Analytical ground state for the three-band Hubbard model

C. Waidacher, J. Richter, R. E. Hetzel, and K. W. Becker
Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany
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For the calculation of charge excitations as those observed in, e.g., photoemission spectroscopy or in electron-energy-loss spectroscopy, a correct description of ground-state charge properties is essential. In strongly correlated systems like the undoped cuprates this is a highly nontrivial problem. In this paper we derive a nonperturbative analytical approximation for the ground state of the three-band Hubbard model on an infinite, half-filled CuO_2 plane. By comparison with projector quantum Monte Carlo calculations it is shown that the resulting expressions correctly describe the charge properties of the ground state. Relations to other approaches are discussed. The analytical ground state preserves size consistency and can be generalized for other geometries, while still being both easy to interpret and to evaluate. [S0163-1829(99)01628-8]

I. INTRODUCTION

The interest devoted to the three-band Hubbard model[1] is due to the fact that it describes the charge properties of a CuO_2 layer, like those found in the high-T_C superconducting cuprates, while still being comparatively simple.[2] The basic assumption that leads to the three-band Hubbard model is that the only relevant orbitals are the Cu $3d_{x^2-y^2}$ and the O $2p_x$ and $2p_y$ orbitals. This granted, the CuO_2 layer may be described by a lattice with one Cu and two O sites per unit cell with hybridization between nearest-neighbor Cu-O pairs and O-O pairs. In the hole picture the three-band Hubbard Hamiltonian reads

$$H = H_0 + H_1, \tag{1a}$$

$$H_0 = \Delta \sum_{j,\sigma} n^p_{j\sigma} + U_d \sum_i n^d_{i\uparrow} n^d_{i\downarrow}, \tag{1b}$$

$$H_1 = t_{pd} \sum_{\langle i,j\rangle \sigma} \phi^{ij}_{pd} (p^\dagger_{j\sigma} d_{i\sigma} + \text{H.c.}) + t_{pp} \sum_{\langle j,j'\rangle \sigma} \phi^{jj'}_{pp} p^\dagger_{j\sigma} p_{j'\sigma}, \tag{1c}$$

where $d^\dagger_{i\sigma}$ ($p^\dagger_{j\sigma}$) create a hole with spin σ in the ith Cu $3d$ orbital (jth O $2p$ orbital), while $n^d_{i\sigma}$ ($n^p_{j\sigma}$) are the corresponding number operators. H_0 is the atomic part of the Hamiltonian with the charge-transfer energy Δ and the on-site Coulomb repulsion U_d between Cu $3d$ holes. H_1 represents the hybridization of Cu $3d$ and O $2p$ orbitals (hopping strength t_{pd}) and of O $2p$ orbitals (hopping strength t_{pp}). The factors ϕ^{ij}_{pd} and $\phi^{jj'}_{pp}$ give the correct sign for the hopping processes,[2] and $\langle ij\rangle$ denotes the summation over nearest-neighbor pairs.

In Eq. (1a) only the most important Coulomb repulsion U_d is included, while O on-site and intersite Coulomb repulsions have been neglected. For explicit calculations the following typical set of values for the parameters involved in Eq. (1a) will be used:[3]

$$\Delta = 3.5 \text{ eV}, \quad U_d = 8.8 \text{ eV},$$
$$t_{pd} = 1.3 \text{ eV}, \quad t_{pp} = 0.65 \text{ eV}. \tag{2}$$

Strong correlations due to U_d are the reason why ground-state properties of Hamiltonian H can be calculated only approximately and/or on finite clusters. Besides analytical approaches like, e.g., different approximations for dynamical Green's functions,[4] mostly numerical simulations[5] have been applied to the three-band Hubbard model. The aim of the present work is to derive an analytical approximation for the ground state of an infinite system at half-filling (i.e., one hole per Cu site) that correctly describes charge properties and is still comparatively easy to evaluate. The resulting approximation does not only allow for a calculation of ground-state properties of the three-band model (1a). It also provides a framework for the investigation of excitations. Furthermore, the approach is sufficiently general to be applied not only to a CuO_2 plane but also to different geometries like, e.g., that of a CuO_3 corner-sharing chain.[6]

Starting point of the approximation is a Néel-ordered ground state of the atomic Hamiltonian H_0, which is denoted by $|\psi_0\rangle$. Due to fluctuations induced by H_1, this atomic ground state $|\psi_0\rangle$ differs from the full ground state $|\Psi\rangle$ of Hamiltonian H. In Sec. III, it will be shown that a perturbative treatment of these fluctuations breaks down for parameter values that are in the physically relevant range. Therefore, ground-state fluctuations have to be treated in a nonperturbative way. In the following, we will present a systematic and nonperturbative scheme to introduce these fluctuations on the background of $|\psi_0\rangle$.

The paper is organized as follows. In Sec. II, the general formalism is presented. As an illustration in Sec. III, this formalism is applied to the (exactly solvable) problem of a single CuO_4 plaquette. The approximative ground state of an infinite, half-filled CuO_2 plane is developed in Sec. IV, and ground-state expectation values are evaluated in Sec. V. In Sec. VI, the results of the analytical approach are compared to projector quantum Monte Carlo simulations. The conclusions are presented in Sec. VII. Finally, a more detailed justification of the approach together with a discussion of its relationship to the cumulant formalism[7] is given in the Appendix.

II. GENERAL FORMALISM

The basic idea is to start with a state $|\psi_0\rangle$ that is a first approximation to the full ground state $|\Psi\rangle$. In the present

case, we will choose $|\psi_0\rangle$ to be a Néel-ordered ground state of the atomic Hamiltonian H_0, Eq. (1b). In $|\psi_0\rangle$, every Cu site is singly occupied and all O sites are empty. Next, fluctuations on the background of $|\psi_0\rangle$ are introduced. These ground-state fluctuations are described by fluctuation operators F_α (introduced below in more detail) that approximately transform state $|\psi_0\rangle$ into the full ground state $|\Psi\rangle$. Under quite general conditions it can be shown[8] that the transformation leading from $|\psi_0\rangle$ to $|\Psi\rangle$ has to be of exponential form

$$|\Psi\rangle = \exp\left(\sum_\alpha \lambda_\alpha F_\alpha\right)|\psi_0\rangle. \tag{3}$$

The parameters λ_α are fluctuation strengths of the fluctuation operators F_α. They are determined using the set of equations

$$0 = \langle\Psi|[H, F_\alpha^\dagger]|\Psi\rangle, \quad \alpha = 1,2,\ldots. \tag{4}$$

Equation (4) follows from the condition that $|\Psi\rangle$ is an eigenstate of the full Hamiltonian H, Eq. (1a). From Eq. (3) all ground-state properties can be evaluated using

$$\langle A\rangle = \frac{\langle\Psi|A|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{5}$$

The ground-state energy, for instance, is calculated from Eq. (5) with $A=H$. Equations (3) and (4), together with an appropriate choice of fluctuation operators F_α, constitute the formal framework to be used in the remainder of this work. The above formalism will be applied to an exactly solvable problem in Sec. III. This serves both as an illustration of the approach and as an indication to which extent a perturbative treatment of ground-state fluctuations is possible.

We finally remark that Eqs. (3) and (4) are closely related to the cumulant formalism (see the Appendix). Therefore, the approach presented in this work preserves size consistency. Thus, for instance, the approximated ground-state energy remains an extensive quantity.

III. APPLICATION TO A SINGLE PLAQUETTE

As an example, the method presented in the last section is now used to find an approximate expression for the ground state of Hamiltonian (1a) for the case of a single CuO_4 plaquette occupied by a single hole. In this case, the unperturbed ground state $|\psi_0\rangle$ of H_0 is a state in which the Cu site is singly occupied while the four O sites are empty. For reasons of symmetry we may use a single fluctuation operator F_1, which describes fluctuations of the hole from the Cu site to the four surrounding O sites j, i.e.,

$$F_1 = -\sum_{j,\sigma} \phi_{pd}^j p_{j\sigma}^\dagger d_\sigma, \tag{6}$$

where ϕ_{pd}^j are the phase factors introduced in Eq. (1c). According to Eq. (3), the full ground state of a hole on a single plaquette is expressed by

$$|\Psi\rangle = \exp(\lambda_1 F_1)|\psi_0\rangle. \tag{7}$$

The norm of this state is

$$\langle\Psi|\Psi\rangle = 1 + 4\lambda_1^2. \tag{8}$$

The fluctuation strength λ_1 in Eq. (7) is determined from condition (4),

$$0 = \langle\Psi|[H, F_1^\dagger]|\Psi\rangle. \tag{9}$$

Nonvanishing contributions in Eq. (9) arise only from terms up to order λ_1^2. The following quadratic equation for λ_1 is obtained:

$$0 = 4t_{pd} - 4(\Delta - 2t_{pp})\lambda_1 - 16 t_{pd}\lambda_1^2. \tag{10}$$

When the positive solution for λ_1 is used in Eq. (7), one obtains the exact ground state. The ground-state energy E_G is calculated using Eq. (5),

$$E_G = -4t_{pd}\lambda_1 = \frac{1}{2}\left[\Delta - 2t_{pp} - \sqrt{(\Delta - 2t_{pp})^2 + (4t_{pd})^2}\right]. \tag{11}$$

For parameter set (2), a value of $\lambda_1 = 0.33$ results. Notice that Eq. (11) contains only a reduced effective charge-transfer energy $\Delta - 2t_{pp}$. The Cu occupation number $\langle n_{\mathrm{Cu}}\rangle = \langle\Psi|n_d|\Psi\rangle\langle\Psi|\Psi\rangle^{-1}$ is given by

$$\begin{aligned}\langle n_{\mathrm{Cu}}\rangle &= \frac{\langle\psi_0|\exp(\lambda_1 F_1^\dagger) n_d \exp(\lambda_1 F_1)|\psi_0\rangle}{\langle\Psi|\Psi\rangle} \\ &= \frac{\langle\psi_0|(1+\lambda_1 F_1^\dagger) n_d (1+\lambda_1 F_1)|\psi_0\rangle}{\langle\Psi|\Psi\rangle} \\ &= \frac{1}{1+4\lambda_1^2}.\end{aligned} \tag{12}$$

From this result one may conclude that a perturbative treatment of F_1 fluctuations (i.e., an expansion in λ_1, see the Appendix), also in infinite systems, is in general not possible. Typically, λ_1 is of the order 1/2. An expansion of Eq. (12) in λ_1, however, diverges for $\lambda_1 \geqslant 0.5$. Condition $\lambda_1 = 0.5$ is equivalent to a vanishing effective charge-transfer energy $\Delta - 2t_{pp} = 0$ and to a Cu occupation number of 1/2. At this point, state $|\psi_0\rangle$ ceases to be a good approximation of the exact ground state $|\Psi\rangle$. This divergence has been observed previously,[9] although its origin was unclear at that time.

IV. APPLICATION TO AN INFINITE CuO_2 PLANE

We now apply the formalism presented in Sec. II to the geometry of an infinite CuO_2 plane. State $|\psi_0\rangle$ is again the Néel-ordered ground state of the atomic Hamiltonian H_0, Eq. (1b). Let us introduce appropriate fluctuation operators F_α. First, operator F_1 from Eq. (6) is generalized to all N Cu sites i,

$$F_{i,1} = -\sum_{j,\sigma} \phi_{pd}^{ij}, p_{j\sigma}^\dagger d_{i\sigma},$$

where the sum is over the four O sites j that surround Cu site i. The remaining operators are constructed in accordance with the following principles: (i) All operators describe delocalizations of a hole initially located at Cu site i. (ii) The final site in the process is reached via the shortest path accessible by Cu-O hopping processes. (iii) A summation over

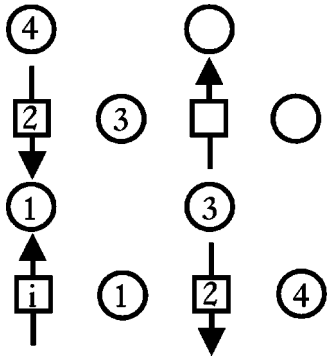

FIG. 1. Final sites of the fluctuation operators $F_{i,\alpha}$. Cu and O sites are symbolized by squares and circles, respectively. Arrows show spin orientation and position of the holes in the atomic ground state. The fluctuations $F_{i,\alpha}$ start from Cu site i and lead to the final sites labeled by $\alpha=1,\ldots,4$. The area shown is a quarter of the full area accessible to the fluctuations.

all equivalent final sites is taken. (iv) The signs of the hopping processes are chosen to be the negative of the phases ϕ_{pd}^{ij} in Hamiltonian (1c) (which guarantees non-negative values for the fluctuation strengths λ_α).

Figure 1 shows final sites reached by fluctuation operators $F_{i,\alpha}$, $\alpha=1,\ldots,4$. For reasons of symmetry only a quarter of the allowed fluctuation range is shown. Fluctuation $F_{i,2}$, for instance, describes the hopping of the hole from Cu site i, via O site j, to the four nearest-neighbor Cu sites k,

$$F_{i,2}=-\sum_{j,k,\sigma}(1-n_{j\sigma}^{p})d_{k\sigma}^{\dagger}d_{i\sigma}.$$

Final states with singly or doubly occupied Cu sites differ by the Coulomb energy U_d. Since U_d is large, we have to distinguish between these two cases. Therefore, we split $F_{i,2}$ into two operators that describe a process leading to a singly or doubly occupied Cu site, respectively,

$$F_{i,2s}=-\sum_{j,k,\sigma}(1-n_{k\sigma}^{d})(1-n_{j\sigma}^{p})d_{k\sigma}^{\dagger}d_{i\sigma},$$

$$F_{i,2d}=-\sum_{j,k,\sigma}n_{k\bar{\sigma}}^{d}(1-n_{j\sigma}^{p})d_{k\sigma}^{\dagger}d_{i\sigma}.$$

Note that it is not necessary to introduce a fluctuation operator, which leads to the nearest-neighbor Cu sites in diagonal direction (e.g., the Cu site without a label in Fig. 1). Due to the Pauli principle, fluctuations to these sites are largely excluded because of antiferromagnetic order. The neglect of fluctuations leading beyond the range shown in Fig. 1 will be justified *a posteriori*. It will be shown that the fluctuation strengths λ_α decrease rapidly with increasing length of the fluctuation processes.

According to Eq. (3), the ground state has the form

$$|\Psi\rangle=\exp\left(\sum_{i,\alpha}\lambda_\alpha F_{i\alpha}\right)|\psi_0\rangle, \tag{13}$$

where α denotes the five fluctuation operators described above. Because of translational symmetry, the parameters λ_α do not depend on the Cu site index i. To simplify Eq. (13), we approximately factorize the exponential function with respect to the fluctuations $F_{i,1}$,

$$|\Psi\rangle=\exp\left(\sum_{i,\alpha>1}\lambda_\alpha F_{i\alpha}\right)\exp\left(\sum_{i'}\lambda_1 F_{i',1}\right)|\psi_0\rangle. \tag{14}$$

This approximation amounts to the assumption that far-reaching fluctuations $F_{i,\alpha>1}$ occur on the background of $F_{i,1}$ fluctuations that in turn are influenced only indirectly (i.e., via λ_1) by the former. The second exponential function in Eq. (14) exactly factorizes with respect to i',

$$|\Psi\rangle=\exp\left(\sum_{i,\alpha>1}\lambda_\alpha F_{i\alpha}\right)\prod_{i'}(1+\lambda_1 F_{i',1})|\psi_0\rangle. \tag{15}$$

In Eq. (15) every hole may fluctuate over a total range of five plaquettes each. Notice that all holes fluctuate simultaneously. This leads to a multitude of many-body effects, i.e., the fluctuation of a hole depends on the configuration of other holes. Basically there are three types of many-body effects that are exemplified in Fig. 2. First, due to the Pauli principle, the fluctuation of a hole may be blocked by the presence of other holes with the same spin, as in the fluctuation process labeled (a) in Fig. 2. Second, there are processes in which holes with the same spin change place, as in process (b). In the following we will call these processes *site-changing processes*. Third, there are strong correlations due to the Hubbard U_d on doubly occupied Cu sites, as in process (c). One common feature of all these many-body effects is that they suppress fluctuations.

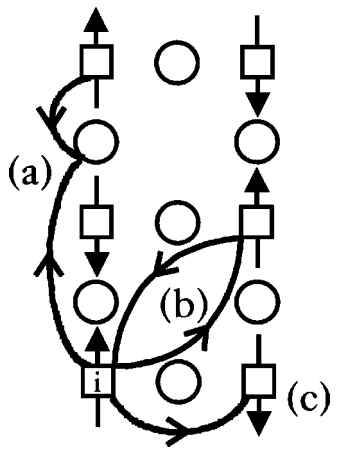

FIG. 2. Examples for many-body effects. There are three types of effects: (a) processes which are excluded by the Pauli principle, (b) site-changing processes, and (c) correlations due to the Hubbard U_d on doubly occupied Cu sites. The approach presented in this work accounts for all effects shown here.

This multitude of many-body effects makes an exact evaluation of expectation values using Eq. (15) impossible. Further approximations are, therefore, necessary. Let us consider processes in which two or more holes simultaneously leave their original plaquette. The fluctuation strengths λ_α for such far-reaching fluctuations turn out to be small compared to λ_1. Therefore, it should be possible to neglect the many-body effects arising in these processes (except for site-changing processes in diagonal direction, see below). In the

case of $F_{i,2d}$ fluctuations, for example, we neglect the possibility that the O site j between the Cu starting and final sites, i and k, may already be occupied by a hole with the same spin. This amounts to the simplification

$$F_{i,2d} = -\sum_{j,k,\sigma} n^d_{k\bar{\sigma}} d^\dagger_{k\sigma} d_{i\sigma}.$$

In this way, all of the aforementioned processes are included, some of them, however, only in a simplified way (i.e., by neglecting many-body effects).

In addition to all many-body effects that are due to processes where only one hole leaves its original plaquette, we furthermore take account of all site-changing processes in diagonal direction, see Fig. 2(b). The suppression of charge fluctuations due to the diagonal sites turns out to be of great importance. On the other hand, site-changing processes involving next-nearest Cu neighbors in horizontal or vertical direction can be neglected for the following reason: During these processes the paths of the holes have to cross at the intermediate O sites (i.e., sites 1 and 4 in Fig. 1). However, since the holes have the same spin, they have to avoid each other due to the Pauli principle. Site-changing processes in horizontal or vertical direction are, therefore, unlikely.

V. EVALUATION OF EXPECTATION VALUES

We now evaluate expectation values with state (15). Using the above approximations the norm of this state is $\langle\Psi|\Psi\rangle = \nu^N$, where N is the number of Cu sites and, in generalization of Eq. (8),

$$\nu = 1 + \sum_\alpha z_\alpha p_\alpha \lambda_\alpha^2. \tag{16}$$

z_α is the number of equivalent final sites of the given process (e.g., $z_{2s}=4$), and p_α is the probability that the configuration of the other holes makes the process possible. This probability is defined by

$$p_\alpha = \frac{\langle\Psi|P_{i,\alpha}|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{17}$$

where $P_{i,\alpha}$ is a projection operator on all configurations that allow for process α. For example, $P_{i,2s}$ projects on states in which the target Cu site of fluctuation $F_{i,2s}$ is empty, whereas $P_{i,2d}$ is the projector on states with a singly occupied final site. Due to translational symmetry, the probabilities p_α do not depend on the site index i. Obviously, Eqs. (16) and (17) have to be solved self-consistently since $|\Psi\rangle$ in Eq. (17) depends on the parameters λ_α. In the case of p_{2s}, for instance, we obtain by explicit calculation

$$p_{2s} = \frac{\langle\Psi|P_{i,2s}|\Psi\rangle}{\nu^N} = \frac{1}{\nu}\sum_\alpha z_\alpha p_\alpha \lambda_\alpha^2 = 1 - 1/\nu.$$

In an analogous way, one finds

$$p_1 = 1, \quad p_{2s} = 1 - 1/\nu, \quad p_{2d} = 1/\nu,$$
$$p_3 = 1 - 2\lambda_1^2/\nu, \quad p_4 = 1 - \lambda_1^2/\nu. \tag{18}$$

The interpretation of Eq. (18) is straightforward. $p_1 = 1$ holds since we assume that far-reaching fluctuations occur on the background of $F_{i,1}$ fluctuations. $1/\nu$ is the probability to find a given hole at its original Cu site. p_{2d} is, therefore, the probability that a target Cu site is singly occupied. This is a necessary prerequisite for the fluctuation process F_{2d}, which leads to a double occupancy, cf. Fig. 2(c). p_{2s}, on the other hand, is the probability that a target Cu site is empty, as required for fluctuation process F_{2s}. The probability to find a given hole at a specific O site on its original plaquette is λ_1^2/ν. Thus, p_4 is the probability that the target O site of fluctuation F_4 is not blocked by the hole of the same spin that resides on the neighboring Cu site, cf. Fig. 2(a). Analogously, p_3 is the probability that the target O site of fluctuation F_3 is not blocked. The additional factor 2 in p_3 (as compared to p_4) is due to site-changing processes, cf. Fig. 2(b).

The fluctuation strengths λ_α are calculated using Eq. (4) for an arbitrary site $i=0$,

$$0 = \langle\Psi|[H, F^\dagger_{0,\alpha}]|\Psi\rangle. \tag{19}$$

One obtains the following nonlinear system of equations:

$$0 = (E_G - \Delta + 2t_{pp})\lambda_1 + t_{pd} + t_{pd}\lambda_{2s}p_{2s} + t_{pd}\lambda_{2d}p_{2d} + 2t_{pp}\lambda_3 p_3 - 2t_{pp}\lambda_1^2\lambda_3/\nu, \tag{20}$$

$$0 = E_G\lambda_{2s} + 4t_{pd}\lambda_{2d}\lambda_1/\nu + t_{pd}\lambda_1 p_{2s} + 2t_{pd}\lambda_3 p_3 p_{2s} + t_{pd}\lambda_4 p_4 p_{2s}, \tag{21}$$

$$0 = (2E_G - U_{dd})\lambda_{2d} + 4t_{pd}\lambda_{2s}\lambda_1 + t_{pd}\lambda_1 + 2t_{pd}\lambda_3 p_3 + t_{pd}\lambda_4 p_4, \tag{22}$$

$$0 = (E_G - \Delta + t_{pp})\lambda_3 p_3 + t_{pp}\lambda_1 p_3 + t_{pd}\lambda_{2s}p_{2s}p_3 + t_{pd}\lambda_{2d}p_{2d}p_3 + t_{pp}\lambda_4 p_3 - (t_{pd} + 2t_{pp}\lambda_1)\lambda_1\lambda_3/\nu, \tag{23}$$

$$0 = (E_G - \Delta)\lambda_4 p_4 + t_{pd}\lambda_{2s}p_{2s}p_4 + t_{pd}\lambda_{2d}p_{2d}p_4 + 2t_{pp}\lambda_3 p_3 - (t_{pd} + 2t_{pp}\lambda_1)\lambda_1\lambda_4/\nu, \tag{24}$$

where $E_G = -4t_{pd}\lambda_1$ is the ground-state energy per Cu site [see Eq. (25)]. This system of equations, together with Eqs. (16) and (18), can be solved self-consistently for all λ_α, p_α and for ν. The solution with the lowest value of E_G is then used in Eq. (15). In the case of $\lambda_\alpha = 0$ for all $\alpha > 1$, Eq. (20) reduces to Eq. (10) for the single plaquette.

Figure 3 shows the delocalization probability $p_\alpha\lambda_\alpha^2/\nu$ of a given hole summed over equivalent final sites as a function of fluctuation length for parameter set (2). In order to demonstrate the convergence of the results, additional fluctuations have been introduced that lead beyond the fluctuation range shown in Fig. 1. The contribution of these additional fluctuations to the ground-state energy amounts to less than 0.1 percent. No significant delocalization beyond the nearest-neighbor plaquette occurs. A similar observation is made when other model-parameter values are chosen within the range, which is relevant for cuprate compounds. These results retrospectively justify the neglect of far-reaching fluc-

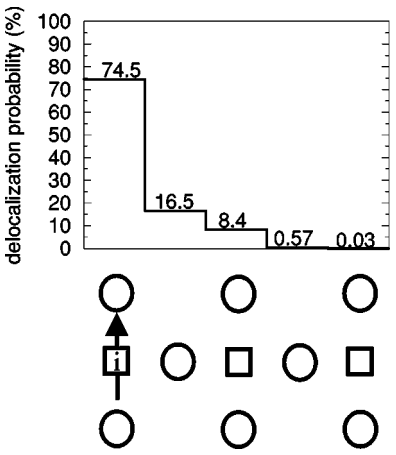

FIG. 3. Delocalization probability as a function of fluctuation length. The graph shows the delocalization probability of a hole that originates from Cu site *i*. The probability is summed over the sites displayed beneath the bars and over all equivalent final sites. The hole remains predominantly on its original plaquette. Delocalization beyond the nearest-neighbor plaquette is negligibly small. The probability has been calculated using Eq. (15) for parameter set (2).

tuations and many-body effects. Notice, however, that the neglect of many-body effects allows for unphysical fluctuations, which may decrease the calculated ground-state energy below the exact value. Thus, in contrast to an exact evaluation of Eq. (5), our approximate solution does not guarantee an upper limit to the exact ground-state energy.

From ground state (15) all expectation values are easily evaluated using Eq. (5). The ground-state energy per Cu site, occupation numbers, and double occupancies of Cu and O sites are

$$E_G = -4t_{pd}\lambda_1, \tag{25}$$

$$\langle n_{\mathrm{Cu}}\rangle = \frac{1}{\nu}(1+4\lambda_{2s}^2 p_{2s}+4\lambda_{2d}^2 p_{2d}), \tag{26}$$

$$\langle d_{\mathrm{Cu}}\rangle = \frac{1}{\nu}(4\lambda_{2d}^2 p_{2d}), \tag{27}$$

$$\langle n_{\mathrm{O}}\rangle = \frac{2}{\nu}(\lambda_1^2+2\lambda_3^2 p_3+\lambda_4^2 p_4), \tag{28}$$

$$\langle d_{\mathrm{O}}\rangle = \frac{1}{4}\langle n_{\mathrm{O}}\rangle^2. \tag{29}$$

The number of holes is conserved, i.e., $\langle n_{\mathrm{Cu}}\rangle + 2\langle n_{\mathrm{O}}\rangle = 1$. By comparison with quantum Monte Carlo calculations, it will be shown in the next section that these results correctly reproduce the charge properties of the ground state. However, magnetic properties like the reduction of sublattice magnetization due to fluctuations are only partly described. We have neglected many-body effects in processes in which two holes simultaneously leave their original plaquette. Therefore, no spin-flip effects are included. Thus, in the (Heisenberg) limit of infinitely large Δ and U_d, ground state (15) reduces to the Néel state.

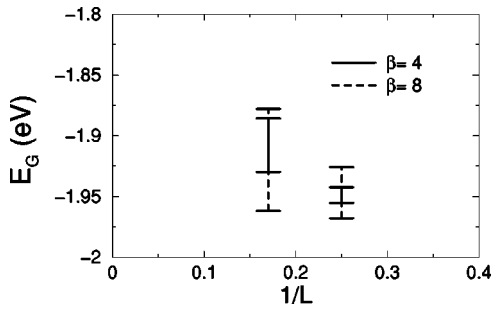

FIG. 4. Convergence of the PQMC calculations with respect to β and the system size. The ground-state energy E_G per Cu site for clusters of 4×4 and 6×6 plaquettes is shown as a function of inverse linear system size L. The solid and broken error bars are the results for $\beta=4$ and $\beta=8$, respectively. The parameters are those of set (2).

VI. DISCUSSION OF THE RESULTS AND COMPARISON TO QUANTUM MONTE CARLO SIMULATIONS

We have carried out numerical simulations of the three-band Hubbard model (1a), using the projector quantum Monte Carlo (PQMC) algorithm,[10] in order to compare them with the analytical result, Eq. (15). In the PQMC approach, the ground state of a finite cluster is projected out from a suitable trial state by applying the exponential operator $e^{-\beta H}$ onto the trial state in the limit $\beta\rightarrow\infty$. However, in numerical calculations only finite values of the parameter β are accessible. Therefore, one has to check convergence of the results with respect to β. Furthermore, one has to account for possible finite-size effects.

In the present study, two different cluster sizes have been investigated. First, we have used a system consisting of 4×4 plaquettes (i.e., 48 sites). This is the smallest cluster that allows for periodic boundary conditions while still being fully two dimensional. Second, we have studied the next largest cluster, a system of 6×6 plaquettes (i.e., 108 sites). We have used a mean-field version of the analytical ground state (15) as trial state. No sign problem occurred.

It turns out that the results obtained for the 4×4 system with $\beta=4$ are already reasonably well converged with respect to both β and system size. As shown in Fig. 4 for the case of the ground-state energy per Cu site, the error bars for different values of β overlap and the values of the 4×4 system differ only slightly from those of the 6×6 system. For this reason, we restrict our simulations to a system of 4×4 plaquettes with $\beta=4$ and compare the results with the analytical approach.

In Figs. 5 and 6, the ground-state energies E_G per Cu site and several occupation numbers calculated using Eqs. (25)–(29) are compared to the results of the PQMC simulations. The number of holes is conserved in both approaches. Thus the O occupation number $\langle n_{\mathrm{O}}\rangle$ is a function of the Cu occupation number $\langle n_{\mathrm{Cu}}\rangle$, and the former is, therefore, not shown. While the values of the model parameters are those of set (2), the charge-transfer energy Δ is varied covering the range of very large charge fluctuations ($\Delta=1.5$ eV) to fairly small charge fluctuations ($\Delta=4.5$ eV). In general, there is good agreement between the analytical and numerical results, especially for larger values of Δ.

With increasing Δ, both E_G and $\langle n_{\mathrm{Cu}}\rangle$ increase while the

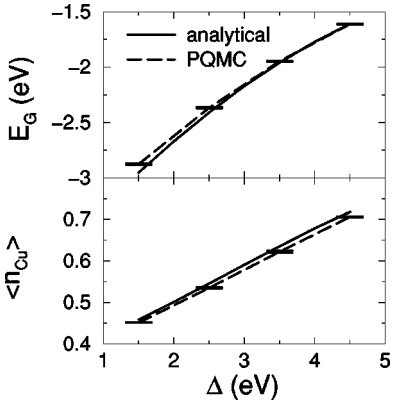

FIG. 5. Comparison of analytically calculated ground-state energies and Cu occupation numbers (solid lines) with the results of PQMC simulations for a cluster of 4×4 plaquettes (error bars connected by broken lines). As a function of Δ, the plots show the ground-state energy E_G per Cu site (upper graph), and the Cu occupation number $\langle n_{\mathrm{Cu}}\rangle$ (lower graph). The other parameters are those of set (2).

O double occupancy $\langle d_{\mathrm{O}}\rangle$ decreases. This behavior is due to the suppression of fluctuations for larger values of the charge-transfer energy. For smaller Δ, the analytical value for the ground-state energy lies below the PQMC result. This can be explained by the neglect of many-body effects in Eq. (15), which allows for more unphysical fluctuations when Δ becomes smaller. These fluctuations also lead to values for $\langle n_{\mathrm{Cu}}\rangle$ that are slightly larger than the PQMC result. However, even for $\Delta=1.5$ eV, the relative deviation for both E_G and $\langle n_{\mathrm{Cu}}\rangle$ amounts to less than 3%.

For larger values of Δ, the decrease of $\langle d_{\mathrm{O}}\rangle$ with increasing Δ is about two times as large as the decrease of $\langle d_{\mathrm{Cu}}\rangle$. The reason for this weaker dependence of $\langle d_{\mathrm{Cu}}\rangle$ on Δ is that an increase in the charge-transfer energy affects $\langle d_{\mathrm{Cu}}\rangle$ only indirectly by reducing the effective Cu-Cu hopping, while—in contrast to $\langle d_{\mathrm{O}}\rangle$—the on-site energy of the final site is not changed. Both analytical and numerical results show a maximum in the Cu double occupancy $\langle d_{\mathrm{Cu}}\rangle$ for intermediate values of Δ. This may be interpreted as the point where Δ is already sufficiently large to force holes from O sites onto already occupied Cu sites but still not large enough to suppress the effective Cu-Cu hopping.

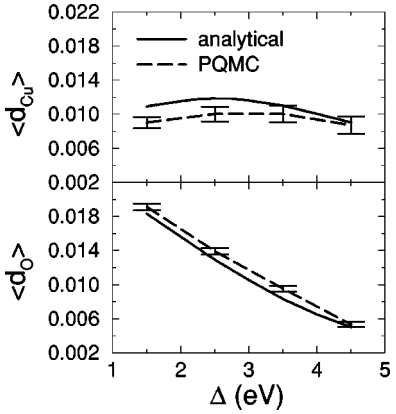

FIG. 6. Comparison of analytically calculated double occupancies (solid lines) with the results of PQMC simulations for a cluster of 4×4 plaquettes (error bars connected by broken lines). As a function of Δ, the plots show the Cu double occupancy $\langle d_{\mathrm{Cu}}\rangle$ (upper graph) and the O double occupancy $\langle d_{\mathrm{O}}\rangle$ (lower graph). The other parameters are those of set (2).

VII. CONCLUSION

Summing up, we have derived an analytical approximation, Eq. (15), for the ground state of the three-band Hubbard model (1a) on an infinite, half-filled CuO_2 plane. The approach uses fluctuation operators F_α and fluctuation strengths λ_α that have a clear physical interpretation. The parameters contained in Eq. (15) are determined self-consistently by solving a nonlinear system of equations. While the approach is nonperturbative and conserves size consistency, expectation values with the approximate ground state are still easy to evaluate. By comparison with projector quantum Monte Carlo simulations, we have demonstrated that Eq. (15) gives a reliable description of charge properties covering the range from small to very large charge fluctuations. Equation (15) can be generalized for other geometries. Furthermore, due to the use of fluctuation operators our approach provides a natural framework for the calculation of charge excitations, for example, by using projection technique. This will be demonstrated in a forthcoming publication.[6]

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APPENDIX: RELATION TO THE CUMULANT FORMALISM

The approach presented above can be formulated in the framework of the cumulant formalism.[7] The cumulant expectation value[11] of a product of operators is a linear combination of different factorizations of expectation values. For example, for two operators A_1 and A_2,

$$\langle\varphi|A_1A_2|\chi\rangle^c=\frac{\langle\varphi|A_1A_2|\chi\rangle}{\langle\varphi|\chi\rangle}-\frac{\langle\varphi|A_1|\chi\rangle\langle\varphi|A_2|\chi\rangle}{\langle\varphi|\chi\rangle^2}.$$

Here and in the following we always assume that the states involved in a cumulant have nonvanishing overlap, i.e., $\langle\varphi|\chi\rangle\neq0$. One of the attractive features of cumulants is that they preserve size consistency.[7]

The cumulant formalism for the calculation of ground-state properties may be formulated as follows. By application of an operator Ω within the cumulant ordering an approximate ground state $|\psi_0\rangle$ can be mapped onto the full ground state $|\Psi\rangle$,

$$|\Psi\rangle^c=\Omega|\psi_0\rangle^c=\exp\left(\sum_\alpha\lambda_\alpha F_\alpha\right)|\psi_0\rangle^c. \tag{A1}$$

The parameters λ_α are determined using the equation[8]

$$0=\langle\varphi|F_\alpha^\dagger H\Omega|\psi_0\rangle^c \tag{A2}$$

for all α and for an arbitrary state $|\varphi\rangle$. These equations follow[12] from the condition that $\Omega|\psi_0\rangle^c$ is an eigenstate of H. The exponential function in Eq. (A1) should be understood in terms of a series expansion in which the operators F_α are subjected to the cumulant ordering. From Eq. (A1), ground-state properties can be calculated using

$$\langle A\rangle=\langle\varphi|A\Omega|\psi_0\rangle^c. \tag{A3}$$

Next we show that Eqs. (3) and (4) can be derived from the above equations when the following identity[12] is used:

$$\langle\varphi|e^{F^\dagger}Ae^F|\chi\rangle^c=\langle e^F\varphi|A|e^F\chi\rangle^c. \tag{A4}$$

Equation (A4) holds for all operators F and A. It allows us to remove the exponential functions from the cumulant ordering and apply them directly onto the states. Using Eq. (A4), Eqs. (3) and (A1) can be directly transformed into each other. In Eq. (A2), on the other hand, we chose $|\varphi\rangle=\Omega|\psi_0\rangle$ and use Eq. (A4) to obtain

$$0=\langle\Omega\psi_0|F_\alpha^\dagger H|\Omega\psi_0\rangle^c.$$

If $|\Omega\psi_0\rangle$ is an eigenstate of H, this equation is equivalent to Eq. (4).

We conclude by pointing out some of the advantages of Eqs. (3) and (4) as compared to other possible approaches within the framework of the cumulant formalism. First, the fact that the exponential operator Ω has been transferred onto the state $|\psi_0\rangle$ amounts to a summation of all orders in the λ_α. Thus, our approach is nonperturbative and avoids (possibly divergent) series expansions of expressions like Eq. (12). The divergence of these series for $\lambda_1\geqslant 0.5$ is equivalent to the violation of condition[13] $|\langle\psi_0|\Psi\rangle|^2>1/2$. Consequently, when $\lambda_1\geqslant 0.5$, within the cumulant ordering no operator Ω exists for state $|\psi_0\rangle$. These difficulties do not occur when Ω has been removed from the cumulant ordering. Second, since in Eq. (4) the full ground state $|\Psi\rangle$ appears as both bra and ket vector, more fluctuations are taken into account. If, for example, Eq. (A2) with $|\varphi\rangle=|\psi_0\rangle$ is used instead of Eq. (4), one always obtains a vanishing value for λ_{2s}.

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