Real-space renormalization-group study of the two-dimensional Hubbard model

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(Received 8 June 1992)

The one-band two-dimensional Hubbard Hamiltonian is analyzed using a real-space renormalization-group block method. The renormalization-group method, previously applied to the one-dimensional case has been extended to two dimensions. It is also shown how to avoid the proliferation of new terms during the process if the shape of the blocks and the symmetries of the kept states are chosen conveniently. We characterize the ground state by its energy per site, the gap of charge excitations, the double occupancy, and the effective hopping. The system shows an insulating behavior in the case of half filling for all nonzero interaction parameter, U, if the hopping is isotropic ($t_y = t_x$); that is to say, the gap opens for all positive U, as in the one-dimensional case. If the hopping anisotropy, $\alpha = t_y/t_x$, is different from unity and zero the ground state is a conductor up to a critical value $(U/t)_{c_1}$, which depends on α. We have analyzed in the same way another filling, $n = \frac{7}{9}$. The system behaves as a conductor, paramagnetic up to a value $(U/t)_{c_2} \sim 2$ and weakly ferromagnetic for higher values of U.

I. INTRODUCTION

The one-electron theory has been able to explain most of the properties of periodic crystals: metals, semiconductors, and insulators. This success could not hide, however, the limits of the so-called "band theory." In this approach one takes into account the Coulomb interactions between the electrons only in a mean-field sense, and one cannot explain some important phenomena such as the itinerant magnetism (Fe ferromagnetism) or some of the metal-insulator (Mott-Hubbard) transitions. Other approaches are then needed in order to understand these phenomena. A few magnetic materials have been described from a microscopical point of view (see Refs. 1 and 2). The mechanism of the Mott-Hubbard transitions is, on the other hand, far from being completely understood (see Ref. 3, Chaps. 4 and 6) even if there are well-established microscopic models. Recently, the discovery of the high-T_c superconductors by Bednorz and Müller[4] has added a new challenge to the understanding of highly correlated electron systems. The phase diagram of these materials at $T = 0$ shows strong parallelism with the Mott-Hubbard insulators at least in what concerns the existence of a conductor-insulator phase transition (see Ref. 5 for an introductory insight on the high-T_c superconductors). There is a general belief[6,7] that the simplest microscopical model providing an account of these surprising properties could be the Hubbard model. This Hamiltonian was proposed 30 years ago by several authors[8–10] in order to describe the transition metal properties. It consists of two parts: a tight-binding band H_t, and an interaction term H_u,

$$H = -\sum_{\langle i,j\rangle,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i c^{\dagger}_{i\downarrow} c_{i\downarrow} c^{\dagger}_{i\uparrow} c_{i\uparrow} = H_t + H_u, \tag{1}$$

where the $\langle\,\rangle$ means hopping restricted to nearest neighbors and $c^{\dagger}_{i,\sigma}$ represents an s-like Wannier orbital. It should be noted here that two important simplifications have been used to obtain this model: the restricted hopping and the intrasite interaction (completely screened in the neighboring sites). The model shows several symmetries if the lattice belongs to the bipartite type.[11] The Schrödinger equation corresponding to (1) is in general very difficult to solve even if we are only interested in the ground-state description. The exact solution is known, however, in the one-dimensional case[12] as well as some of its ground-state properties such as the insulating gap in the half filling[13] case, the susceptibility,[14] the excitation spectra,[15] and, finally, the charge-charge and spin-spin correlation functions.[16]

In two and three dimensions it is no longer possible to apply the Bethe ansatz to the Hubbard model[17] and one has to try other approaches. A physically appealing solution was proposed by Gutzwiller.[8] This solution consists in projecting out an amount of the double occupancy D. Some results of this solution in one dimension[18,19] are in qualitative disagreement with the exact ones: at the half filling the Gutzwiller solution predicts a conducting behavior for all the positive U/t values, which contradicts the insulating nature of the Lieb and Wu ansatz.[12] In two dimensions, where analytical results are not available, Hong and Hirsch[20] have analyzed the bare Hamiltonian and the Gutzwiller function with the aid of the quantum Monte Carlo technique, and they have concluded that the Gutzwiller ansatz does not reproduce the features of the ground state, mainly in what concerns its magnetic behavior. The results can be slightly improved if one takes explicitly into account the spin symmetry breaking,[21] but then one finds a nonzero staggered magnetization even in the one-dimensional case, where we know that the magnetic order does not exist for this model.[16] There are many other variational approaches like the resonating va-

lence bond proposed by Anderson[6] or that of von der Linden and Edwards.[22] The former has been constructed to reproduce a superconducting phase and the latter has been proposed to analyze the ferromagnetic behavior of the Hubbard model, both in the $U/t \rightarrow \infty$ limit. All these variational approaches are reasonable and correct from a physical point of view, that is to say, in order to reproduce the actual behavior of some materials. One could doubt, however, if these functions are able to describe the ground state of the Hubbard Hamiltonian (1). Another analytical approach consists in imposing the existence of an order parameter that can be treated like a mean field[23,24] or in a more sophisticated way as did Schrieffer, Wen, and Zhang[7] and Georges and Yedidia.[25] These two latter groups agree in what concerns the half-filled system (the existence of an antiferromagnetic order) but they are contradictory about the existence of the superconducting phase. So far, we have mainly mentioned analytical methods. There exist, in addition, some numerical techniques such as quantum Monte Carlo[24,26,27] or exact finite-cluster diagonalizations,[28,29] which can be performed without any additional hypothesis (bare Hamiltonian), but it is possible to study the behavior of some variational functions as well (see Refs. 30 and 21, for example). Despite the *a priori* correctness of the numerical methods they are limited to finite-size clusters, which could hide some of the intrinsic properties of the infinite systems like the phase transitions.

It is then reasonable to develop a nonperturbative method with a minimum of constraints able to describe the different phases of a system. This is the aim of the real-space renormalization-group method, which we present in this paper to analyze the nature of the two-dimensional Hubbard model. The renormalization-group techniques have had their main success in the analysis of the Kondo problem by Wilson,[31] who applied the renormalization procedure in the k space. Afterward, Jafarey, *et al.*[32] developed the same idea in real space. The first published paper was, however, by Drell, Weinstein, and Yankielowicz[33] about the iterative construction of the ground state of the $\lambda\varphi^4$ theory. Later, the same ideas were applied to one- and two-dimensional spin systems and finally to the one-dimensional Hubbard model.[34,35] A pedagogical history of the real-space renormalization can be found in Refs. 36 and 37. The present paper is devoted to the renormalization technique applied to a fermion system in two dimensions. Some work has been already reported,[38,39] but the results were not reliable due to the small block size used in the perturbative development (five sites). In Sec. II we discuss the symmetries of the model, which will be used later. Section III describes the block method and the renormalization of the more important quantities: Hamiltonian, double occupancy, etc. We give an outline of the diagonalization of the 3×3 block in Sec. IV, along with some discussion. Finally, Sec. V contains an account of the main results.

II. SYMMETRIES

There are three global symmetries of H independent of the lattice: the total number operator $N_e = \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}$, the projection of the total spin $S_z = \sum_{i,\sigma} \sigma c^\dagger_{i\sigma} c_{i\sigma}$ and the total spin $S^2 = S_z^2 + 1/2(S^+S^- + S^-S^+)$, where $S^+ = \sum_i c^\dagger_{i\uparrow} c_{i\downarrow}$ and $S^- = (S^+)^-$. The rest of the symmetries are lattice dependent, and even if most of them remain in three dimensions we shall focus our attention on the two-dimensional square lattice.

The first symmetry pointed out in the literature is the invariance of the energy spectra under the transformation $t \longrightarrow -t$,[12] which works for many other quantities as well, such as the double occupancy, the local moment, the effective hopping, etc. Another interesting symmetry of the Hubbard model is the pseudospin Z. It was discovered by Castellani *et al.*,[40] analyzed later by Nowak,[41] and applied by others[42,43] in different situations. It consists in a generalization of the spin algebra SU(2) to the charge space.[44] This generalization is, in principle, not possible for an extended system. In the Hubbard model case one can write, however,

$$Z^+ = \sum_{k,k'} d^\dagger_{k\downarrow} d^\dagger_{k'\uparrow} \delta(\varepsilon(k) + \varepsilon(k') - g), \tag{2}$$

where the $d_{k\sigma}$ are the operators that diagonalize the band term

$$H_t = \sum_\sigma \varepsilon(\mathbf{k}) d^\dagger_{k\sigma} d_{k\sigma}, \quad \varepsilon(\mathbf{k}) = -2(t_x \cos k_x + t_y \cos k_y). \tag{3}$$

From (2) and (3) if we choose $g = 0$ and k' so that

$$k' = k + \pi, \tag{4}$$

then we obtain

$$[H_t, Z^+] = 0, \quad [H_u, Z^+] = UZ^+, \tag{5}$$

$$[H, Z^+Z^-] = 0 \tag{6}$$

It is also convenient to write down the explicit form of Z^+ in terms of the Wannier operators $c_{i\sigma}$ in order to get a real-space insight into this pseudospin operator,

$$Z^+ = \sum_i (-1)^i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow}.$$

The Casimir Z^+Z^- is therefore another symmetry of the Hamiltonian (1). It should be noted that (4) is only possible in an $N_s = L \times L$ lattice if L is even (odd) with periodic (free) boundary conditions. The spectra of Z^-Z^+ for a given number of electrons N_e and a spin projection S_z is[41]

$$\gamma_l = (l+1)(N_s - N_e + l),$$

$$l = 0, 1, \ldots, [\tfrac{1}{2}N_e - |S_z|], \tag{7}$$

$$N_e \leq N_s, S_z \leq 0.$$

Finally, we shall use later the spatial symmetry to construct explicitly the Hamiltonian. In the case of the square lattice and an anisotropic hopping $t_y \neq t_x$, H is invariant under the C_{2v} point group.[45] This additional

symmetry enables us to reduce by four the dimension of the greatest subspace defined by N_e and S_z (see also Sec. III).

III. THE BLOCK METHOD

The two main difficulties in treating a many-body problem lie in the huge number of possible configurations and in the complicated task to obtain the eigenvectors of the Hamiltonian, in particular the ground state. We are mainly interested, however, in the macroscopic properties of the system, that is to say, the microscopic fluctuations are not very important to the physical result. We can then, following Kadanoff's idea (see Ref. 46), divide the lattice into blocks of size $(as)^d$, where a is the lattice parameter, d is the dimension of the space, and $s > 1$ is the size factor. Afterward, we average over this block the quantities we are dealing with: the Hamiltonian, the double occupation, etc. In doing so we have neglected the fluctuations down to a size sa. This procedure can be repeated until we reach convergence, the so-called fixed point in the parameter space (t, U).

In order to clarify this process we can visualize it for the two-dimensional case, where we have chosen $s = 3$. We assimilate then each block to a point belonging to a new lattice with a parameter equal to $3a$. So far, we do not know what the Hamiltonian becomes. To have a first insight we label the parameters of the Hamiltonian with a for the original lattice and with $3a$ for the transformed one; there will be then some relations between (t_a, U_a) and (t_{3a}, U_{3a}, J_{3a}):

$$\begin{aligned} t_{3a} &= \varphi_1(t_a, U_a)\ , \\ U_{3a} &= \varphi_2(t_a, U_a)\ , \\ J_{3a} &= \varphi_3(t_a, U_a)\ , \end{aligned} \tag{8}$$

where J_{3a} represents the possible couplings generated by the process.

Furthermore, we are looking for a transformation that conserves the fermionic character of the second quantization operators $c_{i\sigma}$ and, in addition, avoids the proliferation of couplings, i.e.,

$$J_{3a} = 0.$$

A. The effective Hamiltonian

In order to construct the transformation introduced in the preceding section we shall focus our attention on the transformation of the Hamiltonian. Expression (1) can be separated into two terms

$$H = \sum_{\alpha} H_{b\alpha} + \sum_{\langle \alpha,\beta \rangle} V_{\alpha\beta} = H_o + V, \tag{9}$$

where α is a block label, $H_{b\alpha}$ is the intrablock Hamiltonian, and V stands for the hopping part between the blocks. Let us assume that we know how to solve the $H_{b\alpha}$'s and obtain all its eigenvectors $|\phi_{\{i\}\alpha}\rangle$ exactly. We can then formally rewrite H in this basis

$$H = \sum_{\{\psi,\psi'\}} |\psi\rangle\langle\psi|H|\psi'\rangle\langle\psi'|, \tag{10}$$

where $|\psi\rangle = \prod_{\alpha} |\phi_{\{i\}\alpha}\rangle$.

Despite the tautological appearence of (10) it is useful to indicate the first approach of the method: we shall keep four of the eigenvectors in each block from the 4^{N_s} $(N_s = s^d)$, which compose the total Hilbert space. This choice allows us to reduce drastically the number of configurations as well as to conserve the form of the Hamiltonian in the truncated basis. We shall restrict ourselves to the situations where the intrablock term reproduces the structure of the operator $n_\downarrow n_\uparrow$. Each block will be then represented by four states $|\phi_{\{o\}\alpha}\rangle$ that we shall call $|0'\rangle$, $|\downarrow'\rangle$, $|\uparrow'\rangle$ and $|\downarrow\uparrow'\rangle$ by analogy with the original sites. The explicit choice of these states will be done below.

We want now to project H onto the subspace spanned by $|\phi_{\{o\}\alpha}\rangle$'s. If we call P_o the projector on to this subspace,

$$P_o = \sum_{\{\psi_o\}} |\psi_o\rangle\langle\psi_o|, \quad |\psi_o\rangle = \prod_{\alpha} |\phi_{o\alpha}\rangle. \tag{11}$$

We are interested in the explicit expression of the effective Hamiltonian

$$H' = P_o P H P P_o, \tag{12}$$

where P is the perturbed projector of the truncated basis (the perturbation is V). It is now straightforward to get[47,35]

$$H' = \sum_{\psi_o,\psi'_o} |\psi_o\rangle \left\{ E_{\psi_o}\delta_{\psi_o\psi'_o} + \langle\psi_o|V|\psi'_o\rangle + \langle\psi_o|\frac{V(1-P_o)V}{E-H_o}|\psi'_o\rangle + \cdots \right\} \langle\psi'_o|. \tag{13}$$

We have already mentioned that we want to avoid the proliferation of couplings. An inspection of (13) indicates that the two first terms on the right-hand side will reproduce "roughly" the original model, and the third one will introduce some new couplings such as spin-spin interactions and the hopping between next-nearest-neighbor blocks. Hence, we keep the perturbative expression of H' up to the first order in V only.

We want afterward to express the effective Hamiltonian, H', in terms of some second quantization operators $c'_{\alpha,\sigma}$ in order to obtain a Hamiltonian as similar as possible to the original one. We choose then the two first eigenstates as

$$\begin{aligned} |0'\rangle &\equiv |N_e = N_o - 1, s = s_1, S_z = -s_1, \theta = \gamma_1, \Sigma_1, E = E_1\rangle, \\ |\downarrow'\rangle &\equiv |N_e = N_o, s = s_1 + \tfrac{1}{2}, S_z = -s_1 - \tfrac{1}{2}, \theta = \gamma_1 - 1, \Sigma_2, E = E_2\rangle, \end{aligned} \tag{14}$$

where N_o is the number of electrons, s_i the spin, γ_i the pseudospin, and Σ_i stands for the irreducible representations of the spatial group C_{2v}.[45] The symmetries that are not explicitly given in (14) will be provided by the conditions that we shall impose later. We complete the four states by applying the raising spin and pseudospin operators on $|0'\rangle$ and $|\downarrow'\rangle$,

$$\begin{aligned} |\uparrow'\rangle &\equiv S_\alpha^+|\downarrow'\rangle, \\ |\downarrow\uparrow'\rangle &\equiv Z_\alpha^+|0'\rangle, \end{aligned} \tag{15}$$

where α indicates that S^+ and Z^+ are defined on the α block.

The states $|\uparrow'\rangle$ and $|\downarrow\uparrow'\rangle$ are again eigenfunctions of the intrablock Hamiltonian because S^2 and Z^2 are symmetries of the system. The energies E_1 and E_2 will be the lowest compatible with all other symmetries.

B. Renormalization of the Hamiltonian parameters

In order to get the explicit expressions for φ_1 and φ_2 in (8) we need to establish a correspondence such as

$$P_o H_b P_o \longrightarrow H'_u + H'_\mu + K', \tag{16}$$

$$P_o V P_o \longrightarrow H'_t. \tag{17}$$

Here H'_μ represents a chemical potential term and K' is a constant, which will give later the ground-state energy. H'_t stands for the hopping term between nearest-neighbor blocks.

For the intrablock part (16) it is not very difficult to obtain

$$P_o H_{b\alpha} P_o = U' n'_\downarrow n'_\uparrow - \mu'_\downarrow n'_\downarrow - \mu'_\uparrow n'_\uparrow + K'_\alpha,$$

where

$$\begin{aligned} U' &= 2(E_1 - E_2) + U, \\ \mu'_\sigma &= (E_1 - E_2) + \mu_\sigma, \\ K'_\alpha &= E_1 - \mu_\downarrow N_{1\downarrow} - \mu_\uparrow N_{1\uparrow}, \end{aligned} \tag{18}$$

and $N_{1\downarrow} + N_{1\uparrow} = N_o - 1$ and $N_{1\uparrow} - N_{1\downarrow} = 2S_{z1}$. It is now clear why we have to choose only four states to conserve the repulsion term structure: had we chosen eight states, for example, we would have created two kind of electrons and therefore some new couplings.

The projection of the band, $P_o V P_o$, does not transform so clearly. First it is interesting to write the $c_{i\sigma}$ operators on the border of the block in terms of the $|0\rangle_i, \ldots, |\downarrow\uparrow\rangle_i$ states,

$$\begin{aligned} c_{i\sigma} &= c_{i\sigma}(1 - n_{i,-\sigma}) + c_{i\sigma} n_{i,-\sigma} \\ &= |0\rangle_i\langle\sigma|_i + \mathrm{sgn}(-\sigma)\,|-\sigma\rangle_i\langle\uparrow\downarrow|_i, \end{aligned} \tag{19}$$

and then, assuming a natural expansion of the operators on the border of the block α in the subspace spanned by $|0'\rangle, |\downarrow'\rangle, \ldots,$

$$\begin{aligned} c_{i\sigma}(\alpha) &= r_{i_\alpha,\sigma} c'_{\alpha\sigma}(1 - n'_{\alpha,-\sigma}) + v_{i_\alpha,\sigma} c'_{\alpha\sigma} n'_{\alpha,-\sigma} \\ &= r_{i_\alpha,\sigma}|0'\rangle_i\langle\sigma'|_i + \mathrm{sgn}(-\sigma)\, v_{i_\alpha,\sigma}|-\sigma'\rangle_i\langle\uparrow\downarrow'|_i \end{aligned} \tag{20}$$

where the $r_{i_\alpha,\sigma}$'s and the $v_{i_\alpha,\sigma}$'s are real numbers and the other matrix elements, such as $|0'\rangle_i\langle 0'|_i$ vanish. It has been demonstrated[48] that if we choose the $|l\rangle$'s so that

$$Z_\alpha^-|\downarrow'\rangle = 0,$$

with the spatial symmetry given by $\Sigma_1(\Sigma_2) = A_1(A_2)$ the completely symmetric (antisymmetric) irreducible representation and, say

$$|\uparrow'\rangle = \frac{1}{\sqrt{2(s_1 + \frac{1}{2})}} S_\alpha^+|\downarrow'\rangle$$

and, in addition, a convenient shape for the blocks (we restrict ourselves to the case of the 3×3 square block), we get a spin-dependent renormalized hopping,

$$t'_\downarrow = 2(s_1 + \tfrac{1}{2}) t'_\uparrow. \tag{21}$$

In particular for the half-filled band we are looking for the ground state of minimum spin,[42] $s_1 = 0$, so that there is no spin dependence for the renormalized band

$$t'_{x,y} = -2\lambda^2 t_{x,y}, \tag{22}$$

where $\lambda = \langle 0'|c_{i_\alpha\sigma}|\downarrow'\rangle$.

From (22) we notice that the renormalization process preserves the spatial anisotropy and, also, that the hopping parameter changes its sign. This last feature is not important as long as we are interested in obtaining quantities that are invariant under the change $t \to -t$.[12]

C. Renormalization of other quantities

We can extract directly the gap of the charge excitations and the ground-state energy per site from the analysis of (18). The insulating gap is defined for a given N by Refs. 12 and 49,

$$\begin{aligned} \Delta(N) = {} & [E_o(N+1) - E_o(N)] \\ & - [E_o(N) - E_o(N-1)]. \end{aligned} \tag{23}$$

For the half-filled system, in the frame of the renormalization group, we identify the ground state for N electrons to be $|\sigma^{(\infty)}\rangle$ and the $N \pm 1$ electron states to be $|0^{(\infty)}\rangle$ and $|\downarrow\uparrow^{(\infty)}\rangle$. Here the symbol ∞ represents the convergence limit and will be clarified later. The gap (23) is then given by

$$\Delta = U^{(\infty)}. \tag{24}$$

If the system is not half filled $U^{(\infty)}$ does not represent the gap any more because the eigenstate $|\downarrow\uparrow'\rangle$ defined by (15) is no longer the ground state in the $N+1$ subspace. From the constant K' in (18) we obtain the ground-state energy per site

$$\varepsilon_o = \lim_{n\to\infty} \frac{K^{(n)}}{9^n}, \tag{25}$$

where

$$K^{(n+1)} = E_1^{(n)} - (N_o - 1)\mu^{(n)} + 9K^{(n)}. \tag{26}$$

In the free-electron limit it is possible to compare the analytical results from the standard method with those from the real-space renormalization group. We can compare, for example, the exact value of the ground-state energy, $\varepsilon_o^{\rm ex} = -(4/\pi)^2 t = -1.62t$ to that obtained by applying (26), $\varepsilon_o^{\rm rg} = -1.3t$ ($t_y < t_x$). That is, the $\varepsilon_o^{\rm rg}$ is about 80% of the exact one. Another interesting property is the dynamical exponent z defined by

$$t' = s^{-z}t,$$

which tells us how the energy is rescaled depending on the length scaling. In Table I we show the renormalization factors t'/t for two fillings and different hopping anisotropies. From these values we obtain a dynamical exponent that varies at the half filling from $z = 0.89$ in the isotropic case ($\alpha = 1$) to $z = 0.63$ if $\alpha \neq 1$. These results have been obtained as the limiting case of $U \ll 1$ and they already show the odd behavior of the isotropic system at the half filling (see discussion about this anomaly in Sec. V).

When we study highly correlated systems it is also interesting to analyze the qualitative behavior of some quantities such as the double occupancy and the local moment. We need, therefore, to construct an algorithm to obtain these values in the renormalization-group method.

The double occupancy is defined as

$$D = \frac{1}{N}\left\langle \sum_i n_{i\downarrow} n_{i\uparrow} \right\rangle. \tag{27}$$

We use, in fact, a more general expression

$$C(r,s) = \frac{1}{N}\left\langle r\sum_i n_{i\downarrow} n_{i\uparrow} - s\sum_i n_i \right\rangle. \tag{28}$$

After the first iteration, for the 3×3 block, we obtain

$$C(r,s) = r\frac{d_1}{9} - s\frac{N_o - 1}{9} + \frac{1}{9}C'(r',s'),$$

where

$$\begin{aligned} r' &= r + 2r(d_1 - d_2), \\ s' &= s + r(d_1 - d_2), \end{aligned} \tag{29}$$

and

$$d_1 = \langle 0' | \sum_{i=1}^{9} n_{i\downarrow} n_{i\uparrow} | 0' \rangle, \tag{30}$$

$$d_2 = \langle \downarrow' | \sum_{i=1}^{9} n_{i\downarrow} n_{i\uparrow} | \downarrow' \rangle. \tag{31}$$

From (29) it is clear that if we choose $s = r/2$ then this ratio keeps for the following iterations: $s^{(n)} = r^{(n)}/2$. We obtain thus a closed expression for D,

$$D = C(1, \tfrac{1}{2}) + \tfrac{1}{2}(1 - \delta). \tag{32}$$

There are some points where the double occupancy is easy to evaluate, these are the fixed points in the (U,t) space so that

$$\frac{U^{(n+1)}}{t^{(n+1)}} = \frac{U^{(n)}}{t^{(n)}},$$

and then

$$d_1^{(n+1)} = d_1^{(n)}, \quad d_2^{(n+1)} = d_2^{(n)}. \tag{33}$$

In these cases C takes a simple form

$$C_{\rm (fixed)}\left(r, \frac{r}{2}\right) = \frac{r}{9}\left(d_1 - \frac{1}{2}(N_o - 1)\right)(1 + \nu + \nu^2 + \cdots),$$

where

$$\nu = [1 + 2(d_1 - d_2)]/g,$$

and the double occupancy has an analytical expression

$$D_{\rm (fixed)} = \frac{1}{2}\frac{d_2}{4 - d_1 + d_2}. \tag{34}$$

Two of the trivially fixed points are $U/t = 0$ and $U/t = \infty$, where we know that, in the half filling, $D(0) = \frac{1}{4}$ and $D(\infty) = 0$. The results using expression (34) are shown in Table II for $U = 0$ and two different values of the anisotropy ratio, $\alpha = t_y/t_x$ (the limit $U/t = \infty$ does not present any interest because $D = 0$ anyway). It should be noted that for the isotropic system, $\alpha = 1$, the method does not reproduce the expected value, but, when $\alpha \neq 1$ we recover the *a priori* normal result.

Another interesting quantity is the local moment

$$\langle \mathbf{s}_i^2 \rangle = \tfrac{3}{4}\langle {s_{iz}}^2 \rangle = \tfrac{3}{4}\left\langle n_{i\downarrow} + n_{i\uparrow} - 2n_{i\downarrow}n_{i\uparrow} \right\rangle. \tag{35}$$

It can be obtained from the double-occupancy expression

TABLE I. Renormalizing factor of the hopping parameter t'/t for different values of $\alpha = t_y/t$ and two filling cases $n = 1, 7/9$.

α	1	7/9
1	3/8	1/2
0.9	1/2	1/2
0.0001	1/2	1/2
0	1/2	1/2

TABLE II. Total amount of the double occupancy on the 3×3 block ground state in the $N_e = 8$ (d_1) and $N_e = 9$ (d_2) subspaces. We note the difference between the isotropic case, $\alpha = 1$, and the anisotropic one, $\alpha = 0.9$. We report as well the double occupancy per site in the macroscopic limit.

$U = 0$	$\alpha = 0.9$	$\alpha = 1$
d_1	1.812 46	1.671 55
d_2	2.187 46	1.984 34
D	0.2499	0.230

$$\frac{1}{N_s}\sum_i \langle {s_{iz}}^2\rangle = \tfrac{1}{4}n - \tfrac{1}{2}D, \tag{36}$$

and, also, we can construct an algorithm to calculate it with the aid of the renormalization method. In order to appreciate the border effects we shall focus our attention in the central site of the block. The same kind of arguments as in the preceding section leads to a recurrence relation for $\langle \mathbf{s}_i^2\rangle$ (Ref. 34)

$$\langle \mathbf{s}_i^2\rangle = a_1' + \tfrac{4}{3}(a_2' - a_1')\langle \mathbf{s}_i^2\rangle', \tag{37}$$

where the label i stands for the central site and

$$a_1' = \langle 0'|\mathbf{s}_i^2|0'\rangle, \quad a_2' = \langle \downarrow'|\mathbf{s}_i^2|\downarrow'\rangle. \tag{38}$$

IV. DIAGONALIZATION OF AN $L \times L$ BLOCK

We report here the numerical analysis of the Hubbard Hamiltonian in a 3×3 block with free boundary conditions. Some of the results will be valid, however, for an $L \times L$ cluster, where L is an odd integer. The diagonalizations have been carried out by the DSPSV subroutine of the ESSL library in a 3090 IBM computer.

The total number of configurations for such cluster is $4^{L\times L}$, that is 262144 if $L = 3$. However, if we make use of the symmetries of the Hamiltonian mentioned in Sec. II, we are able to reduce the largest dimension of the subspace we want to diagonalize. For example, if we take into account the charge N_e and the spin S_z symmetries the dimension of each of the subspaces so defined is reduced to

$$d(N_e, S_z) = \frac{N_s(N_s-1)\cdots(N_s-N_{e\uparrow}+1)}{N_{e\uparrow}!} \times \frac{N_s(N_s-1)\cdots(N_s-N_{e\downarrow}+1)}{N_{e\downarrow}!}, \tag{39}$$

where $N_{e\uparrow}(N_{e\downarrow})$ stands for the number of spin up (down) electrons. For the 3×3 block the largest matrix corresponding to $N_e = 8(9)$, $S_z = 0(\pm\frac{1}{2})$ subspace has $d(8,0) = d(9,\frac{1}{2}) = 15\,876$.

We could, in principle, use S^2 and Z^2 to reduce even more the largest dimension. Unfortunately, this is not technically useful, but we can add, nevertheless, the total spin and pseudospin in the Hamiltonian input, in order to obtain the eigenstates already classified as spin and pseudospin multiplets. Finally, we explicitly take into account the invariance of H under the elements of C_{2v} in constructing the basis of the Hilbert space. Thus each subspace is labeled by N_e, S_z, Σ, where Σ represents one of the four irreducible representations of C_{2v} (see Table III).

A. Classification in irreducible representations

The Hubbard Hamiltonian can be separated into two parts easy to diagonalize independently, the interaction H_u and the band term H_t. The former is diagonal in the Wannier representation, $c_{i\sigma}$, and the latter can be diagonalized by a basis change (the lattice parameter a is fixed equal to unity)

$$c_{r\sigma} = \frac{2}{L+1}\sum_{k_x,k_y} \sin k_x x \sin k_y y \; d_{k\sigma}, \tag{40}$$

where

$$k_{x(y)} = \frac{\pi}{L+1}p_{x(y)}, \qquad p_{x(y)} = 1, L,$$

and we get the expression

$$H_t = \sum_{k,\sigma} \varepsilon(k) d_{k\sigma}^\dagger d_{k\sigma},$$

where

$$\varepsilon(k) = -2(t_x \cos k_x + t_y \cos k_y). \tag{41}$$

We are able then to rewrite all the operators we need like H_u, $S^{\pm}$, $Z\pm$, N_e, etc., in terms of the $d_{k,\sigma}$, the extended states. It is worth noting that, unlike the standard Bloch functions in an infinite lattice,[51] the $d_{k,\sigma}$ have the full symmetry properties of the spatial group. It is then possible to classify these extended wave functions in irreducible representations depending on the values of $p_{x(y)}$ (see Table IV). Moreover, the representations of C_{2v} are one dimensional, it is then straightforward to construct the Slater determinants $|\phi_\alpha\rangle$ in the subspace defined by N_e, S_z, and Σ,

$$|\phi_\alpha\rangle = d_{k_m\sigma_m}^\dagger \cdots d_{k_1\sigma_1}^\dagger |0\rangle. \tag{42}$$

The three symmetries for $|\phi_\alpha\rangle$ are then directly obtained:

$$N_e = \sum_i^m n_{k_i\sigma_i},$$

$$S_z = \sum_i^m \sigma_i,$$

$$\Sigma = \prod_i^m (\Sigma_i).$$

TABLE III. Character table for the C_{2v} group (from Ref. 45).

C_{2v}	E	C_2	σ_v	$\sigma_{v'}$
A_1	1	1	1	1
B_2	1	−1	−1	1
A_2	1	1	−1	−1
B_1	1	−1	1	−1

TABLE IV. Relationship between the p numbers labeling the extended states (40) and its spatial symmetry.

Representation	p_x	p_y
A_1	Odd	Odd
B_2	Even	Odd
B_1	Odd	Even
A_2	Even	Even

TABLE V. Dimensions of the subspaces belonging to the Hilbert space of the Hubbard Hamiltonian in a 3 × 3 block; for (a) the A_1 and (b) the A_2 representations.

A_1 S_z	0	1/2	1	3/2	2	5/2	3	7/2	4	9/2
N_e										
1	0	4	0	0	0	0	0	0	0	0
2	25	0	8	0	0	0	0	0	0	0
3	0	80	0	16	0	0	0	0	0	0
4	328	0	176	0	30	0	0	0	0	0
5	0	760	0	276	0	36	0	0	0	0
6	1800	0	1128	0	294	0	24	0	0	0
7	0	2664	0	1128	0	200	0	8	0	0
8	3996	0	2616	0	760	0	80	0	1	0
9	0	3960	0	1736	0	328	0	16	0	0

A_2 S_z	0	1/2	1	3/2	2	5/2	3	7/2	4	9/2
N_e										
1	0	1	0	0	0	0	0	0	0	0
2	16	0	8	0	0	0	0	0	0	0
3	0	80	0	24	0	0	0	0	0	0
4	328	0	200	0	36	0	0	0	0	0
5	0	760	0	294	0	30	0	0	0	0
6	1736	0	1128	0	276	0	16	0	0	0
7	0	2616	0	1128	0	176	0	8	0	0
8	3960	0	2664	0	760	0	80	0	4	0
9	0	3996	0	1800	0	328	0	25	0	1

If we take into account these symmetries we can compute the dimension of every subspace for the 3 × 3 block. We show the results for the A_1 and A_2 representations in Table V. The dimensions of the B representations can be calculated from (39), bearing in mind that the B_1 and B_2 subspaces are of equal size.

The extended basis $d_{k\sigma}$ is advantageous because it allows us to separate easily the (N_e, S_z) subspaces in C_{2v} representations. On the other hand, the manipulation of the two-particle operators in this basis is more cumbersome than if we had used the Wannier states $c_{i\sigma}$.

B. Results for the 3 × 3 block

In the analysis of the ground-state properties we first pay our attention to the total symmetries (observables) like total spin and pseudospin. The latter is obtained from $\langle Z^+ Z^- \rangle$ where $\langle\,\rangle$ represents the mean value in the ground state. The results show, as expected, a zero value for all possible subspaces. This seems reasonable as long as we analyze the $N_e \leq N_s$ region.[41]

The total spin presents a more diversified behavior as it can be concluded from the inspection of Table VI. One of the most interesting questions concerning the spin is to know if the Nagaoka theorem[52] is fulfilled in a finite block with free-boundary conditions. The Nagaoka theorem states that for one hole and $U/t = \infty$ the ferromagnetic state is the ground state of the system. We find that the "critical" U/t is near 70, Fig. 1, which agrees with the result of Callaway *et al.*[28] $(U/t)_c = 68$.

We have also computed the double occupancy per site D and the local moment on the central site. The results are shown in Fig. 2 for the double occupancy and in Fig. 3 for the local moment. We present the calculations for two values of the hopping anisotropy $\alpha = t_y/t_x = 1$ and 0.9. The behavior for small U/t values depends on whether the band term is isotropic or not. In the former case the existence of an accidental degeneracy on the Slater determinants (see Table VII) produces a "gap" in the degenerate subspace when the interaction, H_u, is switched on. The lowest state corresponds to a minimization of the double occupancy. This explains the differences between the isotropic and anisotropic cases for small values of U/t.

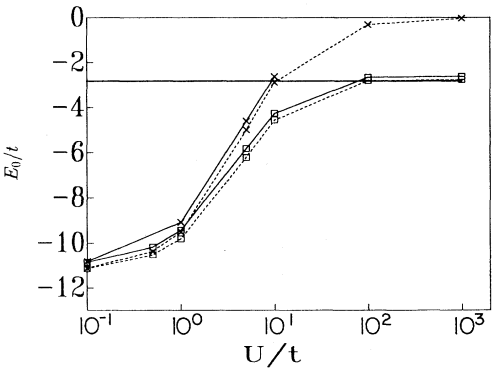

FIG. 1. Ground-state energy for the 3 × 3 cluster computed for $N_e = 8$ (open squares) and $N_e = 9$ (crosses) and for two values of the anisotropy hopping, $\alpha = 1$ (dashed line) and $\alpha = 0.9$ (solid line). The spatial symmetries correspond to A_1 at $N_e = 8$ and A_2 at $N_e = 9$. The horizontal solid line corresponds to the energy of the Nagaoka state at $\alpha = 1$ (A_2 symmetry).

TABLE VI. Ground-state total spin on the 3×3 block for different fillings. They are computed in the symmetric subspace (A_1 representation) except in the $N_e = 9$ case (A_2). In parentheses are shown the values corresponding to the Nagaoka state (A_2 symmetry).

U/t	N_e	2	3	4	5	6	7	8	9
1		0	1/2	0	3/2	0	1/2	0	1/2
10		0	1/2	0	3/2	0	1/2	0	1/2
100		0	1/2	0	3/2	0	3/2	3(4)	1/2
1000		0	1/2	0	3/2	0	3/2	3(4)	1/2

The local moment in the central site presents the same "anomalous" behavior in the $U = 0$ limit: the isotropy enhances the local moment for small U/t values (Fig. 3). In order to get a more pictorial view of the one-hole ground state we plot as well the local moment at the central site from the expression (36).

V. RESULTS AND DISCUSSION

We are interested in the macroscopic properties of the Hubbard Hamiltonian. In the frame of the real-space renormalization the thermodynamic limit would correspond in principle to nearly 16 iterations, so that each site of the renormalized lattice represents close to 7.13×10^{15} original sites (equivalent to Avogadro's number in two dimensions). One can, however, wonder about the necessity to reach this number of iterations to get reliable results. In addition, we have not yet defined (numerically) the concept of fixed point which is crucial to interpret the results. To clarify these two questions we report in Tables VIII and IX the results for $U/t = 0.5$, $\alpha = 1, 0.9$ and different numbers of iterations ($n_{\rm it}$). From the analysis of the data we can conclude the following.

(i) The amount of the quantities per site like energy, double occupancy (extensive ones) does not depend on the iteration number if $n_{\rm it} > 4$.

(ii) On the other hand, the quantities such as the gap are more sensitive to the $U/t(n_{\rm it})$ value and, then, to the number of iterations $n_{\rm it}$ and to the lattice size represented. Therefore, to assure that we have reached a fixed point $U/t(n_{\rm it})$ must be either *zero* or *infinity*. We have chosen our *zero* in determining the number of iterations needed to get $t^{(n_{\rm it})} \sim 10^{-14}$ for $U = 0$. This corresponds to 40 iterations approximately. The *infinity* has been arbitrarily chosen as $U/t = 1000$ because of technical reasons: the CPU time allowed was finite, so we have restricted the diagonalizations to the values of U/t up to 1000.

If we would carry out strictly the renormalization procedure for each group of values (U, t, α) we should diagonalize the Hamiltonian and then, from (18) and (22), we would obtain the input values U', t' of the renormalized Hamiltonian [α does not change in the renormalization process as it is indicated in (22)] and so on. This is, in practice, inoperative because of the size of the matrix and the huge number of iterations we need to realize. We make use then of the fact that U' and t' as functions of U/t are smooth and monotonous (as well as all other properties of a finite system[53]). We can therefore exactly compute these *functions* at some points and use afterward an interpolation algorithm to obtain other values. We restrict the U/t interval to [0, 1000]. Furthermore, to avoid the errors due to the interpolation algorithm

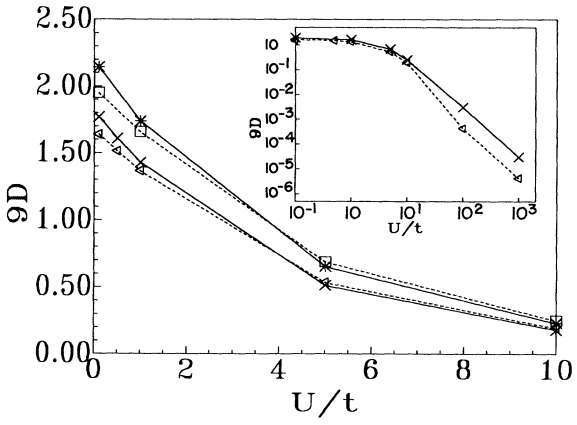

FIG. 2. The double occupancy for $N_e = 9$ (open squares) and $N_e = 8$ (open triangles) both at $\alpha = 1$ and at $\alpha = 0.9$ for $N_e = 9$ (stars) and $N_e = 8$ (crosses). In the inset are shown the $N_e = 8$ and $N_e = 9$ cases at $\alpha = 1$ for a wider range of U/t.

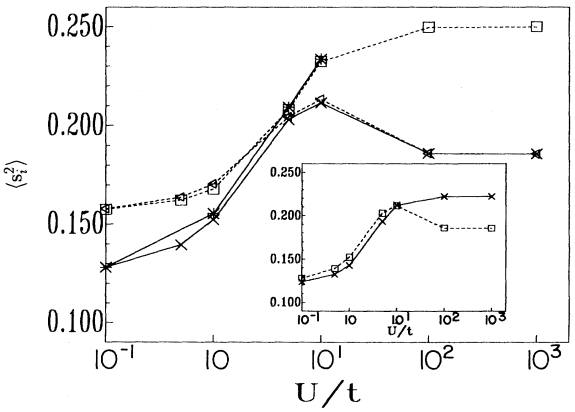

FIG. 3. The local moment measured on the central site [Eq. (35)] in (a) for two different fillings and hopping anisotropies (where the markers have been chosen with the same criteria as that in Fig. 2) and (b) for $N_e = 8$, where we compare the average local moment obtained from Eq. (36) (crosses) to the one on the central site (open squares) both in the isotropic case.

TABLE VII. Degeneracy of the Slater determinants (42) for different fillings. The ν's correspond to the integer numbers we use to write the total energy of a generic determinant: $E(\alpha, N_e) = \sqrt{2}t(\nu_x + \nu_y)$. The odd (even) particle number states belong to the A_2 (A_1) representation and to the $S_z = -1/2$ (0) subspace.

(ν_x, ν_y)	9	8	7	6
$(-6,-2)$	1	1	0	0
$(-4,-4)$	3	3	1	1
$(-2,-6)$	1	1	0	0

the first iteration is done at the points where we have performed the diagonalization.

A. Half-filled system

One of the first tests of a method, not necessarily conclusive, consist in obtaining the ground-state energy per site. In Fig. 4 we present the result obtained with the renormalization-group method for the isotropic system ($\alpha = 1$) to be compared with the lower bound[54] and the trivial upper bound (Hartree-Fock). The renormalization-group energy lies for moderate values of U/t above the limiting interval. This feature is probably due to the neglected terms when we obtained the effective Hamiltonian (13). These terms could enhance the kinetic part and so lower the total energy of the system.

The insulating nature of the ground state in the two-dimensional Hubbard model has not yet been completly understood. There is the general belief that an insulating gap is open for all positives values of U/t. This gap would be induced by the presence of spin-density waves and be roughly proportional to the staggered magnetization.[24,7,25] Another kind of approach consists in obtaining the moment distribution $n(k)$ and analyzing its behavior around the Fermi moment k_F.[50] The continuity of $n(k)$ at this point would imply the existence of no Fermi surface. Unfortunately all these methods have been applied to the isotropic hopping system ($t_x = t_y$), where, as it is well known, the Fermi level coincides (at $U = 0$) with a van Hove singularity. One can wonder if the existence of an antiferromagnetic order still holds if $t_x \neq t_y$ and then if a Mott-Hubbard transition occurs for

TABLE VIII. Renormalization results at $U/t = 0.5$, $\alpha = 1$, and different numbers of iterations. The fixed point in this case is $U/t = \infty$.

n_{it}	$-\varepsilon_0/t$	Δ	D	$(U/t)(n_{it})$
2	1.21069	7×10^{-2}	0.16270	0.548
4	1.21238	1×10^{-2}	0.16269	0.610
10		4×10^{-5}		0.936
15		4×10^{-7}		1.819
20		11×10^{-9}		27.45
22		9×10^{-9}		114495

TABLE IX. The same analysis as in Table VIII in the anisotropic case, $\alpha = 0.9$. The fixed point here is $U/t = 0$.

n_{it}	$-\varepsilon_0/t$	Δ	D	$(U/t)(n_{it})$
2	1.18780	4×10^{-2}	0.13954	0.189
4	1.19075	3×10^{-3}	0.13955	0.054
10	1.19076	7×10^{-7}		0.00087
15		7×10^{-10}		0.00003
40		0		0

a finite U/t in this case.

We have obtained the insulating gap from expression (24) and for two values of α. The results are shown in Fig. 5. It should be noted that for the isotropic case, $\alpha = 1$, the gap opens for all positive U and is exponentially small if $U/t < 1$, in agreement with the results mentioned above. Otherwise, if $t_y = 0.9t_x$ the ground state is found conducting up to $(U/t)_c = 1.8$. The system behaves like an insulator in both cases when U/t is large, where we know that the Hubbard model is equivalent to the Heisenberg model (see Ref. 55, for example) and then there would be no electron motion. Even if we have not computed the gap numerically for the whole anisotropy interval $\alpha \epsilon [0,1]$, we can still guess a qualitative phase diagram in the half-filling case (Fig. 6), where we plot the critical $(U/t)_c$ as a function of α. In fact, we know only three points: $\alpha = 0, 0.9, 1$, but perturbative calculations show that $(U/t)_c$ is, although small, nonzero for all $\alpha \neq 0, 1$ (see Table X). It should be noted here that the results at $U = 0$ are taken as the limit $U/t \to 0$. That is to say, we first obtain the $U \ll t$ result, and we assume the same structure for the ground state at $U = 0$. This procedure avoids the ambiguity in defining the ground state in the degenerate case. In fact,

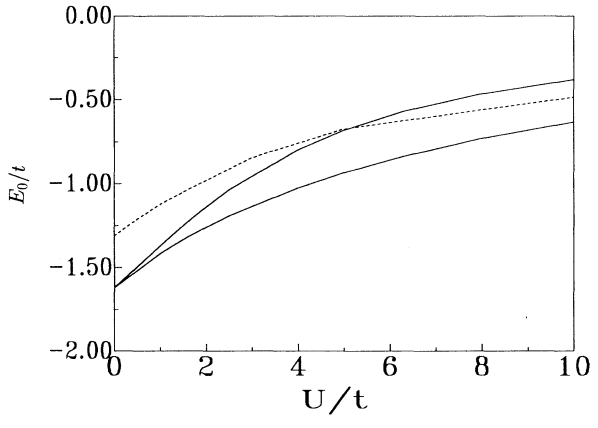

FIG. 4. The ground-state energy per site: renormalization-group result Eq. (25) (broken line) and upper (Hartree-Fock) and lower bound results from Ref. 54 (solid lines). For the values in the interval $U/t\epsilon(5,10)$ only three iterations are possible because off the cutoff $U/t = 1000$ discussed in the text. The actual value of the renormalization-group energy should be therefore even slightly smaller than the one presented here.

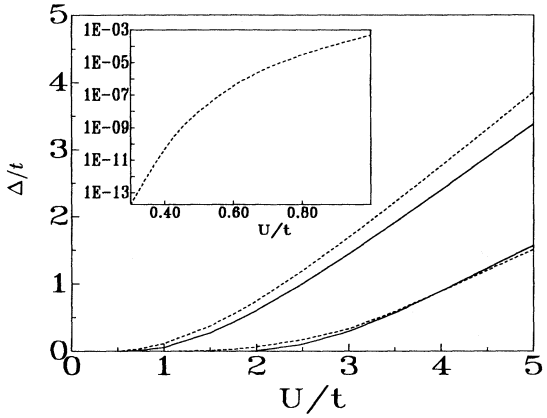

FIG. 5. Variation of the insulating gap with U/t for two values of the hopping, $\alpha = 0.9$ (solid line) and $\alpha = 1$ (broken line). The upper pair of lines correspond to the mean-field results (see, for example, Refs. 54 and 24). The two lower lines represent the renormalization gap (RG). The results for the RG isotropic case for the small values of U/t are shown in the inset.

this ambiguity could be the signature of a nonanalytical behavior of the thermodynamic limit at $U = 0$, similar to the one of the one-dimensional case.[12] Recently Zlatić and Horvatić have pointed out that this nonanalyticity could occur in two dimensions as well in the $n = 1$, $U = 0$ case.[56] To get a more detailed description of the ground state we have determined the double occupancy, the local moment, and the effective hopping.

In Fig. 7 we have plotted the double occupancy obtained by expression (32) for two anisotropy values $\alpha = 0.9, 1$ and compare it with an interpolation formula given by Baereswyl and von der Linden,[50]

$$D = \frac{1 + c_1 U}{4(1 + c_2 U + c_3 U^2 + c_4 U^3)}, \tag{43}$$

with

$$c_1 = 0.491,\ c_2 = 0.594,\ c_3 = 0.216,\ c_4 = 0.026.$$

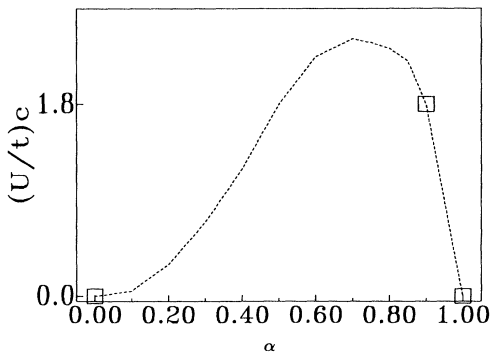

FIG. 6. Phase diagram for the Hubbard model at half filling depending on the anisotropy parameter $\alpha = t_y/t_x$. In fact only three critical values of the interaction strength have been computed, for $\alpha = 0$, 0.9, and 1 (open squares).

TABLE X. Renormalizing factor of the $(U/t)'/(U/t)$ ratio in the $U \ll t$ limit and for three different electronic densities. At half filling there are two marginal cases $\alpha = 1, 0$, which corresponds to an insulating ground state.

α	1	7/9	5/9
1	1	3/4	0
0.9	1/2	3/4	0
0.0001	1/2	3/4	0
0	1	3/4	0

It should be noted that the renormalization-group results agree with (43) if $\alpha \neq 1$. Otherwise, in the isotropic case the degeneracy reduces the double-occupancy amount contrary to the one-dimensional system, where there is no discontinuity in the exact value.[50] We show in Fig. 8 the results for the local moment obtained from (36) and (38). It presents the same behavior as the double occupancy: it is "normal" if $\alpha \neq 1$ and "anomalous" if $\alpha = 1$ as well on the central site as the averaged value.

Another interesting property is the so-called effective hopping defined as[26]

$$\frac{t_{\text{eff}}}{t} = \frac{\langle c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \rangle_U}{\langle c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \rangle_0},$$

which is in turn proportional to the plasmon frequency ω_p.[57] In the frame of the renormalization group this effective hopping becomes

$$\frac{t_{\text{eff}}}{t} = \frac{\varepsilon_o(U/t) - UD}{\varepsilon_o(0)}. \tag{44}$$

We show the results in Fig. 9. We find quantitative agreement with quantum Monte Carlo results.[58] For example, at $(U/t) = 4$ and $n = 1$ we have $D = 0.879$ (0.856) at $\alpha = 1$ (0.9). On the other hand, $D = 0.924$ if $n = \frac{7}{9}$.

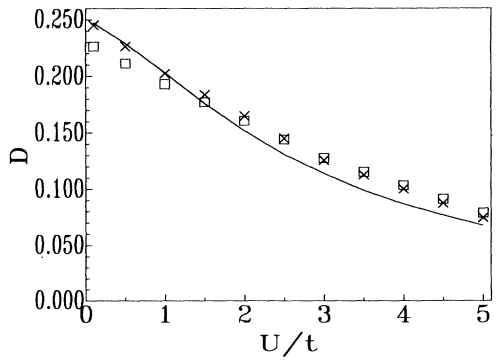

FIG. 7. Double occupancy at the half filling for $\alpha = 1$ (open squares) and $\alpha = 0.9$ (crosses) obtained from the expression (32) in the macroscopic limit. The solid line shows the values obtained by the interpolation expression (43) (Ref. 50).

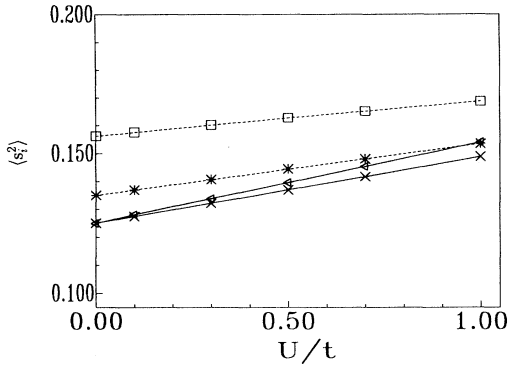

FIG. 8. The local moment in the thermodynamic limit obtained from the recursion expression (37) taken at the central site for $\alpha = 1$ (open squares) and $\alpha = 0.9$ (open triangles) and the local moment computed from Eq. (36) (solid stars and crosses, respectively).

B. Non-half-filled band, $n = \frac{7}{9}$

Away from half filling the expected behavior of the Hubbard Hamiltonian is richer, in particular concerning the magnetic configurations and at least in the mean-field approach.[23] Unfortunately, there are no exact results about the nature of the ground state like the two Lieb theorems[42] except in the limiting case considered in the Nagaoka theorem.[52] We cannot therefore impose a minimum spin in diagonalizing the 3×3 block as in the half-filled case. On the other hand, if we want to apply the same doublet scheme we cannot choose the states with an even number of electrons as a spin doublet: the electronic density should then be $\frac{1}{9}$, $\frac{3}{9}$, $\frac{5}{9}$, or $\frac{7}{9}$. Furthermore, the results when $U \to 0$ have to be consistent with a free-electron system. All these conditions and results reported in Table X allow us to state that the real-space renormalization method, restricted to the choice of four states in each iteration, remains valid only in the $n = \frac{7}{9}$ case. For example, if $n = \frac{5}{9}$ the $|\downarrow'\rangle$ and $|0'\rangle$ states has to be chosen so that $s = \frac{3}{2}$ and $s = 0$, respectively. The renormalized hopping would then be zero; that is to say, the method would predict an insulating ground state for a free-electron system.

The reasons for this behavior have to be sought in an implicit hypothesis on the first approximation: when we had chosen only four states, we implicitly assumed no charge fluctuations. This circumstance is surely correct near the half filling but, far away from this limit it is too naive to represent a block by just four configurations and an effective repulsion. Instead, it would be more natural to imagine the existence of the different exchange terms produced by keeping more than four states. This is however, an ambitious program and for now we will show and interpret the results obtained at $n = \frac{7}{9}$ by the "standard" procedure explained in Sec. II. It should be noted, however, that $|\downarrow\uparrow'\rangle$ does not correspond to the true ground state in the $N_e = 8$ subspace. The actual ground state will have an energy of, say, E_3 smaller than $E_2 + U$ for the state defined in (15);[41] but our choice permits us to avoid, again, the proliferation of couplings in the band term. These couplings are, in addition, energetically unfavorable. We must therefore no longer interpret $U^{(\infty)}$ like a gap but just like a fixed point in the parameter space.

We report in Fig. 10 the results for the ground state energy per site at $n = \frac{7}{9}$, 1 together with the lower bounds found by Valenty, Stolze, and Hirschfield,[59] and the exact result at $U = 0$. In Fig. 9 we show the effective hopping at $n = \frac{7}{9}$, $\alpha = 1$ to be compared to the half-filled case. It should be noted that qualitatively different behavior results depending on whether there is a finite density of holes or not. We expect a zero t_{eff} in the half-filled case at $U/t = \infty$ and a finite value if $n \neq 1$ in the same limit. We can observe this tendency for the results obtained with the renormalization-group method.

We have also estimated the total spin of the system. We have first to reinterpret the renormalization flow of the U/t parameter. Here the $U = 0$ fixed point refers to a paramagnetic state and the $U/t = \infty$ limit corresponds to a weakly ferromagnetic state. For example, if we begin the process already at the infinity limit ($U > 1000t$),

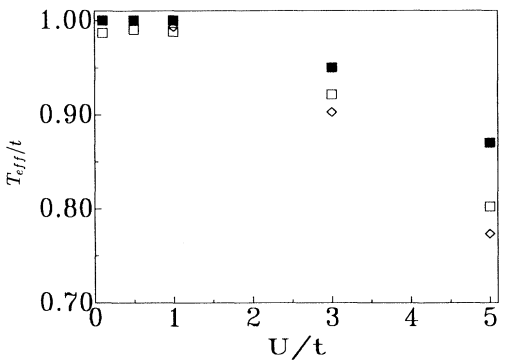

FIG. 9. The effective hopping defined by Eq. (44) at the half filling in the isotropic case (squares) and at $\alpha = 0.9$ (diamonds). The triangles represent the case $n = 7/9$, $\alpha = 1$.

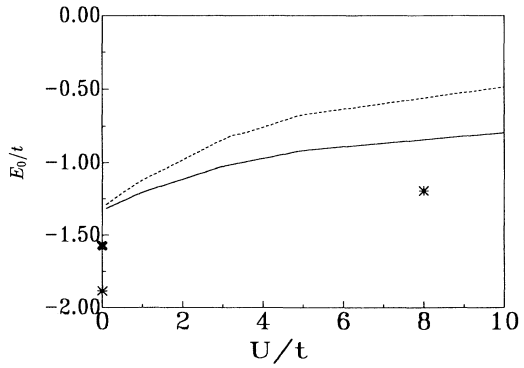

FIG. 10. The ground-state energy per site for $n = 7/9$ (solid line) and $n = 1$ (dashed line) from (25) compared to the exact value at $U = 0$ (the cross) and to the lower bound from Ref. 59 (stars).

the spin per site will be $(\frac{3}{2})(\frac{1}{9}) = \frac{3}{18}$. On the other hand, the $U = 0$ case has zero spin per site value. The intermediate values are separated in two zones by a critical point $(U/t)_c \sim 2$. We have carried out the renormalization procedure as if the ground state were paramagnetic. Additional work is needed to take into account the spin symmetry-breaking explicitly produced by the spin-dependent hopping (21). The lower bound of the total spin is then estimated as the ratio $s^{(n_{it})}/9^{n_{it}}$, where $s^{(n_{it})}$ is the spin of block at $(U/t)(n_{it})$ and $9^{n_{it}}$ represents the size of the lattice at the n_{it} iteration. This estimate is computed from an expression for the total spin per site, which is obtained by the same kind of arguments as those we used to get the total energy and the double occupancy per site: $\langle S_z\rangle/N = \sum_{i=1}^{n} s_o^{(i)}/9^i + \langle S_z^{(n)}/9^n\rangle$.

VI. CONCLUSIONS

Macroscopic description of the ground state is, in general, difficult to infer from microscopical model Hamiltonians by means of analytical or numerical techniques. The real-space renormalization-group analysis of the two-dimensional Hubbard model that we have presented here is an attempt to fill this lacking. We have first improved the understanding of the method itself: we keep the fermionic character of the second quantization operators and, at the same time, we are able to avoid the proliferation of couplings, which is highly desirable in order to keep the computing work up to reasonable limits. Besides, we have outlined the way in which, away from half filling, the spin symmetry can be "naturally" broken in the frame of the renormalization group.

In what concerns the description of the ground state we have studied two electronic density cases: $n = 1$ and $7/9$. At half filling $(n = 1)$ we have analyzed the dependence on the hopping anisotropy $\alpha = t_y/t_x$. We find that the isotropic system $\alpha = 1$ behaves like an insulator for all positives values of the interaction parameter U. On the other hand, if $\alpha < 1$ the ground state becomes a conductor up to a critical value of the ratio $(U/t)_c$. In particular, at $\alpha = 0.9$ we find $(U/t)_c = 1.8$. The one-dimensional insulating behavior is recovered at $\alpha = 0$. One should note the remarkable behavior of the system in the α interval. One could naively think that the half-filled system is insulating in the entire α interval because of the two insulating limits. However, the physical picture is different in the one-dimensional case $(\alpha = 0)$ compared to the isotropic two-dimensional system $(\alpha = 1)$. The former presents a Mott-Hubbard transition at $U = 0$, which can be considered as a one-dimensional feature without spin-broken symmetries. The latter, on the other hand, has a degeneracy at $U = 0$ which induces, even in finite clusters, a different behavior for $U/t \to 0$ and $U/t = 0$ cases. The standard treatment of this degeneracy is done by an explicit spin-broken symmetry (Hartree-Fock), which can be related, in the frame of the one-particle view, with the insulating gap. For the rest of the α values, where no results are known, the system shows a genuine Mott-Hubbard transition, where a broken symmetry is not necessarily implied.

Away from half filling the situation is less clear. We have to interpret in a slightly different manner the two trivial fixed points. At $U/t = 0$ the system represents a conducting paramagnet and if $U/t = \infty$ we still assume the conducting behavior but in a weak ferromagnetic background. The transition between the two regimes is estimated at $(U/t)_{c2} \sim 2$ and the intermediate values have to be viewed as a paramagnet with renormalized parameters if $U < 2t$ or as a weak ferromagnet if $U > 2t$. More work is needed in this region of the density of electrons in order to improve the renormalization procedure. This improvement must be done in two ways. Firstly, the spin-broken symmetry has to be taken into account when the small cluster is diagonalized. Secondly, one should consider the possibility of keeping more than four states in each iteration in order to describe correctly the low-density limits, where a block cannot be assimilated to an s-like atomic orbital.

ACKNOWLEDGMENTS

We wish to thank A.K. Bhattacharjee and R. Jullien for stimulating discussions during the realization of this work. One of us (J.P.C.) was partially supported by Ministerio de Educación y Ciencia (Spain). We acknowledge the CNRS for supporting numerical calculations.

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