\rangle\langle i,2,t| + 2J_T |i,2,0\rangle \times \langle i,2,0| - (3J_S + J_T)|i,2,\pm\rangle\langle i,2,\pm|. \quad (35)$$

The standard Hund's rules correspond to $-J_T < J_S < -5J_T/6 < 0$, when the spin-triplet orbital-singlet configuration has the lowest energy, followed by the spin-singlet orbital doublet with $T_z = \pm 1$. In this case the ideal Mott insulator at half-filling, $n_0 = 2$, represents localized spin-1 moments which should order at low enough temperature to freeze out the spin entropy. On general grounds one expects that the magnetic ordering in the insulator should contaminate the nearby metallic phase so that, as U increases from weak coupling, first a transition from a paramagnetic into a magnetic metal should occur, followed by a Mott transition into a magnetically ordered insulator. Even a mean field approach is in principle able to reproduce the above scenario. In this situation, as we discussed before, the Gutzwiller-projected Hartree-Fock wave function does improve the mean-field solution, providing a better physical description. In Appendix A we analyze in detail the case in which a bipartite lattice stabilizes an antiferromagnetic ordering.

Less conventional is the situation $J_T < -|J_S|$, where the nondegenerate spin singlet with $T_z = 0$, namely,

$$|i,2;S=0;T=1,T_z=0\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{i,1\uparrow}c^\dagger_{i,2\downarrow} + c^\dagger_{i,2\uparrow}c^\dagger_{i,1\downarrow})|0\rangle, \quad (36)$$

is the lowest energy configuration. That would be for instance the case of two Hubbard models (two-chains, two-planes, etc.), coupled by an antiferromagnetic exchange. Here the large U Mott insulator with $n_0 = 2$ describes a collection of on-site singlets, a local version of a valence-bond (VB) insulator. Since it is not degenerate and fully gapped, we expect the VB insulator to be stable at large U against any spin and/or orbital order. Just to avoid unessential complications, we assume that the lattice is sufficiently frustrated to prevent any spin/orbital ordering at any U. This situation is far less trivial than the previous one. In fact, being the Mott insulator not describable by a single Slater determinant, it is inherently unreachable by any mean-field approach, which necessarily leads to some kind of ordered state. According to our previous discussion, we expect in this case that also the GWF is unable to provide a faithful description of the Mott transition.

As we showed in Sec. III, the GWF without any symmetry breaking would undergo a first order metal-insulator transition when the quasiparticle residue

$$Z \simeq \sqrt{\frac{J_T}{6T_0}},$$

namely, when $U = U_*$, being

$$U_* = -6T_0 - 4\sqrt{6T_0 J_T}.$$

We also argued that this result is wrong since a metallic phase is able to enter the regime in which $Z \sim |J_T/T_0|$. Let us now check whether there exists a better broken-symmetry metallic solution. Indeed, even if lattice frustration prevents spin/orbital order, there is still a broken-symmetry GWF which might in principle compete with the above metallic solution.

Superconducting Gutzwiller wave function

When $U = 0$, the multiplet exchange term (35) favors a BCS Hartree-Fock wave-function with the s-wave order parameter

$$\langle \Phi_{BCS}(\Delta_0)|c^\dagger_{i,1\uparrow}c^\dagger_{i,2\downarrow}|\Phi_{BCS}(\Delta_0)\rangle = \langle \Phi_{BCS}(\Delta_0)|c^\dagger_{i,2\uparrow}c^\dagger_{i,1\downarrow}|\Phi_{BCS}(\Delta_0)\rangle \equiv \Delta_0 \leqslant \frac{1}{2}. \quad (37)$$

When $\Delta_0 \to 1/2$, the doubly occupied sites in the spin triplet, $|2,t\rangle$, or in the doublet of spin singlets, $|2,\pm\rangle$, configurations are suppressed by a factor $(1-2\Delta_0)^2$ with respect to the $T_z = 0$ spin singlet, $|2,0\rangle$. Similarly, the probability of singly, $|1\rangle$, or triply occupied, $|3\rangle$, sites vanish like $(1-2\Delta_0)$. This suggests that by Gutzwiller projecting out sites with zero and four electrons, $|0\rangle$ and $|4\rangle$, respectively, through the variational wave function

$$|\Psi_G(\Delta)\rangle = \hat{P}_G|\Phi_{BCS}(\Delta_0)\rangle, \quad (38)$$

one might indeed smoothly connect to the VB insulating state, with $(1-2\Delta_0)$ playing the role of Z. However, even though the uncorrelated BCS wave function has a large order parameter $\Delta_0 \sim 1/2$, the correlated $|\Psi_G\rangle$ should have a much smaller one, $\Delta \sim Z\Delta_0$, since only quasiparticles are involved in superconductivity. In such a case we are therefore obliged to implement the non-Hermitian Gutzwiller correlator in order to get analytical results for large coordination lattices. In other words, we shall work with a Gutzwiller wave function of the same form as Eq. (38) and impose that $|\Psi_G\rangle$ and $|\Phi_{BCS}\rangle$ have the same order parameter Δ through a non-Hermitian $\hat{P}_G$; see Eq. (32). Since this is a novel situation in the Gutzwiller variational approach, we prefer to describe it in detail.

In order to simplify the analysis at half-filling, we assume that the Hamiltonian has particle-hole symmetry and search for solutions which do not break it. This guarantees that there are still two conditions we can impose without losing variational freedom: an overall normalization [Eq. (8)], and a particle-hole symmetry constraint.

To accomplish this job, it is convenient to work not in the original electron basis but in the *natural* basis where the

on-site single-particle density matrix is diagonal. This is done by the following unitary transformation, which is valid at half-filling $n_0=2$:

$$\begin{pmatrix} c_{i,1(2)\uparrow} \\ c^{\dagger}_{i,2(1)\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a_{i,1(2)\uparrow} \\ a^{\dagger}_{i,2(1)\downarrow} \end{pmatrix}.$$

In the natural basis the only nonzero on-site average is

$$\langle \Phi_{BCS}(\Delta) | a^{\dagger}_{i,a\sigma} a_{i,a\sigma} | \Phi_{BCS}(\Delta) \rangle = \frac{1}{2} - \Delta.$$

In order to distinguish the local configurations in the natural from the original basis we will denote the former ones as $|\overline{n},\Gamma_{\overline{n}}\rangle$. The most general local Gutzwiller correlator is, in this case,

$$\hat{\mathrm{P}}_{i,G} = \sum_{\overline{n}} \sum_{\Gamma_{\overline{n}}} \lambda_{\overline{n}\Gamma_{\overline{n}}} |i,\overline{n},\Gamma_{\overline{n}}\rangle\langle i,\overline{n},\Gamma_{\overline{n}}| + \lambda_{\overline{04}} |i,\overline{0}\rangle \times \langle i,\overline{4}| + \lambda_{\overline{40}} |i,\overline{4}\rangle\langle i,\overline{0}|. \tag{39}$$

The last two terms are the only possible off-diagonal elements at half-filling when particle-hole symmetry holds. The normalization condition and the conservation of the single-particle density matrix lead to the following parametrization of the λ's for $\overline{n} \neq 0,4$:

$$\lambda^2_{\overline{n}\Gamma_{\overline{n}}} = \frac{P(\overline{n},\Gamma_{\overline{n}})}{P^{(0)}(\overline{n},\Gamma_{\overline{n}})},$$

where $P(\overline{n},\Gamma_{\overline{n}})$ and $P^{(0)}(\overline{n},\Gamma_{\overline{n}})$ are the correlated and uncorrelated occupation probabilities in the natural basis. For $\overline{n}=0,4$ we have instead

$$\lambda^2_{\overline{0}} P^{(0)}(\overline{0}) + \lambda^2_{\overline{04}} P^{(0)}(\overline{4}) = P(\overline{0}), \tag{40}$$

$$\lambda^2_{\overline{40}} P^{(0)}(\overline{0}) + \lambda^2_{\overline{4}} P^{(0)}(\overline{4}) = P(\overline{4}), \tag{41}$$

$$\lambda_{\overline{0}}\lambda_{\overline{40}} P^{(0)}(\overline{0}) + \lambda_{\overline{04}}\lambda_{\overline{4}} P^{(0)}(\overline{4}) = A(\overline{0};\overline{4}) = A(\overline{4};\overline{0}), \tag{42}$$

where we introduce the transition amplitudes

$$A(\overline{n},\Gamma_{\overline{n}};\overline{m},\Gamma_{\overline{m}}) = \langle \Psi_G | i,\overline{n},\Gamma_{\overline{n}}\rangle\langle i,\overline{m},\Gamma_{\overline{m}} | \Psi_G \rangle.$$

The occupation probabilities in the natural basis are related to those in the original one through

$$\begin{aligned} P(\overline{0}) &= \frac{1}{2}[P(0)+P(2,0)+A(0;4)] + \sqrt{2}A(0;2,0), \\ P(\overline{1}) &= P(1)+A(1;3), \\ P(\overline{2},0) &= P(0)-A(0;4), \\ P(\overline{2},\pm) &= P(2,\pm), \\ P(\overline{2},t) &= P(2,t), \\ P(\overline{3}) &= P(1)-A(1;3), \\ P(\overline{4}) &= \frac{1}{2}[P(0)+P(2,0)+A(0;4)] - \sqrt{2}A(0;2,0), \\ A(\overline{0};\overline{4}) &= \frac{1}{2}[P(0)-P(2,0)+A(0;4)], \end{aligned} \tag{43}$$

where we have used the fact that, by particle-hole symmetry, $P(1)=P(3)$ and $P(0)=P(4)$. The order parameter Δ is given by

$$2\Delta = 2\sqrt{2}A(02+) + A(13),$$

and the following inequalities should be verified:

$$2A(0;2,0)^2 \leqslant P(2,0)[P(0)+A(0;4)],$$

$$A(0;4) \leqslant P(0),$$

$$A(1;3) \leqslant P(1).$$

The big advantage in working with natural orbitals is that the Z reduction factor has the same expression as in Eq. (14), namely,

$$\sqrt{Z(\Delta)} = \sum_{n=1}^{4} \sum_{\Gamma_{\overline{n}},\Gamma_{\overline{n-1}}} \frac{\overline{n}}{4} \frac{g_{\Gamma_{\overline{n}}} g_{\Gamma_{\overline{n-1}}}}{g_{\overline{n-1}}} \left(\frac{1}{2}-\Delta\right)^{\overline{n-1}} \times \left(\frac{1}{2}+\Delta\right)^{4-\overline{n}} \lambda_{\overline{n}\Gamma_{\overline{n}}} \lambda_{\overline{n-1}\Gamma_{\overline{n-1}}}. \tag{44}$$

Once we know how to relate the parameters λ's and Z to the variational occupation probabilities defining the correlated and uncorrelated wave functions, we can solve the most general variational problem by minimizing the energy functional

$$E_G(\Delta) = Z(\Delta)T_0(\Delta) + U[4P(0)+P(1)] + 2J_S P(2,t) + 2J_T P(2,0) - (3J_S+J_T)P(2,\pm), \tag{45}$$

where

$$\langle \Phi_{BCS}(\Delta) | \hat{H}_0 | \Phi_{BCS}(\Delta) \rangle = T_0(\Delta).$$

For the sake of clarity, here we present an analysis based on the following parametrization of the λ's in Eq. (39), although it has less variational freedom:

$$\lambda_{\bar{0}}=\frac{1}{2}(\lambda_0+\lambda_{20})\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{0})}{P^{(0)}_{\Delta}(\bar{0})}},$$

$$\lambda_{\bar{4}}=\frac{1}{2}(\lambda_0+\lambda_{20})\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{4})}{P^{(0)}_{\Delta}(\bar{4})}},$$

$$\lambda_{\bar{0}\bar{4}}=\frac{1}{2}(\lambda_0-\lambda_{20})\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{4})}{P^{(0)}_{\Delta}(\bar{4})}},$$

$$\lambda_{\bar{4}\bar{0}}=\frac{1}{2}(\lambda_0-\lambda_{20})\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{0})}{P^{(0)}_{\Delta}(\bar{0})}},$$

$$\lambda_{\bar{1}}=\lambda_1\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{1})}{P^{(0)}_{\Delta}(\bar{1})}},$$

$$\lambda_{\bar{3}}=\lambda_1\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{3})}{P^{(0)}_{\Delta}(\bar{3})}},$$

$$\lambda_{\bar{2}\bar{0}}=\lambda_0\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{2},0)}{P^{(0)}_{\Delta}(\bar{2},0)}},$$

$$\lambda_{\bar{2}\bar{t}}=\lambda_{2t}\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{2},t)}{P^{(0)}_{\Delta}(\bar{2},t)}},$$

$$\lambda_{\bar{2}\pm}=\lambda_{2\pm}\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{2},\pm)}{P^{(0)}_{\Delta}(\bar{2},\pm)}}. \tag{46}$$

As before Δ_0 is the order parameter of the uncorrelated BCS wave function while Δ is the true order parameter after Gutzwiller projection; see Eq. (38). $P^{(0)}_{\Delta_0}(\bar{n},\bar{\Gamma_n})$ and $P^{(0)}_{\Delta}(\bar{n},\bar{\Gamma_n})$ are the distribution probabilities in the natural basis for the BCS wave functions with order parameters Δ_0 and Δ, respectively. They are explicitly written in Appendix B, Eq. (B4).

The normalization condition as well as the conservation of the single-particle density matrix imply that

$$\lambda^2_{n\Gamma_n}=\frac{P(n,\Gamma_n)}{P^{(0)}_{\Delta_0}(n,\Gamma_n)}, \tag{47}$$

where $P^{(0)}_{\Delta_0}(n,\Gamma_n)=\langle\Phi_{\Delta_0}|i;n,\Gamma_n\rangle\langle i;n,\Gamma_n|\Phi_{\Delta_0}\rangle$ is the occupation probability for configurations in the original electronic basis within the uncorrelated BCS wave function with large order parameter Δ_0 [see Eq. (B5)], while $P(n,\Gamma_n)$ is the same quantity for the correlated wave function. Equation (47) is the most natural generalization of Eq. (10) to a broken-symmetry phase, which is the reason why we have chosen the above parametrization. The true order parameter Δ is defined through

$$\begin{aligned}2\Delta&=P^{(0)}_{\Delta}(\bar{0})+\frac{1}{2}P^{(0)}_{\Delta}(\bar{1})-\frac{1}{2}P^{(0)}_{\Delta}(\bar{3})+P^{(0)}_{\Delta}(\bar{4})\\&=\Delta_0(1+4\Delta_0^2)\sqrt{\frac{P(2,0)P(0)}{P^{(0)}_{\Delta_0}(2,0)P^{(0)}_{\Delta_0}(0)}}\\&\quad+\Delta_0(1-4\Delta_0^2)\frac{P(1)}{P^{(0)}_{\Delta_0}(1)},\end{aligned} \tag{48}$$

which indeed is of order Z when $1/2-\Delta_0\sim Z$, $P(2,0)\sim 1$, $P(1)\sim Z$, and $P(0)\sim Z^2$. The explicit evaluation of the Z reduction factor is presented in Appendix B; see Eq. (B2).

Let us now compare the variational energy as given by Eq. (45) with Z of Eq. (B6), valid for $1/2-\Delta_0=\delta\ll 1$, to the energy of a nonsuperconducting paramagnetic solution [Eq. (45)] with $\Delta=0$, Z being given by Eq. (B3). We find that the Gutzwiller projected BCS wave function has always higher energy by terms roughly of order $Z|T_0|$.

Therefore, even though the Gutzwiller correlator is quite efficient to transform the huge Hartree-Fock energy cost, namely,

$$\begin{aligned}&\langle\Phi_{BCS}(\Delta_0)|\hat{H}|\Phi_{BCS}(\Delta_0)\rangle-\langle\Phi_{BCS}(0)|\hat{H}|\Phi_{BCS}(0)\rangle\\&\quad=T_0(\Delta_0)-T_0(0)+2U\Delta_0^2+4J_T\Delta_0^2\\&\quad\simeq -T_0(0)+\frac{U}{2}+J_T,\end{aligned}$$

into a much smaller one of order $Z|T_0|\sim ZU$ close to the Mott transition, yet it is not able to make superconductivity favorable. That is, the best variational metallic solution remains the one described in Sec. III, with all the drawbacks discussed in Sec. IV. In conclusion, as we anticipated, the Gutzwiller variational approach does not properly describe a mean-field-unlike Mott transition.

In reality we may expect a superconducting phase just before the VB Mott insulator. Recently a model has been studied which shares many common features with the present one, namely, a three-band Hubbard model with inverted Hund's rules,[15] mimicking a strongly dynamical Jahn-Teller effect. For an average number of electrons per site $n_0=2$, the inverted Hund's rules favor, as in our example, a nondegenerate singlet on-site configuration. By a DMFT calculation, a superconducting instability was discovered just before the singlet Mott insulator. However, that instability was found to appear when the quasiparticle residue $Z\sim|J|$ (see Ref. 15). As we discussed at length previously, the simplest metallic Gutzwiller wave function which we have so far considered is unable to reach $Z\sim J$, since it becomes disadvantageous with respect to the insulating one already at $Z\sim\sqrt{J}$. Therefore, we cannot exclude that superconductivity may occur even in the two-band model we have considered.

VII. CONCLUSIONS

In this paper we have analyzed some peculiar features of the Mott transition displayed by a multiband Gutzwiller variational wave function (GWF) in infinite dimensions. The analysis has been carried out by using the generalized GWF introduced in Ref. 11, which allows a simple analytical treatment in infinite dimensions. Moreover, we have extended that wave function to account for broken-symmetry phases.

It is usually assumed that the GWF in infinite dimensions gives a faithful description of the quasiparticle behavior around the Mott metal-insulator transition. We have shown that while this belief is partly true for single-band models, it is incorrect for multiband models. In particular, we have identified at least two major failures of the GWF across the Mott transition. The first concerns the occupation probability $P(n)$ of on-site charge configurations with n electrons different from the integer average one n_0, which is believed to represent just the quasiparticle occupation probability normalized to the quasiparticle residue Z.[15] The GWF in infinite dimensions predicts $P(n)\sim Z^{|n-n_0|}$, close to the Mott transition, while both physical arguments as well as dynamical mean-field theory results suggest a $P(n\neq n_0)\sim Z$, even in infinite dimensions. This apparently innocuous disagreement is instead profound. In fact, the GWF results imply that the quasiparticles remain much more strongly interacting than what the correct $P(n)\sim Z$ behavior suggests.

Another drawback concerns the Mott transition in the presence of a weak multiplet exchange splitting term J. Within the GWF, the Mott transition turns into a first order one and occurs when the quasiparticle residue $Z\sim\sqrt{|J|/W}$, W being the bare bandwidth, much before the quasiparticle gas has had the time to react against J. This happens because the susceptibility to an infinitesimal exchange splitting J diverges at the Mott transition for a GWF. In reality, that susceptibility is finite so that the Mott transition is either second order or weakly first order, in that case occurring when $Z\sim|J|/W$. The main consequence is that the interesting region where the metallic hopping-energy gain $\sim ZW$ competes against the exchange J is not even accessible by a Gutzwiller wave function. Both the above mentioned shortcomings have the same origin: the inability of the GWF to account for spatial correlations of unfavorable charge configurations.

We have then argued, on the basis of a two-band model study, that the GWF is still a good variational wave function in all cases which can be qualitatively described by a mean-field theory, but it fails otherwise, as for instance in the case we have explicitly analyzed where the Mott insulator is a local version of a valence bond insulator. There an improvement of the GWF is necessary.

ACKNOWLEDGMENT

We acknowledge helpful discussions with Joerg Büenemann, Sandro Sorella, and Federico Becca. We are particularly grateful to Claudio Castellani for his invaluable comments and suggestions. This work was partly supported by MIUR COFIN-2001.

APPENDIX A: ANTIFERROMAGNETIC GUTZWILLER WAVE FUNCTION FOR A TWO-BAND MODEL

The best Hartree-Fock wave function $|\Phi_0(m)\rangle$ on a bipartite lattice when the multiplet exchange term favors the spin-triplet configuration is the ground state of a Hamiltonian

$$\hat{H}_{HF}=\hat{H}_0+\mu\sum_i\sum_{a=1,2}(-1)^i(n_{i,a\uparrow}-n_{i,a\downarrow}),$$

which describes an antiferromagnetic insulator with order parameter

$$\langle\Phi_0|n_{i,1\uparrow}-n_{i,1\downarrow}|\Phi_0\rangle=\langle\Phi_0|n_{i,2\uparrow}-n_{i,2\downarrow}|\Phi_0\rangle=2(-1)^i m.$$

We search for the optimal Gutzwiller wave function

$$|\Psi_G\rangle=\prod_i\hat{P}_{i,G}|\Phi_0(m)\rangle,$$

where for a given sublattice, and making use of particle-hole symmetry,

$$\begin{aligned}\hat{P}_{i,G}=&\lambda_0[|i,0\rangle\langle i,0|+|i,4\rangle\langle i,4|]+\lambda_{1+}[|i,1;S_z=1/2\rangle\\&\times\langle i,1;S_z=1/2|+|i,3;S_z=1/2\rangle\langle i,3;S_z=1/2|]\\&+\lambda_{1-}[|i,1;S_z=-1/2\rangle\langle i,1;S_z=-1/2|\\&+|i,3;S_z=-1/2\rangle\langle i,3;S_z=-1/2|]+\lambda_{2\pm}|i,2,\pm\rangle\\&\times\langle i,2,\pm|+\lambda_{20}|i,2,0\rangle\langle i,2,0|\\&+\lambda_{2t+}|i,2;S=1,S_z=1\rangle\langle i,2;S=1,S_z=1|\\&+\lambda_{2t-}|i,2;S=1,S_z=-1\rangle\langle i,2;S=1,S_z=-1|\\&+\lambda_{2t0}|i,2;S=1,S_z=0\rangle\langle i,2;S=1,S_z=0|,\end{aligned}$$

while for the other sublattice + and − interchange. In this particular case the Gutzwiller correlator remains Hermitian since the nonunitary transformation $\hat{U}_i$ is diagonal in the above multiplet basis.

As usual the variational parameters λ's can be expressed in terms of the correlated probability distribution, which we define, for a given sublattice, as

$$P(1,+)=P(1,S_z=1/2)=P(3,S_z=1/2),$$

$$P(1,-)=P(1,S_z=-1/2)=P(3,S_z=-1/2),$$

$$P(2,t+)=P(2,S=1,S_z=1),$$

$$P(2,t-)=P(2,S_z=-1),$$

$$P(2,t0)=P(2,S_z=0),$$

while, for the other sublattice, $S_z\leftrightarrow -S_z$. Through Eqs. (8) and (9), they satisfy the normalization condition

$$\begin{aligned}&2P(0)+2P(1,+)+2P(1,-)+P(2,0)+P(2,\pm)+P(2,t0)\\&\quad+P(2,t+)+P(2,t-)=1,\end{aligned}\tag{A1}$$

as well as the conservation of the order parameter

$$P(1,+)+P(2,t+)-P(1,-)-P(2,t-)=2m. \quad \text{(A2)}$$

The variational energy is then found to be

$$E_G(m)=Z(m)T_0(m)+U[4P(0)+P(1,+)+P(1,-)] +2J_TP(2,0)+2J_S[P(2,t+)+P(2,t0)+P(2,t-)] -(3J_S+J_T)P(2,\pm), \quad \text{(A3)}$$

where

$$T_0(m)=\langle\Phi_0(m)|\hat{H}_0|\Phi_0(m)\rangle$$

and

$$\sqrt{Z(m)}=\frac{2}{\sqrt{1-4m^2}}\Bigg[\sqrt{P(0)}\Bigg(\sqrt{\frac{P(1,+)}{2}}+\sqrt{\frac{P(1,-)}{2}}\Bigg) +\frac{1}{2}[\sqrt{P(1,+)}+\sqrt{P(1,-)}]\Bigg(\sqrt{P(2,\pm)} +\sqrt{\frac{P(2,0)}{2}}+\sqrt{\frac{P(2,t0)}{2}}\Bigg)+\sqrt{\frac{P(2,t+)P(1,+)}{2}} +\sqrt{\frac{P(2,t-)P(1,-)}{2}}\Bigg]. \quad \text{(A4)}$$

For any finite U the optimal solution has always $m\neq 0$ due to the nesting property. For very large U we expect $m\to 1/2$. In this limit we can neglect all P's but $P(1,+)$ and $P(2,t+)$ hence, from Eqs. (A1) and (A2),

$$P(2,t+)=4m-1, \quad P(1,+)=1-2m,$$

which implies that

$$Z(m)\simeq 2\frac{4m-1}{1+2m}.$$

In the same limit the uncorrelated hopping energy has the expression

$$T_0(m)\simeq -2\sqrt{M_2(2-4m)},$$

where

$$M_2=\int d\epsilon\rho(\epsilon)\epsilon^2$$

is the second moment of the uncorrelated density of states per spin and orbital, $\rho(\epsilon)$. Therefore, the variational energy as function of the order parameter m for $U\gg|T_0|$ is

$$E_G(m)\simeq -4\frac{4m-1}{1+2m}\sqrt{M_2(2-4m)}+U(1-2m) +2J_S(4m-1),$$

and it is optimized by

$$m\simeq\frac{1}{2}-\frac{M_2}{(U-4J_S)^2}, \quad \text{(A5)}$$

leading to

$$E_G\simeq 2J_S-\frac{2M_2}{U-4J_S}. \quad \text{(A6)}$$

APPENDIX B: EVALUATION OF THE Z FACTOR FOR THE TWO-BAND MODEL

The explicit expression of the Z reduction factor in the two-band model of Sec. VI allowing for a superconducting order parameter is, through Eq. (44),

$$\sqrt{Z}=\lambda_{\bar{0}}\lambda_{\bar{1}}\left(\frac{1}{2}+\Delta\right)^3+\frac{3}{2}\lambda_{\bar{1}}\lambda_{\bar{2t}}\left(\frac{1}{2}+\Delta\right)^2\left(\frac{1}{2}-\Delta\right) +\lambda_{\bar{1}}\lambda_{\bar{2}\pm}\left(\frac{1}{2}+\Delta\right)^2\left(\frac{1}{2}-\Delta\right)+\frac{1}{2}\lambda_{\bar{1}}\lambda_{\bar{20}}\left(\frac{1}{2}+\Delta\right)^2\left(\frac{1}{2}-\Delta\right)+\frac{3}{2}\lambda_{\bar{3}}\lambda_{\bar{2t}}\left(\frac{1}{2}+\Delta\right)\left(\frac{1}{2}-\Delta\right)^2+\lambda_{\bar{3}}\lambda_{\bar{2}\pm}\left(\frac{1}{2}+\Delta\right)\left(\frac{1}{2}-\Delta\right)^2+\frac{1}{2}\lambda_{\bar{3}}\lambda_{\bar{20}}\left(\frac{1}{2}+\Delta\right)\left(\frac{1}{2}-\Delta\right)^2+\lambda_{\bar{3}}\lambda_{\bar{4}}\left(\frac{1}{2}-\Delta\right)^3. \quad \text{(B1)}$$

If we parametrize the λ's according to Eq. (46) and make use of Eq. (47) we find

$$\sqrt{Z}=\frac{2}{\sqrt{1-4\Delta^2}}\Bigg\{\frac{1}{4}\sqrt{P(0)P(1)}\Bigg[\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{0})P^{(0)}_{\Delta_0}(\bar{1})}{P^{(0)}_{\Delta_0}(0)P^{(0)}_{\Delta_0}(1)}} +\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{4})P^{(0)}_{\Delta_0}(\bar{3})}{P^{(0)}_{\Delta_0}(0)P^{(0)}_{\Delta_0}(1)}}+\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{2},0)P^{(0)}_{\Delta_0}(\bar{1})}{P^{(0)}_{\Delta_0}(0)P^{(0)}_{\Delta_0}(1)}} +\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{2},0)P^{(0)}_{\Delta_0}(\bar{3})}{P^{(0)}_{\Delta_0}(0)P^{(0)}_{\Delta_0}(1)}}\Bigg]+\frac{1}{4}\sqrt{P(2,0)P(1)} \times\Bigg[\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{0})P^{(0)}_{\Delta_0}(\bar{1})}{P^{(0)}_{\Delta_0}(2,0)P^{(0)}_{\Delta_0}(1)}}+\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{4})P^{(0)}_{\Delta_0}(\bar{3})}{P^{(0)}_{\Delta_0}(2,0)P^{(0)}_{\Delta_0}(1)}}\Bigg] +\Bigg[\frac{\sqrt{3}}{4}\sqrt{P(2,t)P(1)}+\frac{\sqrt{2}}{4}\sqrt{P(2,\pm)P(1)}\Bigg] \times\Bigg[\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{1})}{P^{(0)}_{\Delta_0}(1)}}+\sqrt{\frac{P^{(0)}_{\Delta_0}(\bar{3})}{P^{(0)}_{\Delta_0}(1)}}\Bigg]\Bigg\}. \quad \text{(B2)}$$

When $\Delta=\Delta_0=0$, the above expression reduces to the Z factor for a paramagnetic nonsuperconducting solution, namely,

$$\sqrt{Z}=2\sqrt{P(0)P(1)}+\sqrt{3}\sqrt{P(1)P(2,t)}+\sqrt{2}\sqrt{P(1)P(2,\pm)} +\sqrt{P(1)P(2,0)}. \quad \text{(B3)}$$

The uncorrelated probabilities distributions in the natural basis with order parameter Δ_0 (analogous expressions hold for Δ) are

$$
\begin{aligned}
P^{(0)}_{\Delta_0}(\overline{0}) &= \left(\frac{1}{2}+\Delta_0\right)^4 \simeq 1-4\delta+6\delta^2,\\
P^{(0)}_{\Delta_0}(\overline{1}) &= 4\left(\frac{1}{2}+\Delta_0\right)^3\left(\frac{1}{2}-\Delta_0\right) \simeq 4\delta-12\delta^2,\\
P^{(0)}_{\Delta_0}(\overline{2};0) &= \left(\frac{1}{2}+\Delta_0\right)^2\left(\frac{1}{2}-\Delta_0\right)^2 \simeq \delta^2,\\
P^{(0)}_{\Delta_0}(\overline{2};\pm) &= 2\left(\frac{1}{2}+\Delta_0\right)^2\left(\frac{1}{2}-\Delta_0\right)^2 \simeq 2\delta^2,\\
P^{(0)}_{\Delta_0}(\overline{2};t) &= 3\left(\frac{1}{2}+\Delta_0\right)^2\left(\frac{1}{2}-\Delta_0\right)^2 \simeq 3\delta^2,\\
P^{(0)}_{\Delta_0}(\overline{3}) &= 4\left(\frac{1}{2}+\Delta_0\right)\left(\frac{1}{2}-\Delta_0\right)^3 \simeq 0,\\
P^{(0)}_{\Delta_0}(\overline{4}) &= \left(\frac{1}{2}-\Delta_0\right)^4 \simeq 0,
\end{aligned}
\tag{B4}
$$

where the last expressions on the left hand side correspond to the limit $\Delta_0 = 1/2-\delta$ with $\delta \ll 1$. The uncorrelated occupation probabilities in the original electronic basis are readily obtained by the latter upon inverting Eq. (43):

$$
\begin{aligned}
P^{(0)}_{\Delta_0}(0) &= P^{(0)}_{\Delta_0}(4) = \left(\frac{1}{4}+\Delta_0^2\right)^2 \simeq \frac{1}{4}-\delta+2\delta^2,\\
P^{(0)}_{\Delta_0}(1) &= P^{(0)}_{\Delta_0}(3) = 4\left(\frac{1}{16}-\Delta_0^4\right) \simeq 2\delta-6\delta^2,\\
P^{(0)}_{\Delta_0}(2,0) &= \frac{1}{16}+\frac{3}{2}\Delta_0^2+\Delta_0^4 \simeq \frac{1}{2}-2\delta+3\delta^2,\\
P^{(0)}_{\Delta_0}(2,\pm) &= 2\left(\frac{1}{4}-\Delta_0^2\right)^2 \simeq 2\delta^2,\\
P^{(0)}_{\Delta_0}(2,t) &= 3\left(\frac{1}{4}-\Delta_0^2\right)^2 \simeq 3\delta^2.
\end{aligned}
\tag{B5}
$$

In the limit of small δ, by inserting Eqs. (B4) and (B5) into Eq. (B2) one finds, at leading order (recalling that $\Delta \sim Z \ll 1$),

$$
\begin{aligned}
\sqrt{Z} \simeq & \sqrt{2}\sqrt{P(0)P(1)}(1+\delta)+\sqrt{P(1)P(2,0)}\\
& +\left[\sqrt{\frac{3}{2}}\sqrt{P(1)P(2,t)}\sqrt{P(1)P(2,\pm)}\right](1+\delta).
\end{aligned}
\tag{B6}
$$

[1] N.F. Mott, Proc. Phys. Soc., London, Sect. A **62**, 416 (1949).

[2] A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

[3] G. Kotliar, S.Y. Savrasov, G. Palsson, and G. Biroli, Phys. Rev. Lett. **87**, 186401 (2001); M.H. Hettler, M. Mukherjee, M. Jarrell, and H.R. Krishnamurthy, Phys. Rev. B **61**, 12 739 (2000).

[4] M.C. Gutzwiller, Phys. Rev. **134**, A923 (1964); **137**, A1726 (1965).

[5] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989); Phys. Rev. B **37**, 7382 (1988).

[6] F. Gebhard, Phys. Rev. B **41**, 9452 (1990).

[7] E. Plekhanov, S. Sorella, and M. Fabrizio, Phys. Rev. Lett. **90**, 187004 (2003).

[8] C. Gros, Phys. Rev. B **38**, 931 (1988).

[9] A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **87**, 217002 (2001).

[10] S. Sorella, G.B. Martins, F. Becca, C. Gazza, L. Capriotti, A. Parola, and E. Dagotto, Phys. Rev. Lett. **88**, 117002 (2002).

[11] J. Bünemann, W. Weber, and F. Gebhard, Phys. Rev. B **57**, 6896 (1998).

[12] J.P. Lu, Phys. Rev. B **49**, 5687 (1994); Int. J. Mod. Phys. B **10**, 3717 (1996).

[13] T. Okabe, J. Phys. Soc. Jpn. **65**, 1056 (1996).

[14] H. Hasegawa, J. Phys. Soc. Jpn. **66**, 1391 (1997).

[15] M. Capone, M. Fabrizio, and E. Tosatti, Phys. Rev. Lett. **86**, 5361 (2001); M. Capone, M. Fabrizio, C. Castellani, and E. Tosatti, Science **296**, 2364 (2002).

[16] Y. Ono Bulla, M. Potthoff, and R. Bulla, cond-mat/0206508 (unpublished).

[17] S. Florens, A. Georges, G. Kotliar, and O. Parcollet, Phys. Rev. B **66**, 205102 (2002).

[18] M. Rozenberg, Phys. Rev. B **55**, R4855 (1997).

[19] A. Koga, Y. Imai, and N. Kawakami, Phys. Rev. B **66**, 165107 (2002).

[20] T.A. Kaplan, P. Horsch, and P. Fulde, Phys. Rev. Lett. **49**, 889 (1982).

[21] C. Gros, R. Joynt, and T.M. Rice, Phys. Rev. B **36**, 381 (1987).

[22] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987); **56**, 3582 (1987).

[23] P.G.J. van Dongen, F. Gebhard, and D. Vollhardt, Z. Phys. B: Condens. Matter **76**, 199 (1989).

[24] In other words, Γ_n is a multiplet of g_{Γ_n} states, labeled for instance by integers $\alpha_{\Gamma_n}=1,\ldots,g_{\Gamma_n}$ and

$$|i,n,\Gamma_n\rangle\langle i,n,\Gamma_n| \equiv \sum_{\alpha=1}^{g_{\Gamma_n}} |i,n,\alpha_{\Gamma_n}\rangle\langle i,n,\alpha_{\Gamma_n}|.$$

[25] J.E. Hirsch, Phys. Rev. B **31**, 4403 (1985).

[26] This property follows from the simple fact that the leading terms in the variational energy involving the probability $P(n_0 \pm m)$, $m>0$, are of the order

$$T_0\sqrt{P(n_0)P(n_0+1)}\sqrt{P(n_0\pm m)P(n_0\pm m\mp 1)},$$

for the hopping energy, and

$$UP(n_0 \pm m),$$

for the Hubbard repulsion. Comparing the two opposite in sign contributions, one gets

$$P(n_0\pm m) \sim \frac{|T_0|}{U}P(n_0\pm m\mp 1)P(n_0)P(n_0+1),$$

thus leading to

$$P(n_0 \pm m) \sim Z^m,$$

since one expects $P(n_0) \sim 1$ and $P(n_0 \pm 1) \sim Z$.

[27] P. Fazekas and K. Penc, Int. J. Mod. Phys. B **1**, 1021 (1988).
[28] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **59**, 3669 (1990).
[29] L. Laloux, A. Georges, and W. Krauth, Phys. Rev. B **50**, 3092 (1994).
[30] In reality this is already commonly done in numerical simulations when the *t*-*J* model is analyzed as representative of a strong coupling Hubbard model; see Refs. 8–10 and 31.
[31] S. Sorella, Phys. Rev. B **64**, 024512 (2001).