Small-cluster calculations for the simple and extended Hubbard models

J. Callaway, D. P. Chen, D. G. Kanhere,* and Qiming Li
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001
(Received 6 November 1989; revised manuscript received 12 March 1990)

The single-band Hubbard model (both with and without first-neighbor interactions) is studied by exact diagonalization on several one- and two-dimensional clusters, ranging from four to nine sites, including rings and arrangements of squares. Occupancies include the half-filled band (one electron per site) and configurations with one and two holes in the half-filled band. Ground-state properties are determined for a wide range of parameters. We discuss the phase diagram in the (U,V) plane and consider spin, charge, and pairing correlations. The binding of a pair of holes is investigated. Circumstances in which binding and pairing are enhanced by first-neighbor interactions are described.

I. INTRODUCTION

In this paper, we report the results of investigations of the "one-band" Hubbard model defined by the Hamiltonian

$$H = t\sum_{ij\sigma} c_{i\sigma}^{\dagger}c_{j\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{\langle ij\rangle} n_i n_j \ . \tag{1}$$

We use a basis of localized states with one orbital per site. The operator $c_{j\sigma}$ ($c_{j\sigma}^{\dagger}$) destroys (creates) an electron of spin σ on site j. The quantity t is the transfer integral. The sum connects nearest-neighbor sites. The second term represents the Coulomb repulsion between electrons on the same site. The first two terms give the (ordinary) Hubbard model; inclusion of the third term, which describes the Coulomb interaction between electrons on nearest-neighbor sites, produces the extended model.

This Hamiltonian has been of interest in the development of one-dimensional (1D) models of organic semiconductors.[1-3] (It would be beyond the scope of this paper to review this specific application here.) Our studies concern the properties of the ground state of H, which we find by exact diagonalization, considering small clusters of various geometries for wide ranges of parameters and of electron occupancies.

Important general features of the phase diagram for 1D extended Hubbard model when there is one electron per site (half-filled band) are generally accepted:[2-7] (1) In the range $U,V>0; 0<V<U/2$ antiferromagnetic correlations are important, and the ground state is often described as a spin-density wave (SDW). However, (2), for $V>U/2$, charge correlations dominate and the ground state is described as a charge-density wave (CDW). Strong charge correlations characterize the system even when U is negative as long as V is positive. There has been some controversy concerning details of the transition between SDW and CDW regimes: Is it first or second order and does it occur exactly on the line $U=2V$, or can there be some displacement? It is also generally agreed (3) that in the third quadrant of the (U,V) plane in which $U<0$ and $V<0$, pairing correlations (superconductivity) are important close to the negative U axis; whereas for large negative V, a condensed state will be formed in which the particles are clustered together in some region of physical space. A simple argument can be given to determine the boundaries of this region. (4) In the fourth quadrant ($U>0$, $V<0$) SDW correlations dominate as long as $|V|$ is not too large, but for sufficiently negative V, one encounters the condensed state.

The discovery of high-temperature superconductivity in cuprates has attracted much attention to the Hubbard model in general, with special emphasis on the 2D square lattice. Topics of major interest include the existence of long-range antiferromagnetic order in the ground state of the half-filled band, and the effect of holes on magnetic correlations. Of course, one would particularly like to know whether the ground state can be superconducting. We cannot attempt to review or even simply reference the formidable literature that has developed on this topic (but see White *et al.*[8] for recent "state of the art" numerical results). Rather less attention has been devoted to the extended model in two dimensions, although there were early suggestions that some high-T_c materials might be close to CDW instabilities.[9-11] We note results of a quantum Monte Carlo calculation[12] which gives results for the square lattice in the half-filled band case which are quite similar to those obtained previously for the 1D case except that the transition between SDW and CDW states occurs close to the line $U=4V$ rather than $U=2V$.

Although the early proposals that a soft phonon mode associated with a near CDW instability might be responsible for high-T_c superconductivity have found little support, it remains interesting to examine the effects of the interaction between charges on neighboring sites on a system in which there are some holes in a half-filled band. This interaction does play a significant role in some theories of superconductivity.[13-15]

The exact diagonalization calculations we describe in this paper involve systems of four, six, eight, and nine sites, as illustrated in Fig. 1. The study of systems with different numbers and geometrical arrangements of sites

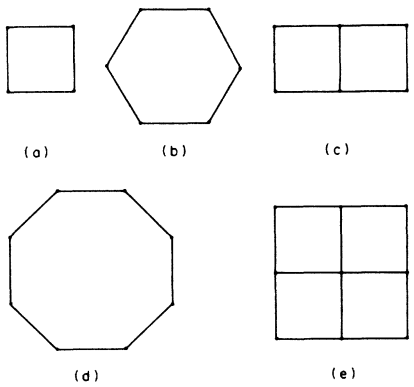

FIG. 1. Clusters considered in this paper: (a) square, (b) hexagon, (c) two squares, (d) octagon, (e) four squares.

helps one to understand which results are characteristic of the model in general and which are sensitive to structure. We thought it would be interesting to see whether typical differences between large one- and two-dimensional systems (for example, the existence of a saturated ferromagnetic ground state as $U \rightarrow \infty$ for one hole in an otherwise half-filled band) would be apparent in small clusters. However, the greatest emphasis is placed on results for the two- and four-square systems of Figs. 1(c) and 1(e) (occasionally referred to as 2×3 and 3×3). We consider electron occupancies corresponding to the half-filled band, and this with one or two holes.

The dimension of the Hamiltonian matrix increases very rapidly with the number of sites and the number of particles. For example, the number of states in the subspace with $S_z=0$ for 6 particles on 6 sites is 400; for 8 particles on 8 sites, 4900; for 9 on 9 sites, 15 876; for 16 on 16, 16 563 690, and so on. The growth in size of the Hamiltonian matrix limits the size of the cluster that can be investigated by exact diagonalization. Of course, one can employ improved algorithms (e.g., the Lanczos method), or use spatial and spin symmetries which reduce the size of the matrix whose eigenvalues have to be determined, but cluster size limitations are always a problem for calculations of this type. Considerably larger clusters can be studied if one forbids the double occupancy of any site. Then one must consider a different Hamiltonian—the so-called t-J model. We have not done this, as it appears that the t-J model gives results which represent the underlying Hubbard model accurately only for fairly large positive U (say $U > 10$).

Instead of considering the largest possible clusters, we have attempted instead to cover a large region of the U, V parameter space for those we considered. This requires a large number of calculations, so that the time required for a single one has to be limited. We think that the reader will find some of the results concerning pairing and spin coupling, for the case in which these are two holes in a half-filled band, to be both surprising and unusually interesting. And, as suggested above, we discuss the dependence of the results on the assumed geometry.

This paper is organized as follows: In the next section we describe our procedures and give definitions for the specific correlation functions that we calculate. Our results are presented in Sec. III. Section III A contains some discussion of the ordinary one-band Hubbard model (with $U > 0$). The extended model is described in Sec. III B. Our conclusions are summarized briefly in Sec. IV.

II. PROCEDURE

We consider the Hamiltonian of Eq. (1) on a basis of localized states, i.e., states which are eigenstates of the n_{is}. For convenience, one of the parameters of Eq. (1) can be set equal to 1 in magnitude. We take this to be t. This means that the parameters and energies of the Hamiltonian are in effect $U/|t|$, $V/|t|$, and $E/|t|$. In addition, the systems we consider in this paper are such that the energies are independent of the sign of t, and we may thus consider t to be positive. Interchanging electrons and holes ($c_{is} \leftrightarrows b_{is}^{\dagger}$) merely displaces the energies by a constant, which we ignore.

In this work, we will consider the ground-state properties of the system only and do not address questions concerning finite-temperature behavior. The clusters are treated as free: periodic boundary conditions are not imposed. (For some of the clusters considered we found that imposition of periodic boundary conditions produced severe distortions in the spectrum of single-particle states.) The properties of the system will be described on the basis of correlation functions and related structure factors. The correlation functions are spin

$$L_{ij} = \tfrac{1}{4}\langle G|(n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow})|G\rangle \tag{2}$$

and charge

$$D_{ij} = \langle G|n_i n_j|G\rangle \ , \tag{3}$$

in which $|G\rangle$ is the ground-state vector. We note that the D_{ij} satisfy the sum rule

$$\sum_{ij} D_{ij} = n_e^2 \ , \tag{4}$$

where n_e is the number of electrons in the system. We also consider pairing-correlation functions P_{ij},

$$P_{O,ij} = \langle G|O_i O_j^{\dagger}|G\rangle \ . \tag{5}$$

Hirsch[16] has defined a set of operators O:

local singlet

$$O_i = c_{i\uparrow}c_{i\downarrow} \ , \tag{6a}$$

extended singlet

$$O_i = \frac{1}{\sqrt{2}}(c_{i\uparrow}c_{i+x\downarrow} - c_{i\downarrow}c_{i+x\uparrow}) \ , \tag{6b}$$

triplet

$$O_i = c_{i\uparrow}c_{i+x\uparrow} \ , \tag{6c}$$

triplet antiparallel

$$O_i = \frac{1}{\sqrt{2}}(c_{i\uparrow}c_{i+x\downarrow} + c_{i\downarrow}c_{i+x\uparrow}) \ . \tag{6d}$$

Our calculations will emphasize local singlet pairing. It has to be observed that, in the presence of repulsive interactions, this is not necessarily the most significant. However, up to this point, our calculations have not shown convincing evidence for the importance of other pairings.

Some confusion can arise because the pairing-correlation functions defined above may not be zero in the case of a noninteracting electron system. A possible way to correct for this is to subtract a single-particle contribution defined as that obtained by factoring P_{ij}. Consider the corrected local singlet pairing function $P^C_{L,ij}$ defined by

$$P^c_L = \langle G|c_{i\uparrow}c_{i\downarrow}c^\dagger_{j\downarrow}c^\dagger_{j\uparrow}|G\rangle - \langle G|c_{i\uparrow}c^\dagger_{j\uparrow}|G\rangle\langle G|c_{i\downarrow}c^\dagger_{j\downarrow}|G\rangle \ . \tag{7}$$

Note that the local singlet pairing involves the transfer of an "up-down" electron pair between two sites. In the case $i=j$, involving the same site,

$$P^C_{L,ii} = \langle G|n_{i\uparrow}n_{i\downarrow}|G\rangle - \langle G|n_{i\uparrow}|G\rangle\langle G|n_{i\downarrow}|G\rangle \ . \tag{8}$$

This function clearly contains spin and charge fluctuation contributions. In the simple case in which a half-filled "band" (one electron per site) is considered and all the sites are identical, then

$$P^C_{L,ii} = \langle G|n_{i\uparrow}n_{i\downarrow}|G\rangle - \tfrac{1}{4} \ . \tag{9}$$

This measures the double-occupancy probability with respect to that in a uniform system. Hence, we expect

$$P^C_{L,ii} = -\tfrac{1}{4} \ ,$$

in the large-U limit of the Hubbard model and

$$P^C_{L,ii} = 0 \ ,$$

as $U \to 0$. If U is negative, the double occupancy increases and $P^C_{L,ij}$ becomes positive. However, the negative-U Hubbard model is known to be superconducting. Hence, we do not think it is desirable to exclude the one-site pairing term when the possibility of superconductivity is considered. However, if single-particle correction is not included, $P^C_{L,ij}$ will be positive and will increase as U decreases ($U>0$). If misinterpreted, an incorrect prediction of superconductivity for $U>0$ may be made.

As the number of sites increases, there are many different correlation functions to be considered, and it becomes convenient to introduce structure factors. In the case of spin, we have, on introducing a wave vector $\mathbf{q}$,

$$S_s(\mathbf{q}) = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}L_{ij} \ . \tag{10}$$

Similar structure factors are defined for density

$$S_c(\mathbf{q}) = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}D_{ij} \ , \tag{11}$$

and pairing. We consider the local singlet

$$S_L(\mathbf{q}) = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}P_{L,ij} \ , \tag{12}$$

and the single-particle corrected local singlet

$$S^c_L(\mathbf{q}) = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}P^C_{L,ij} \ . \tag{13}$$

If the geometry of the system is such that all sites are equivalent, the $1/N$ and one sum may be deleted. In a small system, only a limited set of wave vectors $\mathbf{q}$ have any significance. We consider only $\mathbf{q}=0$ for the pairing correlations but for spin and charge structure factors, we consider alternating cases; $\mathbf{q}=\pi$ in one dimension or $\mathbf{q}=(\pi,\pi)$ in two dimensions. Some authors emphasize the possibility of more complicated $\mathbf{q}$-dependent structure factors in superconductivity such as "d wave."[8]

If the nearest-neighbor interaction V is sufficiently negative, a condensed or droplet state will be formed. The particles occupy the smallest possible number of contiguous sites. In the case of a half-filled one-dimensional system in which all sites are identical by symmetry, Lin and Hirsch[6] proposed to use a structure factor

$$S(Q_m) = \frac{1}{N}\sum_{i=0}^{N-1}\exp(iQ_m\cdot\mathbf{R}_i)\sum_{j=1}^{N}(D_{i,i+j}-\langle n_i\rangle\langle n_{i+j}\rangle) \tag{14}$$

in which $Q_m = 2\pi/N$. We believe it may be simpler for the small systems of interest here which are not necessarily half-filled, to use the parameter

$$C = \sum_{j=-M}^{M}\left[D_{i,i+j} - \left[\frac{n_e}{N}\right]^2\right] , \tag{15a}$$

in which n_e is the number of particles ("electrons") in the system, N is the total number of sites, and

$$M = \frac{1}{2}\left[\frac{n_e}{2}-1\right] , \tag{15b}$$

if the quantity on the right is an integer, otherwise M is the next integer larger than that quantity. A positive value of C indicates condensation. In a system in which the sites are not geometrically equivalent, C should be redefined after determining the sites on which condensation occurs.

In the case of systems of less than eight sites, we used a program that actually computed all the eigenvalues and eigenvectors of H. For larger (eight- and nine-site) systems, we used a Lanczos algorithm program which makes proper allowance for the possibility of degeneracies (often realized).[17] In this case we obtained typically the lowest four eigenvalues and eigenvectors for the lowest two spin states.

III. RESULTS

A. Simple Hubbard model

We begin with some results for the simple Hubbard model [$V=0$, in Eq. (1)] for positive U. Although this model has been extensively studied through Monte Carlo calculations, the present results are interesting in that we consider different geometries, and there is no limitation

on the size of U/t.

In Fig. 2 we show, for the half-filled case, our results for the antiferromagnetic spin structure factor $S_s(\pi)$. The following points should be noted: (1) The structural factor increases with the size of the system; one expects that $S_s(\pi) \sim N$. (2) In the case of the two six-site systems shown, $S_s(\pi)$ is slightly larger for two squares than for the hexagon. (3) The structure factor increases with U in a qualitatively similar fashion for all systems; it is close to its large-U limit for $U/t = 20$. This value may be regarded, roughly, as defining the large-U limit.

The average double occupancy in the ground state, scaled by the square of the number of electrons in the system

$$d_2 = \frac{N}{n_e^2} \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle \ , \tag{16}$$

is shown in Fig. 3 for the half-filled band for three of the systems studied. It is obvious that the same general tendencies are exhibited by all systems. For U larger than about 10, the dependence is essentially t/U^2. In Fig. 4, d_2 is plotted as a function of the number of holes N_h for the four-square system. Notice that d_2 is almost independent of N_h up to $N_h = 4$. The one-hole systems behave quite similarly to the half-filled band, except that those which become ferromagnetic (have a high-spin ground state) at large U, have zero double occupancy for U larger than the critical value for ferromagnetism.

Most of the systems considered have a maximum spin ground state in the large-U limit when there is one hole in a half-filled band. We give in Table I the critical value of the U/t for the maximum spin state for several systems (some of these results are taken from our previous publications).[18,19] However, the ground state for five electrons in a hexagon is not ferromagnetic for any U/t.[20] These results are qualitatively consistent with Nagaoka's theorem,[21] which, however, explicitly applies only to infinite systems. In addition, Riera and Young[22] have found that the ground state is ferromagnetic with maximum spin for infinite U in $\sqrt{8}\times\sqrt{8}$, $\sqrt{10}\times\sqrt{10}$, and 4×4 square lattice clusters with one hole.

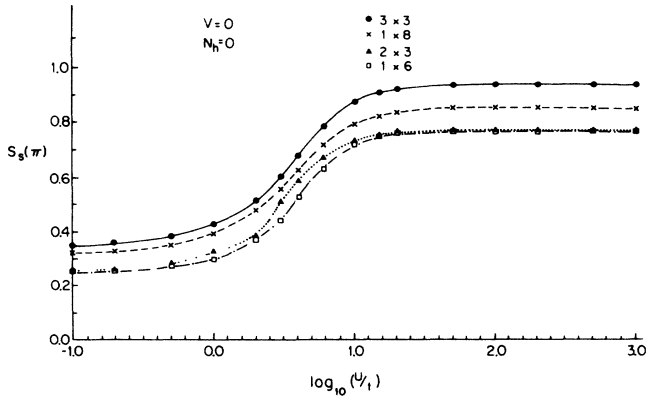

FIG. 2. Ground-state antiferromagnetic spin structure factor $S_s(\pi)$. Open squares, hexagon; solid triangles, two squares; crosses, octagon; solid circles, four squares.

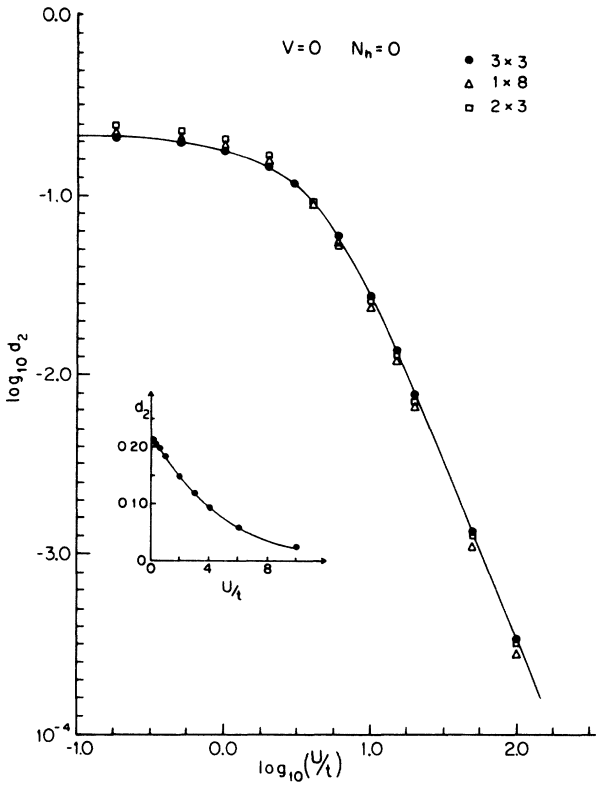

FIG. 3. The average double occupancy, scaled by the square of the number of electrons in the system, is shown for the half-filled band: squares, two square system; triangles, octagon; solid circles, four squares. The inset shows the same quantity (four squares only) on a linear scale.

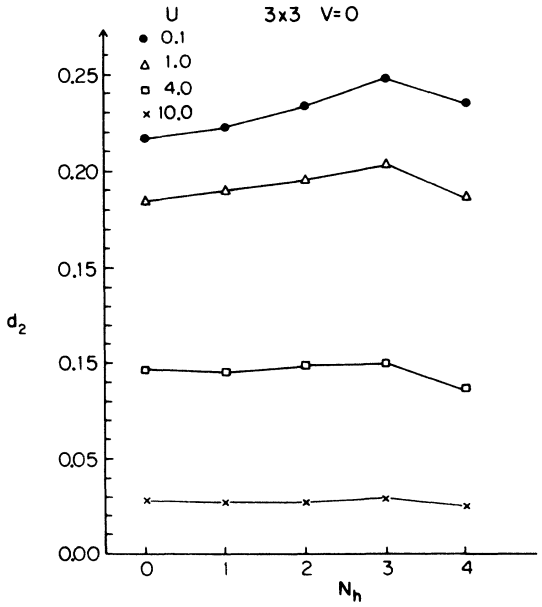

FIG. 4. The dependence of the scaled averaged double occupancy [Eq. (16)], on the number of holes for the four-square system for several values of U.

TABLE I. Critical value of U_c/t for a maximum spin ground state in the case of one hole in the half-filled band. Note that the maximum spin state is never the ground state for a hexagon or an octagon (but the latter has an intermediate spin, $S=\frac{3}{2}$, ground state for sufficiently large U).

	U_c/t
Square	13
Octahedron	11
Two squares	52
Cube	39.5
Four squares	68

A characteristic feature of the Hubbard model in all geometries is the formation of local moments when U/t is large. This occurs because, by aligning the spins on each site, the system avoids the large repulsive energy that would otherwise occur when electrons of opposite spin are on the same site. Thus, for $U/t > 10$ (roughly), the local moment, normalized by the number of electrons in the system (and averaged over sites if these are not all equivalent),

$$\bar{m} = 4\langle S_{iz}^2 \rangle N/n_e \tag{17}$$

is nearly independent of geometry and occupancy (n_e). The limiting value, 1, is approached smoothly. On the other hand, the coupling between moments on different sites depends strongly on geometry and occupancy, and has been the subject of much recent interest.

Figure 5 shows the dependence of the antiferromagnetic structure factor $S_s(\pi)$ for the four-square system of Fig. 1(e) on U/t and the number of holes in the system. The curve for zero holes is reproduced from Fig. 2 for comparison purposes. One observes the significant reduction in $S_s(\pi)$ when one or two holes are present in the system. This reduction is much larger than can be accounted for according to Eq. (17), and indicates the reduction of the coupling between sites, i.e., the reduction of magnetic order. The curves for one- and two-hole systems are terminated at the value of U/t at which the spin of the ground state increases beyond the lowest possible value. This occurs for the two-hole system (as well as for the one-hole case noted earlier). The two-hole ground state has $S=\frac{3}{2}$ for $37 < U/t < 85$ and $S=\frac{5}{2}$ for $U/t > 85$. However, Riera and Young[22] found a singlet ground state as $U \to \infty$ for the square clusters they considered including 4×4. Evidently the existence of a magnetic ground state at large U for two holes is sensitive to the precise size and geometry considered. It should also be noted that in the 3×3 geometry the single-hole system has a triplet ground state for small U ($0 < U/t < 2.8$).

Figure 6 shows first- and second-neighbor spin-correlation functions for a ring of eight sites (octagon) for the half-filled band and for two holes in a half-filled band. In the half-filled case at large U/t, the second-neighbor correlation function is in magnitude, 43% of the first-neighbor function and of opposite sign. In the case of two holes, the first-neighbor correlation function is, for large U/t, 52% of that for the half-filled band, but the second-neighbor function has only 23% of the magnitude of the half-filled band and is of opposite sign. Magnetic correlations are thus greatly reduced in strength beyond first neighbors and are not describable in terms of alternating ↑ and ↓ spins.

The geometric simplicity of the octagon makes possible a simple interpretation of the spin correlations in the one-hole case when U is fairly large but the ground state still has $S=\frac{1}{2}$. Each site has $\frac{7}{8}$ of a single electronic moment. This local moment is almost exactly compensated by negative spin correlation on the two nearest-neighboring sites, these functions being close to $(-\frac{1}{2})$ of the single-site moment.

We now turn to the question of the binding of two

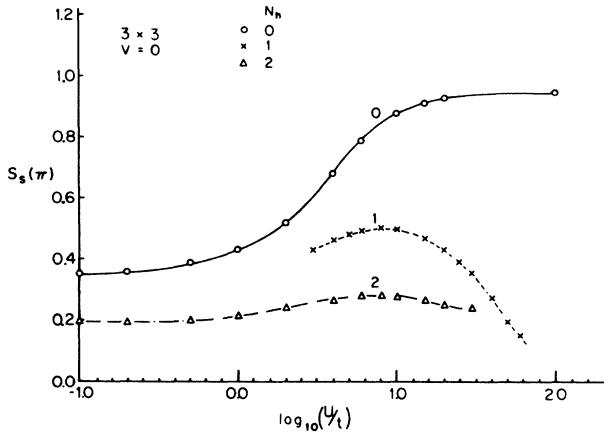

FIG. 5. Dependence of the antiferromagnetic structure factor $S_s(\pi)$ on U/t for the four-square system of Fig. 1(e). The curves are labeled by the number of holes in a half-filled band. The lower two curves are terminated at the value of U/t such that the ground state is not the low-spin state.

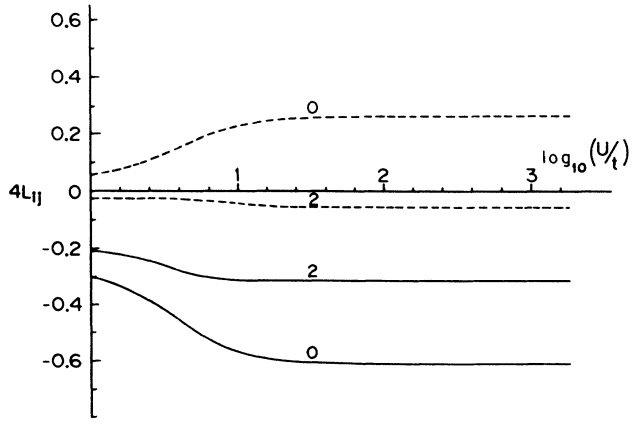

FIG. 6. Comparison of ($4\times$) first-neighbor (solid curves) and second-neighbor spin-correlation functions (dashed lines) for an octagonal cluster. Curves are labeled by the number of holes in the "half-filled band."

holes. This is described in terms of the quantity

$$E_B = E(0) - 2E(1) + E(2) , \tag{18a}$$

in which $E(0)$ is the ground-state energy of the half-filled band, $E(1)$ refers to one hole in the half-filled band, and $E(2)$ to two holes. A negative value of E_B is taken to indicate binding. This quantity has been investigated by Riera and Young for the simple one-band Hubbard model for an eight-site cluster.[23] They found binding for small to moderate U for this system. A recent preprint reports binding for two holes in a 4×4 lattice for $0 < U < 7$.[24]

Our results do not show binding for most, but not all, of the clusters we have considered. For example, binding is also not found for the two-square systems of Fig. 1(c), or for the four-square system [Fig. 1(e)], but weak binding is found for the octagon. Our results for the four-square system and the octagon are shown in Fig. 7. We have also considered quantities

$$E_{B3} = E(0) + E(3) - E(1) - E(2) \tag{18b}$$

and

$$E_{B4} = E(0) - 2E(2) + E(4) . \tag{18c}$$

The first would be negative if a three-hole cluster were to be stable against a two-hole cluster and a single hole; the second if two two-hole clusters would bind. In fact, these are strongly positive for the simple Hubbard model in the cases we considered, but some regions where they are negative occur for the extended Hubbard model. An example will be shown below.

The presence or absence of binding of a pair of holes is not a general characteristic of the Hubbard Hamiltonian: its presence or absence depends on the geometry of the physical system. It turns out that binding is strongly influenced by the presence of the first-neighbor interaction V in the Hamiltonian. We will discuss this below.

The single-band Hubbard Hamiltonian can also be considered for negative U. An on-site attraction replaces repulsion. Anderson[25] argued that such a description might be appropriate for some defects in semiconductors. In the case of negative U, the Hubbard Hamiltonian leads to pairing and to superconductivity.[26] This superconductivity is of the BCS type for $|U|$ small, and goes over to that resulting from the Bose condensation of pairs (which exist above T_c) when $|U|$ is large.[27] It has been argued that cuprate superconductors may be negative-U systems.[28]

Scarlettar *et al.* have discussed the phase diagram for the negative-U Hubbard model on a (2D) square lattice.[29] They find that the ground state at half-filling shows both superconducting and charge-density-wave order, and that away from half-filling there is a transition at a finite temperature into a superconducting state.

Our results show the coexistence of pairing and CDW correlations for negative U for all of the systems considered. An example of this is shown in Fig. 8 where we plot the single-particle local singlet pairing structure factor and the charge structure factor for four electrons in the two-square system of Fig. 1(c). We have subtracted from the charge structure factor the value for noninteracting electrons ($U=0$) in the same system so both curves pass through the origin. The results show the enhancement of both singlet and pairing correlations for negative U. We will return to the subjects of pairing and binding below in connection with our discussion of the extended model.

B. Extended Hubbard model

Because much of the work on the extended Hubbard model has been concerned with the half-filled band situa-

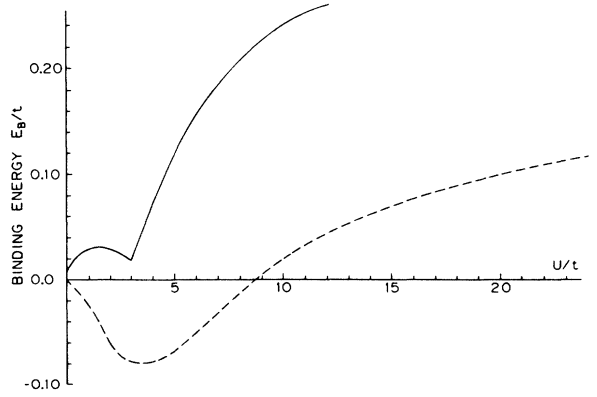

FIG. 7. The binding energy for two holes [Eq. (18)] is shown for the four-square system of Fig. 1(e) (solid line) and for the octagon (dashed line).

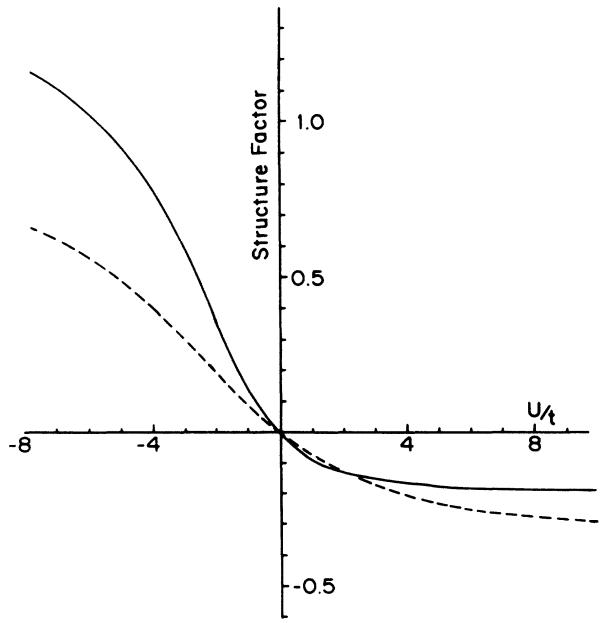

FIG. 8. The corrected local singlet pairing structure factor (solid line) and the charge structure factor (from which the value for $U=0$ has been subtracted) (dashed line) are shown for the two-square system of Fig. 1(c).

tion in a one-dimensional system, we begin our considerations of the effects of the first-neighbor interaction by showing results for six electrons in a six-site hexagonal system in Fig. 9. This system exhibits all of the features mentioned in the Introduction. To show this effectively, we have plotted the spin, charge, and singlet pairing structure factors, and the condensation parameter as a function of angle θ,

$$\theta=\tan^{-1}(U/V) ,$$

going around an ellipse defined by

$$U^2+4V^2=a^2 .$$

We have chosen to associate U with $2V$ in this figure because, qualitatively, one thinks of V as twice as effective as U in determining the properties of one-dimensional systems. We chose $a=8t$ in order to describe a system with reasonably strong interactions, but not in a strong-interaction limit.

Specifically, the system shows the expected transition from spin-density-wave to charge-density-wave behavior in the first quadrant for V slightly greater than $U/2$. (This is also true for the octagon.) The CDW structure factor is dominant through the second quadrant. Pairing is important in a small region in the third quadrant close to the negative-U axis. It should be noted that singlet pairing is slightly enhanced by a weak attractive first-neighbor interaction: the maximum of the pairing structure factor as V varies occurs just below, not on, the negative-U axis. As V becomes more negative, a condensed state is formed which persists into the fourth quadrant. However, as the magnitude of the negative V decreases in the fourth quadrant, the SDW state reappears. The SDW structure factor $S_s(\pi)$ has its maximum with respect to V not at $U=0$ but for slightly negative V. Thus, SDW ordering is also enhanced by a small negative V. In addition, the local singlet pairing structure factor is shown for this system for two holes in the half-filled band. This quantity is enhanced with respect to that for the half-filled band, and maintains a significant value throughout the regime of CDW order.

The two-dimensional clusters of Figs. 1(c) and 1(e) show the antiferromagnetic to CDW transition for values of V significantly smaller than $U/2$. For a large two-dimensional system, the transition would be expected to occur close to $V=U/4$.[12] Figure 10 shows the spin and charge structure factors for the four-square system of Fig. 1(e) as a function of V for $U=2t$. In this case, a sharp transition between spin and charge ordering occurs at $V=0.555t$.

The sharpness of the SDW-CDW transition also depends on geometry. We describe a transition in a finite system as sharp if it involves the crossing (in energy) of two eigenstates which have to be of different symmetry, as a parameter in the Hamiltonian is varied. Otherwise, a single state can evolve continuously although rapidly. In this sense, a sharp SDW-CDW transition occurs for the half-filled system in the (four-site) square, exactly on the line $U=2V$. A sharp transition is also found in the four-square system as shown in Fig. 10, but not in the other clusters (hexagon, two square, octagon) considered in this paper. The transition becomes more rapid [in the sense that $\partial S_c(\pi)/\partial V$ becomes larger] as U increases.

It will also be noticed that Fig. 10 shows a second transition at negative V, at (roughly) $V=-0.71$. This transition leads to the disappearance of the SDW order, the appearance of double occupancy, particularly on the central

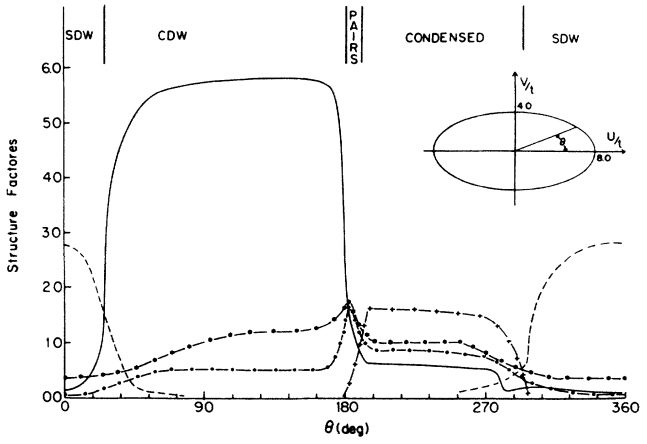

FIG. 9. The charge structure factor (solid line) $S_c(\pi)$, (4×) spin structure factor (dashed line), local singlet pairing structure factor (dashed line with circles) $S_P(0)$, and condensation parameter (dashed line with +) are shown for the six electrons in a hexagon. Quantities are plotted as functions of angle θ around an ellipse $U^2+4V^2=64t^2$ (inset). In addition, the local singlet pairing structure factor is shown for four electrons in the same system (dashed line with *). Regions of dominance of spin-density waves, charge-density waves, pairing, and condensation are marked at the top of the figure.

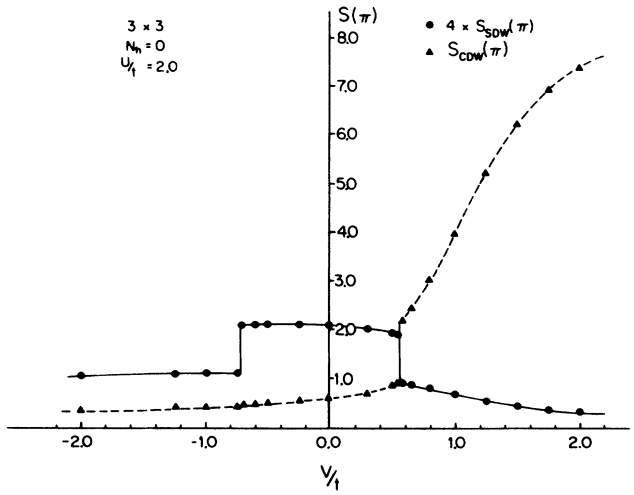

FIG. 10. The dependence of (4×) the antiferromagnetic and the charge structure factor for the four-square system of Fig. 1(e) in the half-filled band case on the nearest-neighbor interaction V is shown for a fixed value of U ($U=2.0t$). A sharp transition between antiferromagnetic and CDW states occurs at $V/t=0.555$. Another transition occurs close to $V/t=-0.71$.

atom, and thus to the development of a condensed state.

Our most striking results for the extended model concern the case in which there are two holes in the half-filled band. The inclusion of first-neighbor interactions can favor either spin alignment or pairing for certain ranges of parameters. In some geometries, notably the two-square and four-square systems we find two regions in the (U,V) plane where alignment occurs. The first is along and below the U axis for large U, as illustrated in Fig. 11. For $V=0$ and large U, the ground state for four electrons in the two-square has $S=1$. The spin alignment is rapidly suppressed for positive V, but is favored for negative V, and the region in which the ground state is a triplet extends below the U axis as far as (roughly) $U=9$. In addition, there is another region at large U and V, where the ground state has $S=1$. In this case, the spin alignment exists in the presence of CDW order, as shown in Fig. 11.

For negative V, a condensed state forms. In the two-square, four-electron system, the ground state for large negative V and positive U is characterized by single occupancy of the two middle sites [see Fig. 1(c)], while the two pairs of end sites have equal probability ($\frac{1}{2}$) of being occupied. The charge correlation functions indicate that if the left pair is occupied, the right pair is vacant, or vice versa. The ground state contains both possibilities symmetrically. The condensation begins to develop below the U axis, and the occupancy pattern is already apparent below about $V=-1.1$ over a wide range of U. Because none of the sites are doubly occupied, condensation develops in the presence of spin correlations. However, if V becomes sufficiently negative, the system becomes unstable in a sense pointed out by del Bosch and Falicov.[7] If the system were to be connected to a reservoir of particles, it would fill up. This occurs when the energy per particle in the system when all sites are doubly occupied ($U/2+7V/3$) is lower than the energy per particle in the four-electron system. The latter quantity is close to V when $U>0$. The stability line defined in this way is shown in Fig. 11. For large U, the line is well approximated by $V=-3U/8$. It should be noted that this line lies well below the onset of condensation: in this system condensation does not necessarily imply instability. Similar features are found in the four-square system.

We have also examined the binding energy of two holes, given by Eq. (18a). There is a region of binding in the first quadrant for small U and moderate to large V. This is indicated in Fig. 11. Binding coexists with the CDW order. The binding extends throughout the second quadrant. The situation is similar in the four-square system as is illustrated in Fig. 12. We have investigated pairing correlations in this region, and find positive values of the corrected local singlet pairing structure factor in the region in which E_B is negative, as shown in Fig. 13. However, the possibility of phase separation of the holes has to be considered seriously, as the two-pair binding energy E_{B4} also becomes negative in this region (as does also E_{B3}, which is not shown). There is a small range in the neighborhood of $V=1$ where S_L^c is positive,

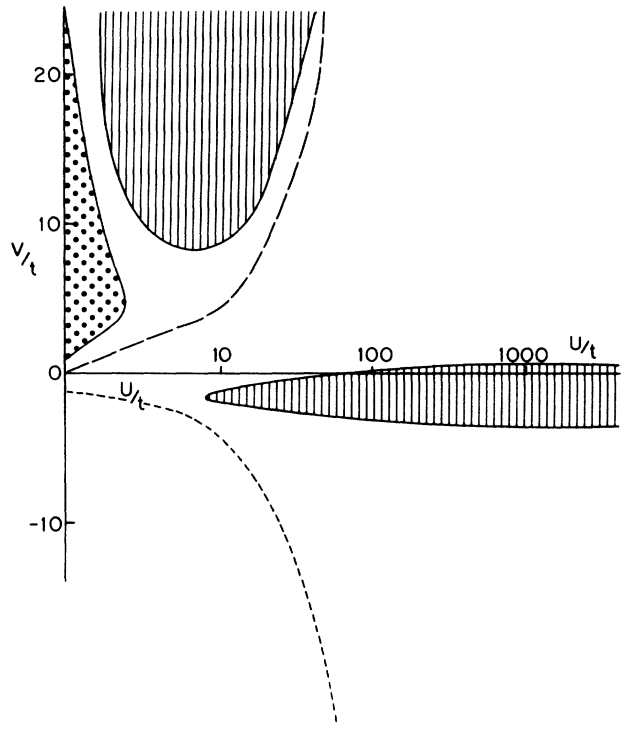

FIG. 11. Partial phase diagram for two holes in the half-filled band for the two-square system of Fig. 1(c). The regions with vertical shading are those in which the two holes have parallel spin; the region with circles is that in which the two-hole binding energy is negative. Note that the scale of U changes from linear to logarithmic at $U/t=10$. The long-dashed line in the upper part of the plane is the CDW boundary. The CDW order occurs above and to the left of this line. The system is unstable in a manner described in the text below the short-dashed line in the lower part of the figure. A condensed state develops between the negative-U axis and this line.

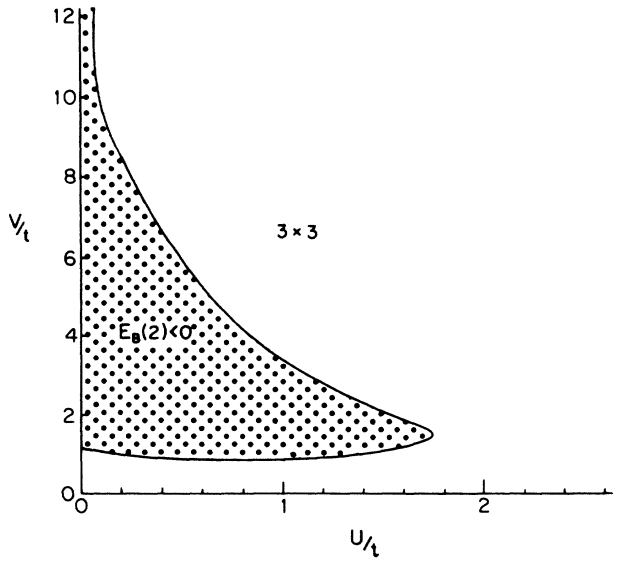

FIG. 12. The region of hole binding for seven electrons in the nine-site system is indicated by circles.

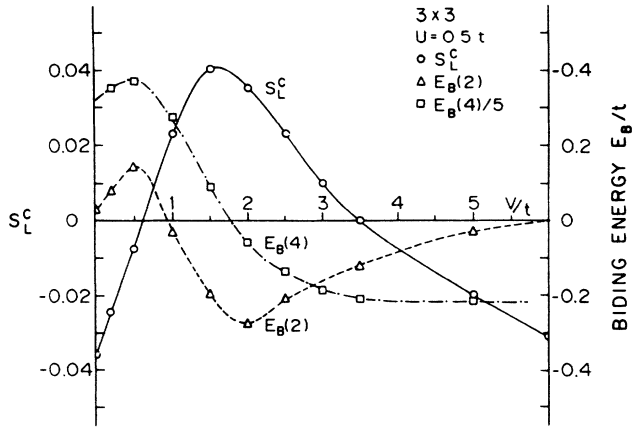

FIG. 13. The corrected local singlet structure factor for seven electrons in the nine-site four-square system (solid curve, left-hand scale) is shown as a function of V/t for $U=0.5t$. The pair binding energy E_B is shown (dashed line, right-hand scale) as is the two-pair energy E_{B4} (divided by 5, dotted line, right-hand scale).

E_B is negative, and E_{B3} and E_{B4} are still positive. The pairing described here coexists with the SDW order.

It remains for future investigations to determine whether the enhancement of pairing by repulsive first-neighbor interactions also occurs in larger systems, and whether there is any relevance to high-T_C superconductivity as actually observed. However, several other groups have found hole binding in systems where a first-neighbor interaction is added to a Hubbard model for CuO_2 planes.[30–32] The particular interest of the present results is that pairing occurs in a parameter region in which U and V are of modest size.

IV. CONCLUSIONS

We have studied the one-band Hubbard and extended Hubbard models on several lattices by exact diagonalization. In general, our results are limited to fairly small clusters (quantum Monte Carlo calculations are possible for larger systems), but there are no restrictions in our work concerning the occupancy or the size of the parameters that we can consider, and the calculations can be performed using the exact ground state, rather than requiring an extrapolation from finite temperatures. Our findings may be summarized as follows.

A. Simple Hubbard model

1. Half-filled band

In this well-studied system, our results agree with those of other calculations, including quantum Monte Carlo simulations for larger clusters. We find antiferromagnetic alignment of local magnetic moments, with a structure factor that increases with the size of this cluster. However, our work extends to much larger values of U than have been considered in Monte Carlo calculations. Our results for $U/t > 20$ for the nine-site system should be quantitatively rather reliable here in the sense that finite-size effects should be small, and enable a determination of the amount of double occupancy as a function of U in a region which is not easily accessible to the Monte Carlo calculations. For negative U we observe the coexistence of the CDW order and local singlet pairing.

2. One and two holes in a half-filled band

For moderate values of U, we see the expected reduction in the range of magnetic alignment. At large U, we find ferromagnetic alignment in the quasi-two-dimensional systems, where there is one hole, consistent with Nagaoka's theorem, but in the one-dimensional systems the ground state is not a saturated ferromagnet. We have determined the critical value of U defining the ferromagnetic region for several different geometries. In the case of two holes, we have found, in the quasi-two-dimensional systems, a region of unsaturated ferromagnetism at large U, and believe this should be considered seriously as a possibility in larger systems. Local singlet pairing is found for negative U.

B. Extended Hubbard model

In the half-filled band case, our results are consistent with previous work. We have studied the entire phase diagram, including the condensed state for large negative V. The new results concern the case when there are a pair of holes in the half-filled band.

(1) For negative values of V too small in magnitude to produce a condensed state, we find that, for positive U, local moments are enhanced, and spin alignment is strengthened. The region of unsaturated ferromagnetism is extended to smaller values of U.

(2) An unexpected region of spin pairing has been discovered in the upper first quadrant of the (U,V) plane where it coexists with the CDW order.

(3) We find, in the quasi-two-dimensional systems, a region local singlet pairing, and in which two holes bind, for moderate and large values positive values of V, and small positive values of U (also for negative U). Although there is certainly a tendency toward phase separation in this region, we find in some of the clusters that there is a window in which two holes bind and pair, but larger hole clusters do not bind. Although other authors using different models, more explicitly relevant to CuO_2 planes, have found the binding of pairs under rather similar circumstances for specific parameter values, we believe this is the first calculation to determine the portion of the phase diagram in which binding occurs. The possible relevance of this region of parameters to high-T_c superconductors remains to be studied.

There is another way of looking at the results which is also of interest. From the studies of clusters of different geometry, one can recognize properties which are characteristic of this type of model in general, and those which show a pronounced dependence on sample geometry.

In the first category of generic results we place (1) formation of local spin moments for strong on site interactions, (2) existence of SDW or antiferromagnetic correlations in the ground state of a half-filled band system, (3)

reduction of the range of spin correlations by hole doping except when a ferromagnetic ground state is formed, (4) occurrence of local singlet pairing for negative U, (5) a transition to the CDW order for sufficiently repulsive nearest-neighbor interactions, and (6) enhancement of magnetic correlations for positive U and of pairing correlations for negative U by weakly attractive first-neighbor interactions.

The second category of geometrically sensitive results includes, obviously, the precise numerical values of the parameters at which the transitions occur. Moreover, some qualitative features are also dependent on geometry including: (1) the presence or absence of saturated ferromagnetism in the large-U limit for systems with one hole in a half-filled band (this has been recognized for many years), (2) the occurrence of a ground state with $S>0$ or $\frac{1}{2}$ for a system of two holes in the same limit, and (3) the binding of two holes for small U.

ACKNOWLEDGMENTS

This work was supported in part by the Louisiana Educational Quality Support Fund and in part by the National Science Foundation under Grant No. 8810249.

*Permanent address: Department of Physics, University of Poona, Pune 411007, India.

[1]J. Hubbard, Phys. Rev. B **17**, 494 (1978).
[2]V. J. Emery, Phys. Rev. B **14**, 2989 (1976).
[3]V. J. Emery, in *Highly Conducting One Dimensional Solids*, edited by J. Devreese, R. Evrard, and V. van Doren (Plenum, New York, 1979).
[4]J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984).
[5]B. Fourcade and G. Spronken, Phys. Rev. B **29**, 5096 (1984).
[6]H. Q. Lin and J. E. Hirsch, Phys. Rev. B **33**, 8155 (1986).
[7]L. M. del Bosch and L. M. Falicov, Phys. Rev. B **37**, 6073 (1988).
[8]S. B. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).
[9]J. D. Jorgensen, H. B. Schuttler, D. G. Hinke, D. W. Capone II, K. Zhang, M. Broedsky, and D. J. Scalapino, Phys. Rev. Lett. **58**, 1024 (1987).
[10]J. Yu, A. J. Freeman, and J. H. Xu, Phys. Rev. Lett. **58**, 1035 (1987).
[11]L. F. Mattheiss, Phys. Rev. Lett. **58**, 1028 (1987).
[12]Y. Zhang and J. Callaway, Phys. Rev. B **39**, 9397 (1989).
[13]C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. **68**, 681 (1987).
[14]J. Callaway, D. G. Kanhere, and P. K. Misra, Phys. Rev. B **36**, 7141 (1987).
[15]V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987); V. J. Emery and G. Reiter, Phys. Rev. B **38**, 4547 (1988).
[16]J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985).
[17]J. K. Cullum and R. A. Willoughby, *Lanczos Algorithms for Large Symmetric Eigenvalue Computations* (Birkhäuser, Boston, 1985).
[18]J. Callaway, D. P. Chen, and R. Tang, Z. Phys. D **3**, 91 (1986); Phys. Rev. B **35**, 8723 (1987).
[19]J. Callaway, D. P. Chen, and Y. Zhang, Phys. Rev. B **36**, 2084 (1987).
[20]The large-U ground state for seven electrons in an octagon has $S=\frac{3}{2}$ (instead of $S=\frac{1}{2}$ or $\frac{7}{2}$); apparently an exceptional case.
[21]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[22]J. A. Riera and A. P. Young, Phys. Rev. B **40**, 5285 (1989).
[23]J. A. Riera and A. P. Young, Phys. Rev. B **39**, 9697 (1989).
[24]E. Dagotto, A. Moreo, R. L. Sugar, and D. Toussaint, Phys. Rev. B **41**, 811 (1990).
[25]P. W. Anderson, Phys. Rev. Lett. **34**, 953 (1975).
[26]P. Pincus, P. Chaikin, and C. F. Coll, Solid State Commun. **12**, 1265 (1965).
[27]P. Nozieres and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1986).
[28]J. A. Wilson, Int. J. Mod. Phys. B **3**, 691 (1989).
[29]R. T. Scarlettar, E. Y. Loh, J. Gubernatis, A. Moreo, S. R. White, D. J. Scalapino, R. L. Sugar, and E. Dagotto, Phys. Lett. **62**, 1407 (1989).
[30]J. E. Hirsch, S. Tang, E. Loh, and D. J. Scalapino, Phys. Rev. Lett. **60**, 1668 (1988).
[31]C. A. Balseiro, A. G. Rojo, E. R. Gagliano, and B. Alascio, Phys. Rev. Lett. **60**, 1668 (1988); Phys. Rev. B **38**, 9315 (1988).
[32]W. H. Stephan, W. v. d. Linden, and P. Horsch, Phys. Rev. B **39**, 2924 (1989).