Superconductivity near phase separation in models of correlated electrons

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Numerical and analytical studies of several models of correlated electrons are discussed. Based on exact diagonalization and variational Monte Carlo techniques, we have found indications that the two-dimensional t-J model superconducts near phase separation in the regime of quarter-filling density, in agreement with previous results reported by Dagotto and Riera [Phys. Rev. Lett. **70**, 682 (1993)]. At this density the dominant channel is $d_{x^2-y^2}$, but a transiton to s-wave superconductivity is observed decreasing the electronic density. In addition, the one-band t-U-V model has also been studied using a mean-field approximation. An interesting region of $d_{x^2-y^2}$ superconductivity near phase separation is observed in the phase diagram, and its implications for recent self-consistent studies of d-wave condensates in the context of the high-T_c cuprates are briefly discussed. Finally, the two-band Hubbard model on a chain is also analyzed. Superconducting correlations near phase separation exist in this model, as it occurs in the t-J model. Based on these nontrivial examples it is conjectured that electronic models tend to have superconducting phases in the vicinity of phase separation, and this regime of parameter space should be explored first when a new model for superconductivity is proposed. Reciprocally, if it is established that a model does not phase separate, even in an extended parameter space, then we believe that its chances of presenting a superconducting phase are considerably reduced.

I. INTRODUCTION

The study of high-temperature superconductors continues to attract much attention.[1] On the experimental side, steady progress is being made in the preparation of single-crystal samples of high quality for several compounds. The common features of the cuprates are experimentally well established, especially the "anomalous" behavior of several observables in the normal state like the dc resistivity, optical conductivity $\sigma(\omega)$, Hall coefficient, and others.[2] New compounds have been recently discovered with a critical temperature of ~ 133 K, increasing our expectations that the cuprates may become technologically relevant in the near future.[3] On the theoretical side, considerable progress has also been achieved in recent years in the study of models of correlated electrons. Powerful numerical techniques have shown that some of the anomalous properties of the cuprates may be explained by simple one-band Hubbard and t-J models.[4,5] The midinfrared band of $\sigma(\omega)$ observed in $La_{2-x}Sr_xCuO_4$ and other compounds[6] may be produced, at least in part, by the spin excitations that heavily dress the hole carriers.[4] The temperature dependence of the magnetic susceptibility[7] can also be explained by models of holes moving in a strong antiferromagnetic background.[8] The appearance of states in the charge-transfer gap upon doping[9] can be mimicked using the one-band Hubbard model.[10] Mean-field theories of

the t-J model[11] have contributed to the understanding of the incommensurate peaks observed in $La_{2-x}Sr_xCuO_4$,[12] and they are in good agreement with numerical studies of the same model.[13] Unfortunately, other anomalous properties are still unexplained, like the linear behavior of the resistivity with temperature, and the pinning of the chemical potential with doping in some compounds.[14] Nevertheless, the theoretical progress described above should be considered as an important step towards the development of a microscopic theory of the high-T_c cuprates.

In spite of this progress in the description of normal-state properties, the presence of superconductivity in the ground state of models of correlated electrons is still a subtle and much debated issue. Numerical studies of the t-J model on large enough lattices have shown that holes in an antiferromagnetic background tend to form bound states in the $d_{x^2-y^2}$ channel.[15] Similar results have been obtained in the context of the one-band Hubbard model using self-consistent approximations which suggest the existence of d-wave pairing at very low temperatures.[16] However, no convincing quantum Monte Carlo numerical evidence has been found that the model indeed superconducts at low temperatures and hole density.[17] These numerical results can be interpreted in two ways. On the one hand, it may occur that the Hubbard model indeed does not superconduct. This negative result is not at all excluded. On the other hand, it may occur that present day numerical techniques are not accurate enough to find out the (weak) signals of a superconducting condensate in this model. It is clear that analyzing a two-hole problem is simpler than searching for a condensate, where the subtle coherence and overlap effects between pairs is crucial for its existence. In particular, note that for a finite lattice of, e.g., 16 sites, a realistic electronic density of $\langle n \rangle = 0.875$ corresponds to only one pair of holes, which, of course, cannot produce a superconducting signal alone. Then, it may simply occur that close to half-filling the clusters accessible to numerical studies do not have enough pairs to produce a clear signal of superconductivity as an output. Actually, Monte Carlo studies of the attractive Hubbard model[18] (which has a well-established superconducting ground state) have shown that in the regime of low electronic density (and thus low pair density) it is difficult to observe a numerical evidence of superconductivity in the ground state. A similar situation may occur in the t-J and repulsive Hubbard models near half-filling where the density of pairs is small.

Based on these ideas, two of us[19] recently started the search for indications of superconductivity in the ground state of the two-dimensional t-J model in a novel regime of parameter space, namely $\langle n \rangle = \frac{1}{2}$ (which by analogy with the Hubbard model, it will be called "quarter-filling" in this paper), and large coupling J/t. The main motivation for such a study in a region of parameter space which is not realistic for the cuprates is that in this regime the number of carrier pairs is maximized (closer to half-filling there are fewer holes, and near the empty system fewer electrons). In addition, it is well known that there are attractive forces operating in this model since the system phase separates at large J/t. Also note that at low electron density, two electrons on an otherwise empty lattice minimize their energy by forming a tight singlet bound state.[20] Then, densities of quarter-filling or less and couplings close to phase separation seem the most optimal regime to search for superconductivity in the two-dimensional (2D) t-J model, as reported by Dagotto and Riera.[19] A strong indication of superconductivity was found by these authors in the equal-time pairing correlations, with a signal which is maximized in the $d_{x^2-y^2}$ channel in agreement with the results for two holes close to half-filling,[15] and with the self-consistent approximations.[16]

One of the purposes of this paper is to discuss in more detail the results found in Ref. 19 for the 2D t-J model. We provide numerical evidence showing that the region of d-wave superconductivity near quarter-filling is robust and likely to survive the bulk limit. In addition, we found a novel transition from $d_{x^2-y^2}$-wave to s-wave superconductivity as a function of density. This transition was expected in order to make compatible the results of Emery, Kivelson, and Lin[20] suggesting s-wave superconductivity at very low density (based on the presence of two-electron s-wave bound states on an empty lattice), and those of Dagotto and Riera[19] at quarter-filling, suggesting a $d_{x^2-y^2}$ condensate. The numerical evidence for these results is based on a variational Monte Carlo calculation on large clusters, and it is consistent with the results obtained with the Lanczos approach on smaller clusters. The success of this search for superconductivity in the t-J model opens the possibility for the existence of superconductivity in the realistic regime of small J/t and $\langle n \rangle \sim 1$, as discussed below in the text.[21]

Actually, this paper has a more general purpose. We will argue that for a given electronic model, the region in parameter space where superconductivity has the highest chances of being stable is in the neighborhood of phase separation.[22] Moreover, we believe that the attractive force responsible for phase separation also leads to the strong pairing correlations in its neighborhood (similar ideas have been recently discussed by Emery and Kivelson, see Ref. 23). In this regime it is energetically favorable to form pairs of holes rather than larger clusters of holes, due to the gain in kinetic energy obtained by giving mobility to those pairs. Reciprocally, if the model does not have phase separation, not even in an extended parameter space (without explicitly changing the repulsive or attractive character of the potential), then it is difficult to imagine that it will present a superconducting phase. This is a *conjecture* that is presented and discussed in this paper. As with any conjecture, we do not have a rigorous mathematical proof of its validity, but here we provide several examples that illustrate the main ideas behind it. This conjecture has practical implications since it is well known that establishing the presence of phase separation for a given model is usually simpler than finding a superconducting ground state. Then, once phase separation is found, the region to search for pairing is considerably reduced. To support our ideas, in addition to the two-dimensional t-J model, in this paper we also discuss the attractive Hubbard model which naively seems a

counter-example to our conjecture, i.e., it superconducts but does not phase separate. However, it can be shown that in an extended parameter space (i.e., including attractive density-density correlations which are usually spontaneously generated by any renormalization group procedure), the regime of s-wave superconductivity of the negative U Hubbard model is in contact with a robust region of phase separation. As a bonus of this study, an interesting region of $d_{x^2-y^2}$ superconductivity in the extended t-U-V one-band Hubbard model was observed. This phase may have important implications for recent efforts to describe the cuprates with effective Hamiltonians based on the interchange of magnons.[16] Finally, we briefly present results for the two-band Hubbard model in a one-dimensional chain showing that also in this case strong superconducting correlations appear near phase separation. All these examples give strong support to our conjecture. In addition, note that recent experimental work[24] has shown that in some cuprates with an excess of oxygen there is phase separation and is not caused just by a chemistry problem (the oxygens are very mobile). Theoretical ideas by Emery and Kivelson[23] have been presented linking phase separation and superconductivity in the cuprates, and thus the type of studies described in this paper may have implications for real materials.

The organization of the paper is the following: In Sec. II, the t-J model in two dimensions is studied at different densities. The interesting transition from $d_{x^2-y^2}$-wave to s-wave superconductivity is discussed. In Sec. III, mean-field results for the t-U-V model are presented, and its rich phase diagram discussed at half-filling. In Sec. IV, we briefly discuss results for the two-band Hubbard model on a chain. Conclusions are presented in Sec. V, and finally in the appendices we discuss measurements of the superfluid density for the one-band Hubbard model, and the influence of the fermionic statistics on the phase diagram of the 2D t-J model.

II. t-J model in two dimensions

A. Density $\langle n \rangle = \frac{1}{2}$

As discussed in the Introduction, recently it has been suggested by two of us[19] that the t-J model in two dimensions may have a superconducting phase near phase separation, and at density $\langle n \rangle = \frac{1}{2}$. The numerical evidence for these conclusions was based on an exact diagonalization study of finite clusters, analyzing the equal-time pairing correlations, the superfluid density (discussed briefly in Appendix A), and the anomalous flux quantization. For completeness, in this section some of those results are reproduced from Ref. 19. New information for other cluster sizes and parameters is provided. The t-J model is defined by the Hamiltonian

$$H = J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j) - t \sum_{\langle ij \rangle, s} (\bar{c}^{\dagger}_{i,s} \bar{c}_{j,s} + \text{H.c.}) , \qquad (1)$$

where $\bar{c}^{\dagger}_{i,s}$ denote *hole* creation operators; $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ are number operators for electrons; and the rest of the notation is standard. In the numerical studies of this model described below, square clusters of N sites have been used (with periodic boundary conditions). In order to search for indications of superconductivity in the ground state, let us define the pairing operator

$$\Delta_i = c_{i,\uparrow}(c_{i+\hat{x},\downarrow} + c_{i-\hat{x},\downarrow} \pm c_{i+\hat{y},\downarrow} \pm c_{i-\hat{y},\downarrow}) ,$$

where $+$ and $-$ corresponds to extended-s and $d_{x^2-y^2}$ waves, respectively, and $\hat{x}, \hat{y}$ are unit vectors along the axis. Note that the pairing operator is constructed using electronic operators (not hole operators). The pairing-pairing correlation function defined as $C(\mathbf{m}) = (1/N) \sum_i \langle \Delta_i^{\dagger} \Delta_{i+\mathbf{m}} \rangle$, and its susceptibility $\chi^{\alpha}_{\text{sup}} = \sum_{\mathbf{m}} C(\mathbf{m})$ have been calculated (where $\alpha = d$ corresponds to the $d_{x^2-y^2}$ wave, and $\alpha = s$ to the extended-s wave). $\langle\ \rangle$ denotes the expectation value in the ground state, which is obtained accurately using the Lanczos method. Note that the pairing operator used here is not strictly a spin singlet but actually the sum of a singlet and a triplet. This operator allows us to study the two spin sectors at the same time. Once a large signal in the pairing correlations is observed in some region of parameter space, it is trivial to implement rigorous spin singlet or triplet operators to find out which one carries the strongest correlation. In practice, we found that the results obtained using the operator Δ_i defined above at all distances larger than zero, are quantitatively very similar to the results obtained using a spin-singlet operator. Even at zero distance the difference is only about 15%. Then, the results below using Δ_i should be considered approximately equal to those obtained using the proper singlet operator Δ_i^S (where $\Delta_i^S = \Delta_i - \hat{I}\Delta_i$, and $\hat{I}$ is the operator that inverts the z direction spin projection for each electron).

Working on a 4×4 cluster, and density $\langle n \rangle = \frac{1}{2}$, the numerical results are shown in Fig. 1. The d-wave susceptibility presents a sharp peak at coupling $J/t = 3$, suggesting that strong pairing correlations exist in this region of parameter space [Fig. 1(a)]. We have verified explicitly that the abrupt reduction of the signal after $J/t = 3$ is caused by a transition to the phase separation region which is expected at large couplings[20] (this conclusion was obtained studying numerically the compressibility). However, it is important to remark that a large superconducting susceptibility (or rather, zero-momentum pairing correlation function) is not sufficient to guarantee the presence of long-range order, but an increase of χ^{d}_{sup} with the lattice size is required. Unfortunately, it is difficult to study lattices much larger than the 4×4 cluster, and thus such an explicit analysis is not possible with present day computers. Nevertheless, we can study the existence of long-range order in this model by explicitly calculating the pairing correlations as a function of distance. A robust tail in the correlation would suggest long-range order (or at least a correlation length larger than the lattice size). The results for the t-J model are shown in Fig. 1(b), both for the $d_{x^2-y^2}$- and extended-s wave correlations. Similar correlations are also shown in Fig. 1(c) for the d-wave channel, parametric with the coupling J/t. These results indicate that most of the signal in the susceptibility does *not* come from the on-site correlation, but from its tail. Although

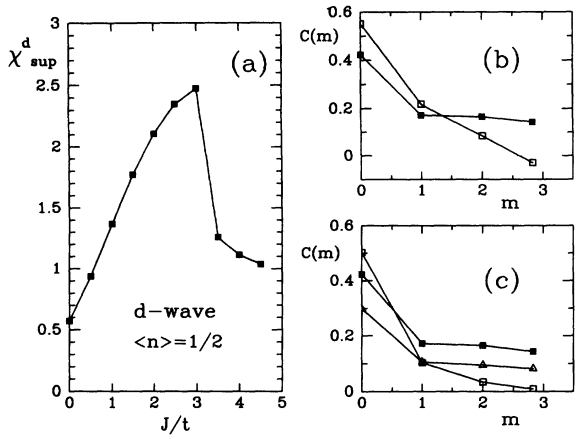

FIG. 1. (a) Superconducting susceptibility $\chi^d_{\rm sup}$ corresponding to $d_{x^2-y^2}$ correlations (defined in the text) as a function of J/t for the 2D t-J model, at quarter-filling density. The results are obtained on a 4×4 cluster; (b) pairing correlations $C(\mathbf{m})$ as a function of distance m, at $J/t=3$ [i.e., where $\chi^d_{\rm sup}$ peaks in (a)], $\langle n\rangle=\frac{1}{2}$, using a 4×4 cluster. The full squares are results for $d_{x^2-y^2}$ symmetry, while the open squares correspond to extended s wave; (c) same as (b) but for different values of J/t, and using only the $d_{x^2-y^2}$ correlations. The full squares correspond to $J/t=3$, the triangles to $J/t=1$, and the open squares to $J/t=4$ (region of phase separation). These results are taken from Dagotto and Riera [Phys. Rev. Lett. **70**, 682 (1993)], and reproduced here to make the paper self-consistent.

this is not a rigorous proof, such a result strongly suggests that long-distance pairing correlations are developing in this region of parameter space. Further studies at other densities and couplings show that the results of Figs. 1(b) and 1(c) are indeed robust, and in regions where no superconductivity exists, the pairing correlations decay very abruptly with distance, typically being compatible with zero at about two lattice spacings. This is precisely the case of the repulsive Hubbard model in two dimensions studied with quantum Monte Carlo techniques.[17] Then, the reader should notice that the correlations shown in Figs. 1(b) and 1(c) are perhaps the strongest numerical signals of superconductivity reported thus far in the literature of the 2D t-J and Hubbard models, using unbiased numerical techniques.

What is the physical reason for the presence of strong pairing correlations in this region of parameter space? To begin with, note that there are attractive forces between electrons operative in the t-J model which are responsible for the existence of phase separation. Such forces can be roughly described in the two limits of low and high electronic density. For example, it is well known that two holes in an antiferromagnetic background at large J/t tend to bind in a $d_{x^2-y^2}$-wave bound state in order to minimize the number of antiferromagnetic missing bonds.[15] This force leads to clustering of holes at a finite hole density. In the other limit of low electronic density, it can be shown that two electrons in an otherwise empty lattice form a bound state at coupling $J/t>2$, since the Heisenberg term acts like an explicitly attractive force. Increasing further the coupling and working at finite density, phase separation occurs.[20] This special case is interesting since it shows that at low electronic density there are bound states whose kinetic energy forbids the clustering effect until a large coupling is reached. We believe that a similar scenario holds at quarter-filling $\langle n\rangle=\frac{1}{2}$, namely, that the force that produces phase separation for $J/t>3$ also produces pairing at smaller coupling. The gain in kinetic energy of the mobile pairs forbids phase separation in this regime.

Another qualitative argument to help understanding the presence of pairing is the following: suppose a repulsive density-density interaction $V\sum_{\langle ij\rangle} n_i n_j$ is added to the Hamiltonian of the t-J model. Such a term has been analyzed by Kivelson, Emery, and Lin[25] in the large V/t limit, and by Dagotto and Riera[26] numerically for all values of V/t. These authors showed that at large V/t a tendency to form an ordered arrangement of dimers (spin singlets formed by two electrons at a distance of one lattice spacing) exists. Analytic calculations, supported by numerical results, show the existence of this dimer lattice very clearly. The introduction of a hopping term t induces superconducting correlations.[25] The exact diagonalization results[26] suggest a smooth connection between large and small V/t, and thus some remnants of dimers may exist in the pure t-J model at this density (although now in a spatially disordered state). The phase diagram obtained numerically in the plane V/t-J/t is shown in Fig. 2 (the points represent the position of the maximum in the superconducting susceptibility evaluated on a 4×4 cluster). However, a more subtle issue forbids a completely smooth connection between the two regimes: at large V/t there is a robust spin gap in the spectrum due to the formation of dimers, and thus the s-wave correla-

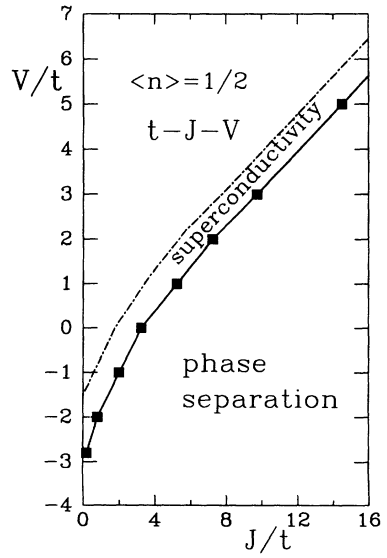

FIG. 2. Phase diagram of the t-J-V model at quarter-filling. The full squares denote the positions of the peaks in $\chi^d_{\rm sup}$ obtained using a 4×4 cluster. The other boundary of the superconducting regime (dot-dashed line) should not be considered quantitative, but only schematic.

tions dominate. However, at $V/t=0$ the $d_{x^2-y^2}$ correlations are dominant and the presence of nodes in the spectrum (in the bulk limit) allow for the possibility of creating low-energy spin triplets (i.e., zero spin gap). Then, if our numerical results are valid in the bulk limit, a transition between *s*- and *d*-wave ground states should exist as a function of V/t, near phase separation (the verification of this idea certainly deserves more work). The closing of the spin gap as a function of this coupling has indeed been observed by Troyer *et al.* in the one-dimensional version of the *t-J-V* model.[27] In the next section, it will be shown that a transition from *d*- to *s*-wave condensates also exists as a function of density in the pure 2D *t-J* model.

It would be important to study larger clusters in order to verify that the strong tail of the correlations as a function of distance shown in Figs. 1(b) and 1(c) are not a mere finite-size effect. Unfortunately, such a study is difficult with present day computers since the memory requirements needed to carry out a Lanczos study of the *t-J* at quarter-filling grow exponentially with the cluster size.[28] In spite of this problem we managed to study a tilted cluster of 20 sites[29] as that shown in Fig. 3(a). Although not obvious to the eye, it can be shown that this cluster is invariant under rotations in $\pi/2$ about a site, and thus it can be used to explore the presence of superconductivity in the *d* channel.[30] However, the 20-site cluster has a disadvantage for the particular problem studied in this section. The trouble is schematically shown in Fig. 3(a): considering the *t-J-V* model in the limit of large V/t, the five dimers that could, in principle, be formed in the cluster do not have space to minimize the energy unless a V energy larger than 5 V is paid. This is purely an artifact of the shape of the cluster that does not occur in square $L\times L$ lattices. Since on the 4×4 cluster a smooth connection was observed between large and small V/t, the lack of a proper V/t limit for the 20-site cluster implies that the signal for superconductivity in the other limit of $V/t=0$ may be spuriously reduced compared to that of the 16-site cluster. This conclusion was verified by an explicit numerical study of the $N=20$ cluster. The normalized signal for *d*-wave pairing correlation shown in Fig. 3(b) is reduced by approximately a factor of 2 when the lattice size is increased from $N=16$ to 20 sites. Rather than considering this as a negative result for our scenario, we believe the reason for this reduction is the topology of the $N=20$ cluster as explained before. In spite of this problem, note that even for the $N=20$ lattice, there are no indications that the correlation will decay to zero at large distances since the signal is fairly flat. Of course, studies on larger clusters that satisfy the proper V/t limit would be important to verify our assumptions, but we believe that the evidence discussed in this section suggesting the existence of superconductivity in the quarter-filled 2D *t-J* model is strong, and may survive the bulk limit. Finally, we would like to remark that "dynamical" studies of this condensate would be very important. Actually, we have already carried out studies of the dynamical pairing correlation in the *d*-wave channel. It shows a sharp peak at the bottom of the spectrum, as expected from a *d*-wave condensate. Other dynamical properties are currently being analyzed by Maekawa *et al.*[31]

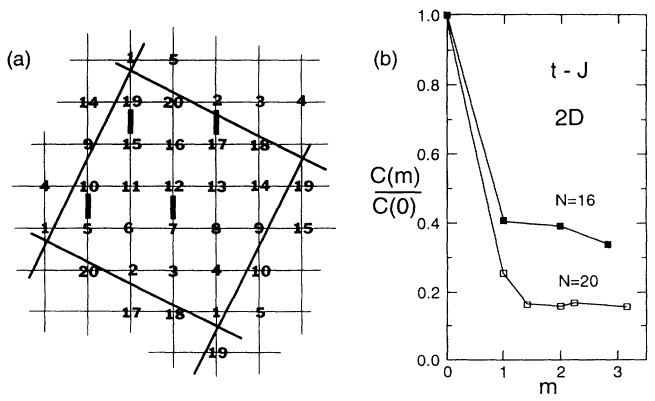

FIG. 3. (a) Cluster of 20 sites used in this paper. The sites are numbered such that the neighbors can be identified once periodic boundary conditions are applied. The four thick links represent dimers formed in the large V/t limit as discussed in the text; (b) $d_{x^2-y^2}$ pairing correlations (normalized to one at distance zero), as a function of distance for $J/t=3$ and $\langle n\rangle=\frac{1}{2}$, obtained on a 4×4 cluster (full squares) and on a 20-site cluster (open squares).

B. Low electronic density, $\langle n\rangle<\frac{1}{2}$

It is interesting to extend the results obtained in the previous subsection to other densities. Here, the region $\langle n\rangle<\frac{1}{2}$ will be explored. In this regime the problem associated with the lattices of 20 sites does not hold anymore since four or less dimers can be accommodated in the cluster of Fig. 3(a) without trouble at large V/t, and thus results for a lattice slightly larger than a 4×4 cluster become available. In addition, there is a physical motivation for the study of low electronic densities: from the work of Emery, Kivelson, and Lin[20,32] it is known that at $J/t=2$ a bound state of two electrons appears due to the attractive spin-spin interaction in the Hamiltonian that favors the formation of a spin-singlet state. Then, it is natural to expect that a finite (but small) density of these bound states may Bose condense at low temperatures in the *s*-wave channel.[20,25] This argument is very persuasive, but the numerical results in favor of a *d*-wave condensate at quarter-filling are also fairly strong.[19] Thus, the only solution to this apparent paradox is that the ground state of the 2D *t-J* model exhibits a transition from *s* wave at low densities to *d* wave at higher densities. Here, evidence based on exact diagonalization and variational Monte Carlo (VMC) studies is presented to support this conjecture.[33] Then, the phase diagram of the *t-J* model seems very rich indeed showing *d*- and *s*-wave superconducting condensates, phase separation, antiferromagnetism, ferromagnetism, and paramagnetic phases in the $\langle n\rangle$-J/t plane.

Consider a 20-site cluster with eight electrons (i.e., $\langle n\rangle=0.4$), and let us evaluate in its ground state the same pairing correlation functions studied at quarter-filling in Figs. 1(b) and 1(c). The results for the $d_{x^2-y^2}$

and extended-s symmetries are shown in Figs. 4(a) and 4(b). At this density, it is clear from the figure that the d-wave pairing correlations are still dominant over s wave, i.e., the d-wave correlations at a distance of approximately three lattice spacings are robust and do not show indications of reduction with distance. In Figs. 4(c) and 4(d) similar correlations are shown at a lower density $\langle n \rangle = 0.2$ (four electrons on the 20-site cluster). The qualitative results are similar to those obtained in Fig. 4(a) although now the correlation at a distance of two lattice spacings in the s-wave channel is larger than at $\langle n \rangle = 0.4$. This suggests a tendency towards the formation of a competing s-wave condensate, but it is not enough to show that such a condensate will become stable upon further reduction of the density. Unfortunately, on this cluster the next density available corresponds to only two electrons which we know cannot be representative of a finite density of particles. Thus, from the exact diagonalization analysis we can only roughly say that the transition from d- to s-wave superconductivity may occur at an electronic density $\langle n \rangle < 0.2$.

It would be very important to verify this result by some other independent calculation. For this purpose, we have implemented a simple VMC simulation, using trial wave functions with an s and d symmetry superconducting condensates, and also states representing a Fermi liquid,

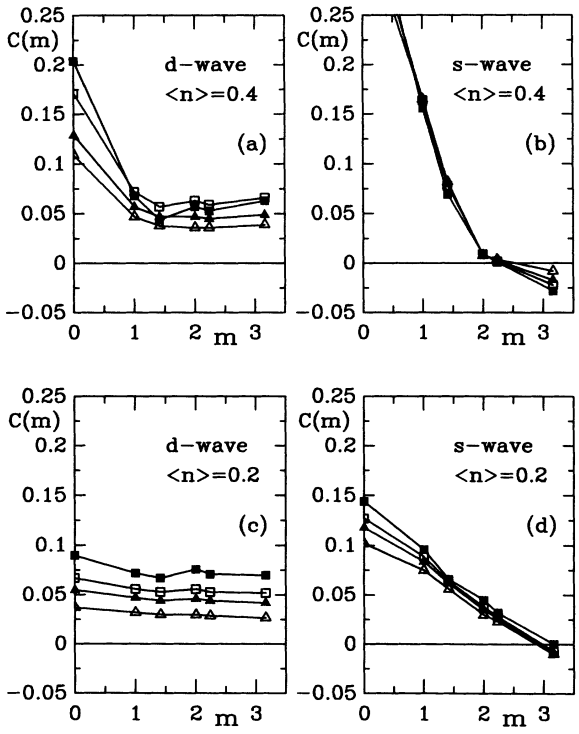

FIG. 4. Pairing correlation $C(\mathbf{m})$ as a function of distance, for the 2D t-J model on a 20-site cluster. The open triangles, full triangles, open squares, and full squares are results at coupling s $J/t=2.1$, 2.7, 3.0, and 3.5, respectively. (a) corresponds to $d_{x^2-y^2}$ symmetry and density $\langle n \rangle = 0.4$, while (b) is for extended-s and the same density. (c) and (d) are the same as (a) and (b), respectively, but at a density $\langle n \rangle = 0.20$.

and the phase-separated regime. From the energy competition between these states, we should be able to extract qualitative information at low densities. The states we have used are a Gutzwiller state, which becomes stable at small values of J/t, and is defined as

$$|\mathrm{GW}\rangle = \sum_{r_1,\ldots,r_{N_e}} P_d \det_\uparrow \det_\downarrow \Pi_{r_i\sigma_i} c^\dagger_{r_i\sigma_i} |0\rangle \ , \tag{2}$$

where $P_d = \Pi_i (1 - n_{i\uparrow} n_{i\downarrow})$ projects outs states with double occupancy, $\det_\sigma$ are Slater determinants of a filled Fermi sea corresponding to spin σ, and the sum in front denotes all possible electronic configurations (with the spin index omitted). N_e is the number of electrons, while the rest of the notation is standard, and follows the recent work of Valenti and Gros on variational wave functions.[34]

As superconducting condensates we use the states previously introduced by Gros *et al.*[35] For the α-wave condensate ($\alpha = s$ or d) we define

$$|\alpha\rangle \sim P_d \left[\sum_k a_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right]^{N_e/2} |0\rangle \ , \tag{3}$$

where $a_k = \Delta_k / (\epsilon_k + \sqrt{\epsilon_k^2 + \Delta_k^2})$, and $\epsilon_k = -2t(\cos k_x + \cos k_y) - \mu$ (μ is the chemical potential). The parameter $\Delta_k = \Delta_V$ corresponds to an s wave, while $\Delta_k = \Delta_V(\cos k_x - \cos k_y)$ is a $d_{x^2-y^2}$ wave. Δ_V is a $\mathbf{k}$-independent variational parameter [note that this state can be rearranged in the form of a resonating valence bond (RVB) state, see Ref. 35]. Finally, a variational state for the phase-separated region was used, which simply has all the electrons clustered in an antiferromagnetic state (whose energy density can be easily obtained from Monte Carlo calculations of the spin-$\frac{1}{2}$ Heisenberg model in two dimensions[36]).

The actual variational calculations have been carried out using the Monte Carlo technique on an 8×8 cluster, and for 10, 26, 42, and 50 electrons (that correspond to closed-shell configurations). About 10 000 Monte Carlo sweeps for each density and coupling were performed. The results for the energy of each one of these variational states are shown in Figs. 5(a)–5(c). At low electronic density $\langle n \rangle = 0.156$, Fig. 5(a) shows that the s-wave state is energetically better than the corresponding d-wave state approximately in the interval $4 < J/t < 5.5$. For smaller values of the coupling, the Gutzwiller state dominates, while for larger values of J/t the phase-separated state is stable, as expected. The dominance of s-wave correlations near phase separation at low fillings is compatible with the ideas discussed before, namely, that electrons in an otherwise empty lattice bound in s-wave states, and thus at least for $\langle n \rangle \ll 1$ and low temperatures we would expect a Bose condensation of these s-wave pairs.[20,37]

Figure 5(b) shows results for a higher electronic density $\langle n \rangle \sim 0.406$. In this case, the s wave is no longer stable, and the d wave minimizes the energy in the region $2.5 < J/t < 3.8$. This result is to be expected based on our exact diagonalization analysis near quarter-filling. Then, as a function of density a transition from s-wave to d-wave pairing has been observed. Increasing further the filling to $\langle n \rangle = 0.656$, the d-wave state still dominates be-

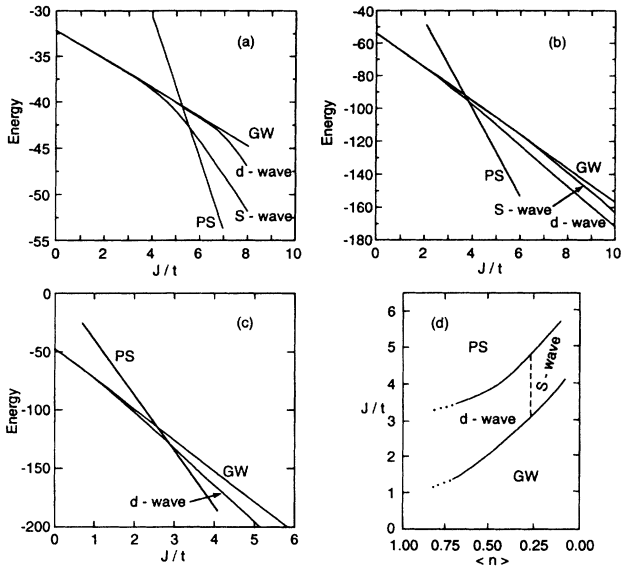

FIG. 5. Results obtained using the variational Monte Carlo technique on an 8×8 cluster applied to the 2D t-J model, as described in the text. GW corresponds to the energy of the Gutzwiller state Eq. (2), while the energies of the s and $d_{x^2-y^2}$ states are denoted by "s wave" and "d wave," respectively. The energy of the phase-separated state is labeled PS. (a) corresponds to density $\langle n\rangle=\frac{10}{64}\approx0.156$; (b) $\langle n\rangle=\frac{26}{64}\approx0.406$; and (c) $\langle n\rangle=\frac{42}{64}\approx0.656$; (d) rough phase diagram of the 2D t-J model predicted by the VMC approach.

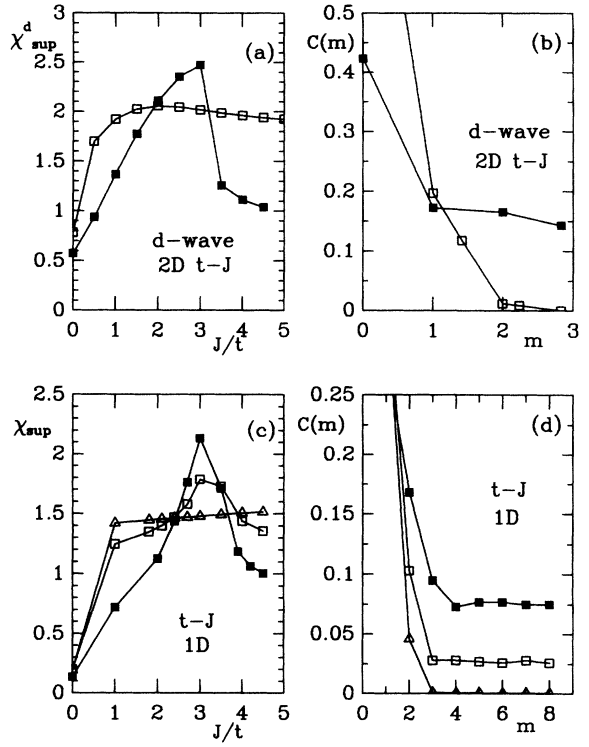

FIG. 6. (a) d-wave pairing susceptibility as a function of J/t for the 4×4 cluster. The full squares correspond to $\langle n\rangle=0.50$, while the open squares are for $\langle n\rangle=0.75$; (b) d-wave pairing correlations at $J/t=3$ and $\langle n\rangle=0.50$ (full squares); and $J/t=2$ and $\langle n\rangle=0.75$ (open squares); (c) similar results as those shown in (a), but for the 1D chain at $J/t=3$. Full squares denote results at $\langle n\rangle=0.50$, open squares at $\langle n\rangle=0.75$, and triangles at $\langle n\rangle=0.875$; (d) shows explicitly the pairing correlation as a function of distance for the 1D t-J chain, at $J/t=3$. The notation is as in (c).

tween $1.5<J/t<3.0$. A rough and qualitative phase diagram obtained with the VMC method is shown in Fig. 5(d). Results at densities close to half-filling are not shown since the variational energies for different states are very close to each other in this region, and thus corrections to each state cannot be neglected.

C. High electronic density, $\langle n\rangle>\frac{1}{2}$

After analyzing the region of small electronic density, it is important to study the more realistic regime of high densities. It is clear that the t-J model was originally introduced to qualitatively mimic the behavior of the high-T_c cuprates, and thus the physically interesting regime corresponds to small hole density (i.e., $\langle n\rangle$ slightly smaller than one), and small values of J/t (since the cuprate compounds are known to be in the strong-coupling regime, and if the one-band Hubbard Hamiltonian is used to model the materials, we should work in the region $U/t\gg1$, which corresponds to $J/t\ll1$). Then, it is quite important to carry out a numerical study for densities $\langle n\rangle>\frac{1}{2}$. The results for four holes on the 16-site cluster are shown in Figs. 6(a) and 6(b), where they are compared with the results for eight holes. The susceptibility at $\langle n\rangle=0.75$ is much flatter than at quarter-filling, and the actual correlations as a function of distance are very close to zero already at a distance of two lattice spacings. Then, our numerical results do not show indications that the interesting superconducting region observed at $\langle n\rangle\leq\frac{1}{2}$ can be extended towards the realistic regime of densities closer to half-filling.

However, we would like to point out that this negative result is not definitive. There are many arguments suggesting that a calculation similar to that of Figs. 6(a) and 6(b), but carried out on a larger lattice may show more positive signals of superconductivity. To begin with, note that the VMC calculation described in the previous section on a larger lattice still predicts the dominance of a d-wave condensate over other states. Although variational calculations are generally uncontrollable (since it is difficult to judge how accurate the trial states are), the interesting qualitative agreement found with the exact diagonalization results at other densities suggests that the wave functions we used may be quantitatively accurate. The "size" in real space of the pairing operators is another possible reason for the small correlation found in Figs. 6(a) and 6(b). In a typical BCS condensate, the size of a pair depends on the density of carriers, even with a strong local attractive potential. The lower the density, the larger the pair size to maintain the coherence among pairs. Then, it may occur that the local operator used in our study does not have a large overlap with the actual more extended pairing operator that may exist in this model.

Finally, we would like to point out an analogy between our results for the 2D lattice, and those obtained for the 1D t-J chain. As it is well known, a numerical analysis of the t-J model in one dimension has shown a region where superconducting correlations are dominant[38] in the sense that they decay the slowest as a function of distance. This region is a strip bordering phase separation (very similar to that found in our two-dimensional study), and it covers a wide range of densities between small $\langle n \rangle$, and $\langle n \rangle$ as large as 0.875. Although no long-range order can occur in 1D at any temperature, and even the statistics of the particles is not important in one dimension, since fermions and hard-core bosons produce the same phase diagram (in two dimensions the situation is drastically different, see Appendix B), the results on a chain are still very instructive to guide our intuition in the more realistic 2D problem. The 1D results are based on a study of K_ρ which is a parameter based on conformal field theory, that controls the decay of the correlation functions with distance. This quantity can be obtained from a study of spin and charge velocities, and it is believed to be affected by finite-size effects less severely than actual pair correlations. In Figs. 6(c) and 6(d) we show the pair susceptibility and correlation function for the case of eight, four, and two holes on a 16-site one-dimensional chain. The case of two holes corresponds to a nominal density $\langle n \rangle = 0.875$, i.e., where superconductivity should still be dominant. However, Fig. 6(d) clearly shows that for this density an analysis of the pair correlation shows no indications of the superconductivity dominated ground state implied by K_ρ (this is not surprising since two holes can form only one pair). This example tells us that a superconducting ground state cannot be identified easily using finite clusters when only a few number of pairs is available. It may occur that the regime of $\langle n \rangle = 0.75$ in 2D is analog to $\langle n \rangle = 0.875$ in 1D.

Thus, we conclude that due to the limitations of numerical studies based on exact diagonalizations, the regime of small hole density is difficult to analyze (unfortunately, there are no stable quantum Monte Carlo techniques to study the 2D t-J model at low temperatures). Then, we believe that in order to make further progress closer to half-filling, it would be important to develop a good variational wave function to describe the regime of quarter-filling (where results can be compared with the exact diagonalization predictions), and then carry out calculations with the same wave function at densities closer to half-filling.[39] Note also that other terms in the Hamiltonian like a t' hopping may shift the d-wave region towards even smaller densities.

D. Phase diagram of the 2D t-J model

Based on the numerical results discussed in the previous sections, we believe that the phase diagram of the two-dimensional t-J model is schematically as shown in Fig. 7. Clearly there is a large region of phase separation at large J/t for all values of the density. The boundaries of this phase are in good agreement with results from high-temperature expansions.[40] The novel result discussed in this paper, and before in Ref. 19, is the existence of a region of d-wave superconductivity (in the $d_{x^2-y^2}$ channel) that extends from low to high electronic densities, with a numerical signal that is maximized at quarter-filling (where the numbers of pairs is also maximized). Numerically it is difficult to find the boundary of the d-wave phase at large electronic densities, i.e., close to half-filling. Even the phase-separated region boundary is controversial (and thus we only write "AF" in Fig. 7 in that regime, to show that antiferromagnetic correlations are important but we do not know the details of the phase diagram). However, we have presented arguments suggesting that it may be possible that the d-wave region survives as a narrow strip following phase separation, even in the regime close to half-filling. After all, two holes in an antiferromagnetic background form a $d_{x^2-y^2}$ bound state,[15] and thus the most economical hypothesis is to link the numerical strong signals at quarter-filling with the bound states at half-filling. Of course, the verification of this hypothesis needs, and deserves, more work.

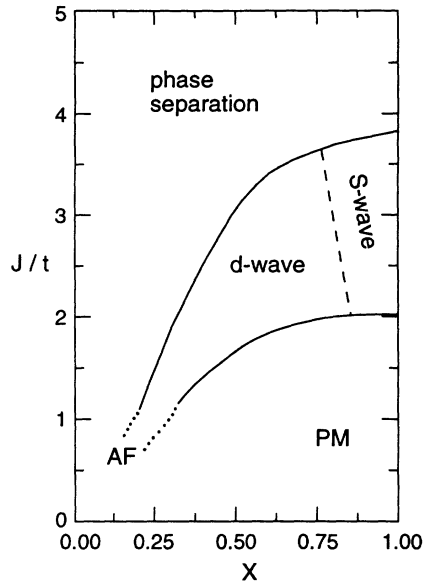

FIG. 7. Phase digram of the 2D t-J model. "d wave" denotes the phase where the $d_{x^2-y^2}$ correlations were found to be strong in the numerical study presented in this paper. "s wave" denotes the regime where the VMC approach showed the presence of a stable s-wave condensate. The dashed line separating d wave from s wave is schematic since we only have results at a small number of electronic densities. AF denotes the antiferromagnetic region close to half-filling. In this regime we do not have enough accuracy in our analysis to complete the phase diagram. The d-wave superconducting phase may or may not extend into the small J/t region. Finally, PM denotes a paramagnetic state.

In the other limit of low electronic density, an interesting change in the symmetry of the condensate is observed (which was unknown to two of us in a previous publication[19]). This is compatible with the observation that two electrons on an empty lattice form an s-wave bound state

for $J/t > 2$.[20] This region of condensed dimers may be similar to that found at large density-density repulsion $V/t \gg 1$ in previous work.[25,26] We believe that in the three-dimensional parameter space J/t, V/t, $\langle n \rangle$, the s-wave region of the pure t-J model at low electronic density, and the s-wave region at quarter-filling of the t-J-V model may be analytically connected. A similar behavior may occur in one dimension where a spin-gap phase[38,41,42] was observed at low densities for the t-J model, and at large V/t and quarter-filling for the t-J-V model.[25,26] Such a rich phase diagram certainly deserves more work. The d-wave region found in this work seems disconnected from those two limiting cases with s-wave symmetry, and should be considered as a new phase. Finally, the paramagnetic PM region resembles much a noninteracting gas of particles (and thus a Fermi liquid, at least at low densities), but a careful study of the wave-function renormalization Z is needed to clarify this issue.

It is important to remark that the region of s-wave superconductivity at small electronic density shown in Fig. 7 may be larger than what is shown in the figure. In constructing the boundary of phase separation in Fig. 7 we used the discrete version of the second derivative of the ground state with respect to density. However, the error bars at small $\langle n \rangle$ are large using this procedure. Then, in the region $\langle n \rangle \ll 1$ we used the results obtained from the high-temperature expansions[40] to complete the boundary of phase separation. Although with this technique the study of pairing correlations has not been addressed yet, their predictions for the phase-separation boundary seem accurate at intermediate densities where the results can be contrasted with exact diagonalization predictions. Nevertheless, here we want to warn the reader that if the formation of a bound state of four electrons on an otherwise empty lattice is used as a criterion for phase separation, then the critical value near the empty system becomes $J/t = 4.85$ as claimed by Lin,[32] instead of a number slightly smaller than four as shown in Fig. 7. In addition, using exact diagonalization methods we have evaluated the energy of the ground state at a fixed and low electronic density, and from there calculated numerically the second derivative with respect to the coupling J/t to search for indications of a phase transition. Our results suggest that phase separation may start at J/t as large as ~ 5.5. Then, the error bars at small density of the phase diagram Fig. 7 may be large. More work is needed to obtain quantitative results, but nevertheless we believe that the qualitative features of the phase diagram are properly captured by our prediction Fig. 7.

III. STUDY OF THE t-U-V MODEL

To continue our study of electronic models and the presence of superconductivity near phase separation, let us consider the t-U-V model on a square lattice. This model is the standard one-band Hubbard model extended to include a nearest-neighbor density-density interaction (in the study below we will analyze both an attractive and repulsive V term). There are several reasons to consider this model in detail. First, it will illustrate the conjecture presented in this paper, namely, the rule that superconducting phases of purely electronic models typically appear near a regime of phase separation. Actually, we will discuss below that even for the attractive Hubbard model, which naively seems to superconduct without phase separation in its phase diagram, a small negative V term is enough to induce an instability towards phase separation. Thus, even the attractive Hubbard model, and thus the BCS model satisfies the rule described above in an extended parameter space (keeping the attractive character of the potential). In addition, we have found that one of the superconducting phases of this model corresponds to a $d_{x^2-y^2}$ condensate. The possible existence of d-wave superconductivity in the high-temperature superconductors has recently received considerable attention.[43,16] Then, it becomes important to have a toy model with a condensate in this d channel for further studies of its dynamical properties.[44] Finally, we believe that a possible effective model to describe holes in the t-J model will include an attractive density-density interaction at distance of one lattice spacing, and a strong repulsion on site. Such an effective interaction is natural at least in the large J/t limit where two holes form a tight bound state at a distance of one lattice spacing (and of course, they cannot occupy the same site). Then, the t-U-V model in strong coupling, with $V<0$ and $U \gg 1$ is a natural candidate for such an effective theory.[45] The fact that indeed it produces a $d_{x^2-y^2}$ condensate gives more support to this conjecture.

The t-U-V model is defined as

$$H = -t \sum_{\langle ij \rangle} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_{i} (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}) + V \sum_{\langle ij \rangle} (n_i - 1)(n_j - 1) , \quad (4)$$

where the notation is standard. It is assumed in this section that we are working on an $N \times N$ cluster with periodic boundary conditions. The study will be limited to the half-filled density, which is enough to illustrate our main results. In this regime, the mean-field approximation used to describe the spin-density-wave (SDW) state of the repulsive Hubbard model is expected to provide reliable information also for the t-U-V model.[46] Since our analysis goes beyond the Hubbard model to include a density-density V interaction, new phases are expected to appear in parameter space, and thus in addition to a mean field for the SDW state, we will discuss a generalization for a charge-density wave (CDW), an s-wave BCS superconducting state (SS), and a d-wave superconducting state (DS). The appearance of SDW, CDW, and SS orders are natural since they can be obtained by perturbation theory starting from the atomic limit ($t=0$) in the regimes $V=0$, $U \gg 1$; $U=0$, $V \gg 1$; and $V=0$, $U<0$, $|U| \gg 1$, respectively. On the other hand, the d-wave phase is more difficult to predict intuitively.[47] Finally, a regime with phase separation (PS) exists when $V<0$ and $|V| \gg 1$. In this region, the energy is minimized by forming a large cluster of double occupied sites. Of course, numerical techniques like those presented in the previous sections are important to verify the accuracy of the rough mean-field predictions. For example, it is clear that the

region of phase separation will not present such a sharp division between the region with double occupancy and the empty part of the lattice, especially at finite V. However, the computer work for this model is highly nontrivial, and such an analysis will be postponed for a future publication.

Here, we will briefly describe the mean-field approach for the case of the SDW and CDW states.[46] For more details see Ref. 48. First, let us rewrite exactly the interaction term of Eq. (4) in momentum space as

$$H^{UV}=U\sum_{i} n_{i\uparrow}n_{i\downarrow}+V\sum_{\langle ij\rangle} n_i n_j$$
$$=\frac{U}{4N}\sum_{q}(n_q n_{-q}-\sigma_q^z\sigma_{-q}^z)+\sum_{q} V(q)n_q n_{-q}\ , \qquad (5)$$

where we have introduced the standard definitions of the density and spin operators, namely, $n_q=\sum_{k\sigma} c^{\dagger}_{k+q\sigma}c_{k\sigma}$ and $\sigma_q^z=\sum_{k\sigma}\sigma c^{\dagger}_{k+q\sigma}c_{k\sigma}$. The potential in the density-density interaction is of the form $V(q)=(V/N)(\cos q_x+\cos q_y)$, and we have used the definition $c^{\dagger}_{k\sigma}=(1/\sqrt{N})\sum_j e^{ik\cdot j}c^{\dagger}_{j\sigma}$ in the Fourier transformation. For the mean-field approximation corresponding to a SDW state, we introduce the ansatz $\langle n_{i\sigma}\rangle=\frac{1}{2}[1+\sigma S(-1)^{i_x+i_y}]$ [where S is a parameter whose value will be fixed by energy minimization, and $i=(i_x,i_y)$], which after some straightforward algebra can be shown to be equivalent to $\langle\sigma_q^z\rangle=SN\delta_{q,Q}$, where $Q=(\pi,\pi)$. In addition, the constraint that in mean value there is only one particle per site in the ground state at half-filling, can be formally expressed as $\langle n_q\rangle=N\delta_{q,0}$. For the CDW, the proposed ansatz is $\langle n_{i\sigma}\rangle=\frac{1}{2}[1+\rho(-1)^{i_x+i_y}]$, which is σ independent, and ρ is a mean-field parameter similar to S for the SDW. Such an ansatz is equivalent to requiring that $\langle n_q\rangle=N\delta_{q,0}+\rho N\delta_{q,Q}$, and $\langle\sigma_q^z\rangle=0$, in the mean-field ground state.

Neglecting higher-order terms in the corrections to the mean-field values, the interaction Eq. (5) becomes

$$H_{MF}^{UV}=-\frac{U}{4N}\sum_{q}(\langle n_q\rangle\langle n_{-q}\rangle-\langle\sigma_q^z\rangle\langle\sigma_{-q}^z\rangle)$$
$$+\frac{U}{2N}\sum_{q}(n_q\langle n_{-q}\rangle-\sigma_q^z\langle\sigma_{-q}^z\rangle)$$
$$+\sum_{q} V(q)(-\langle n_q\rangle\langle n_{-q}\rangle+2\langle n_{-q}\rangle n_q)\ . \qquad (6)$$

Specializing now for the SDW state, the whole Hamiltonian Eq. (4) is given by

$$H_{MF}=\sum_{k\sigma}\epsilon_k c^{\dagger}_{k\sigma}c_{k\sigma}-\Delta\sum_{k\sigma}\sigma c^{\dagger}_{k+Q\sigma}c_{k\sigma}+\frac{US^2N}{4}\ , \qquad (7)$$

where $\epsilon_k=-2t(\cos k_x+\cos k_y)$, the gap $\Delta=US/2$, and $\sigma=+1(-1)$ for spin up (down). After a standard Bogoliubov diagonalization of Eq. (7), the ground-state energy is

$$\frac{E_{g.s.}^{SDW}}{N}=-\frac{1}{N}\sum_{k}\sqrt{\epsilon_k^2+\Delta^2}+\frac{\Delta^2}{U}\ , \qquad (8)$$

from which we obtain the self-consistent equation,

$$\frac{1}{2N}\sum_{k}\frac{1}{\sqrt{\epsilon_k^2+\Delta^2}}=\frac{1}{U}\ , \qquad (9)$$

which has a solution for $U>0$ (note that this equation is independent of V at this level of approximation).

The procedure to obtain results for the CDW case is very similar to that followed for the SDW state, and thus we will not repeat it here. The ground-state energy is given by

$$\frac{E_{g.s.}^{CDW}}{N}=-\frac{1}{N}\sum_{k}\sqrt{\epsilon_k^2+\Delta^2}-\frac{\Delta^2}{U-8V}\ , \qquad (10)$$

where we have defined $\Delta=\rho(U-8V)/2$. The self-consistent equation for the CDW state is equal to Eq. (9) if U is replaced by $-U+8V$. The same occurs for the energy, and thus it is clear that the SDW and CDW states will cross at the line $U=-U+8V$, i.e., if $U=4V$, where both U,V are positive. Note also that the results for SDW in the $V=0$, positive U axis are identical to those of the CDW state in the $V=0$, negative U axis, if U is replaced by $-U$. This symmetry is correct even in an exact treatment, since the repulsive Hubbard model can be exactly mapped into the attractive Hubbard model.[18]

Now, let us consider the possibility of superconductivity in the phase diagram. While it is well known that in the $V=0$ and negative U axis, an s-wave condensate exists, other channels may become stable when the on-site attraction is not too strong. The formalism to handle superconductivity at the mean-field level is very standard, and thus we will describe it only schematically. To begin with, it is important to exactly rewrite the interaction term defined in Eq. (5) as

$$H^{UV}=\sum_{pp'q\sigma\sigma'}\left[\frac{U}{2N}\delta_{\sigma-\sigma'}+\frac{V}{N}[\cos(p-p')_x+\cos(p-p')_y]\right]c^{\dagger}_{p\sigma}c^{\dagger}_{-p+q\sigma'}c_{-p'+q\sigma'}c_{p'\sigma}\ . \qquad (11)$$

In Eq. (11) it is convenient to further separate the interaction in two pieces. One of them corresponds to $q=0$, and $\sigma'=-\sigma$, which will lead to the interesting superconducting properties of the ground state. The other terms corresponding to $q\neq 0$ can be rewritten in the mean-field approximation, and after some algebra they become $-UN/4-2NV+(U/2+4V)\hat{N}$, where $\hat{N}$ is the total number operator (in order to implement the constraint of working at half-filling we have explicitly used $\langle n_q\rangle=N\delta_{q0}$). Remember that once the Hamiltonian is

written in a particle-hole symmetric form as in Eq. (4), there is no need to introduce a chemical potential to implement the constraint of working at half-filling. Adding together the potential and kinetic energy of t-U-V Hamiltonian we arrive at

$$H \approx \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{p}\mathbf{p}'\sigma} c^{\dagger}_{\mathbf{p}\sigma} c^{\dagger}_{-\mathbf{p}-\sigma} c_{-\mathbf{p}'-\sigma} c_{\mathbf{p}'\sigma} f(\mathbf{p}-\mathbf{p}') , \tag{12}$$

where

$$f(\mathbf{p}-\mathbf{p}') = \frac{U}{2N} + \frac{V}{N}[\cos(p-p')_x + \cos(p-p')_y] .$$

To proceed with the mean-field treatment, we make the standard ansatz $\langle c^{\dagger}_{\mathbf{p}\uparrow} c^{\dagger}_{-\mathbf{p}\downarrow} \rangle = \langle c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} \rangle = \phi_{\mathbf{p}}$, where ϕ is a real function. The superconducting order parameter is introduced as

$$\Delta_{\mathbf{p}} = -2 \sum_{\mathbf{k}} f(\mathbf{p}-\mathbf{k}) \phi_{\mathbf{k}} . \tag{13}$$

$\Delta_{\mathbf{p}}$ is also real, although a generalization to a complex order parameter is very simple. With these assumptions, the Hamiltonian Eq. (12) can be written in the mean-field approximation as

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}\sigma} c_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{1}{2} \sum_{\mathbf{k}\sigma} \sigma \Delta_{\mathbf{k}} (c_{-\mathbf{k}-\sigma} c_{\mathbf{k}\sigma} + c^{\dagger}_{\mathbf{k}\sigma} c^{\dagger}_{-\mathbf{k}-\sigma}) + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \phi_{\mathbf{k}} . \tag{14}$$

The diagonalization of Eq. (14) is performed following standard techniques, and thus we simply present the results. The ground-state energy is

$$\frac{E_{\mathrm{g.s.}}}{N} = \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \phi_{\mathbf{k}} - \frac{1}{N} \sum_{\mathbf{k}} \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}} , \tag{15}$$

and the self-consistent equation obtained from minimization of the ground-state energy is

$$\Delta_{\mathbf{p}} = -\sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}} f(\mathbf{k}-\mathbf{p})}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}}} . \tag{16}$$

Now, let us specialize the generic results, Eqs. (15) and (16), to the particular case of an isotropic s-wave condensate (SS). This symmetry is certainly relevant for the attractive Hubbard model ($V=0$, $U<0$). For an s wave we can assume $\Delta_{\mathbf{p}}$ to be $\mathbf{p}$ independent, and the self-consistent equation formally becomes again Eq. (9), replacing U by $-U$. The s-wave ground-state energy is

$$\frac{E^{\mathrm{SS}}_{\mathrm{g.s.}}}{N} = \frac{\Delta^2}{|U|} - \frac{1}{N} \sum_{\mathbf{k}} \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2} . \tag{17}$$

Note that this energy, and thus the self-consistent equation derived from it, are independent of V, as in the case of the SDW state. As explained before, it is also interesting to notice that for the purely attractive Hubbard model ($V=0$, $U<0$) the energy of the CDW state and the superconducting SS state are degenerate. This is to be expected since by a simple transformation the attractive and repulsive Hubbard models can be mapped into each other. The CDW (SS) correlations become the spin correlations in the Z (XY) direction. By rotational invariance, the Z and XY spin correlations are identical in the repulsive Hubbard model, implying the degeneracy of the CDW and SS states for the attractive case, even in an exact treatment of the problem.

The gap equation, Eq. (16), also admits solutions in channels other than s wave. Let us consider the ansatz $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y)$ that corresponds to a $d_{x^2-y^2}$ superconductor (Δ_0 is assumed to be momentum independent, and will be obtained by self-consistency). After considerable but straightforward algebra, we arrive to the self-consistent equation for Δ_0:

$$\frac{1}{|V|} = \frac{1}{N} \sum_{\mathbf{k}} \frac{\cos k_x (\cos k_x - \cos k_y)}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_0 (\cos k_x - \cos k_y)^2}} . \tag{18}$$

This equation can be solved iteratively for Δ_0. The ground-state energy for this condensate is

$$\frac{E^{\mathrm{DS}}_{\mathrm{g.s.}}}{N} = \frac{\Delta^2_0}{|V|} - \frac{1}{N} \sum_{\mathbf{k}} \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_0 (\cos k_x - \cos k_y)^2} . \tag{19}$$

Whether this d-wave state becomes stable or not in some region of parameter space depends on its energy competition with the other possible states. Finally, in the region $V<0$ (and for large $|V|$), there is phase separation, i.e., it is energetically preferable to separate the lattice into a region mostly without electrons, and a region where every site is doubly occupied. In this way, the dominant V term of that regime is minimized. Including fluctuations, the separation between the two regions will not be sharp and it may occur that the two dominant states have densities $\langle n \rangle = 1+\delta$ and $1-\delta$, with the parameter δ different from 1 for a finite value of $|V|$. Preliminary quantum Monte Carlo results support this scenario. However, for our rough mean-field approximation, we will assume a "perfect" phase separation with $\delta = 1$ (i.e., where electrons are simply not allowed into the empty part of the lattice), and thus the ground-state energy is simply

$$\frac{E^{\mathrm{PS}}}{N} = \frac{U}{4} + 2V . \tag{20}$$

The phase diagram of the t-U-V model in the mean-field approximation is obtained by comparing the energies of the SDW, CDW, SS, DS, and PS phases given by Eqs. (8), (10), (17), (19), and (20), respectively. The results are presented in Fig. 8, showing that the phase diagram at half-filling is very rich. In the purely repulsive Hubbard regime and its neighborhood, the SDW state has the lowest energy, as expected. Increasing V a transition to the CDW regime is found at $U=4V$, as was explained before. This CDW phase is very robust and is stable also in the presence of a negative U term. Actually, in the purely attractive Hubbard model axis, the CDW state is degenerate with the superconducting state SS. If a small and negative V term is introduced, then this SS state becomes stable, and the CDW-SS degeneracy is broken. However, decreasing further the strength of V (towards more negative values), induces another transition into a

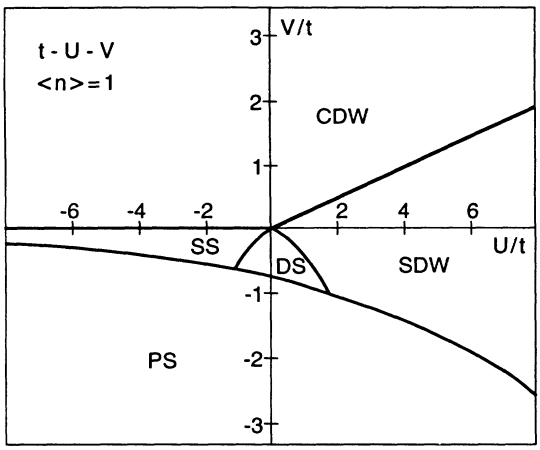

FIG. 8. Phase diagram of the t-U-V model in the mean-field approximation, at half-filling. SDW denotes a spin-density-wave state, CDW a charge-density wave, PS corresponds to phase separation, while SS and DS are superconducting states with s and $d_{x^2-y^2}$ symmetry, respectively.

phase-separated regime. Thus, in this model we also observe the feature discussed in the Introduction, namely, that a superconducting phase appears in the neighborhood of phase separation, as it occurs in the 2D t-J model. In this case it is necessary to extend the parameter space beyond an on-site attractive U/t term, to include further attractive interactions at a distance of one lattice spacing in order to observe this behavior. Such an extension is natural, since a strictly on-site force is somewhat pathological and physically difficult to realize.[49] Phase separation is very robust in this model as shown in Fig. 8, and it exists even for large and positive values of U/t. Finally, it is interesting to observe the presence of an "island" in parameter space where the $d_{x^2-y^2}$ state is stable. This occurs for small values of $|U|$, and negative V. Again, increasing further $|V|$ leads to an instability towards phase separation. Note that for large values of U/t, there is a direct transition from SDW to phase separation. Then, finding phase separation in a given model is not sufficient to guarantee the presence of superconducting in its vicinity. More details about the interesting phase diagram shown in Fig. 8, especially regarding the d-wave condensate, will be presented in a future publication.

IV. TWO-BAND HUBBARD MODEL ON A CHAIN

The presence of superconductivity near phase separation is not restricted to one-band models. The same phenomenon occurs in the ground state of multiband Hamiltonians, and in this section we analyze a particular (and physically relevant) case in detail. The model we will study is the three-band model proposed by Emery,[47] and Varma and collaborators,[50] which is believed to contain the basic ingredients to describe the behavior of electrons in the CuO_2 planes of the high-T_c superconductors. Using the *hole* notation, where the vacuum is defined as having all the d orbitals occupied in the copper sites and the p orbitals occupied in the oxygen sites, the Hamiltonian is

$$H=-t_{pd}\sum_{\langle ij\rangle}p_j^{\dagger}(d_i+\text{H.c.})+\epsilon_d\sum_i n_i^d+\epsilon_p\sum_j n_j^p + U_d\sum_i n_{i\uparrow}^d n_{i\downarrow}^d+U_p\sum_j n_{j\uparrow}^p n_{j\downarrow}^p+V\sum_{\langle ij\rangle}n_i^d n_j^p\ , \quad (21)$$

where p_j are fermionic operators that destroy holes at the oxygen sites labeled j, while d_i corresponds to hole annihilation operators at the copper sites i. $\langle ij\rangle$ refers to pairs of nearest-neighbors i (copper) and j (oxygen) sites (and t_{pd} is the corresponding hybridization between copper and oxygen). U_d and U_p are positive constants that represent the repulsion between holes when they are located at the same d and p orbitals, respectively. V corresponds to the Coulombic repulsion when two holes occupy adjacent Cu-O links. The importance of this term has been remarked by Varma and collaborators.[50] In principle, interactions at larger distances should also be included in the Hamiltonian, but such an analysis will not be carried out in this paper.[51] ϵ_d and ϵ_p are the energies of each orbital (with the charge-transfer constant defined as $\Delta=\epsilon_p-\epsilon_d$, which for the cuprates is a positive number). The doping fraction is defined as $x=n_h/N$, where $n_h=(N_h-N)$ is the number of holes doped away from half-filling, N_h is the total number of holes, and N is the number of Cu-O cells. At half-filling $N_h=N$, as in the insulating parent cuprates. Below, only the region $0\le x\le 1$ will be explored which is relevant for hole-doped materials.

It is generally accepted that U_d is the largest parameter of the model. In particular, $U_d>\Delta$, which is consistent with the charge-transfer character of the copper oxides. It is also generally accepted that in the undoped case there is one hole in each Cu site, while upon doping, additional holes are introduced into the oxygen sites. Under these assumptions (supplemented with $V=0$), Zhang and Rice[52] derived the t-J model as an effective low-energy Hamiltonian of the more general three-band model. In the region of parameter space where this derivation is valid, the conclusions we reached for the t-J model in the previous sections will also apply to the more general Emery-Varma Hamiltonian Eq. (21). However, the three-band model is more general than the t-J model and thus it is worth exploring the behavior of its ground state in regions of parameter space that cannot be mapped into a simplified one-band Hamiltonian. For example, in the particular case $U_d=\infty$, an interesting regime of phase separation was studied with the slave-boson approach for finite V, and superconducting instabilities were observed in its vicinity.[22] Then, phenomena similar to those described in Secs. II and III also take place in the multiband Hubbard model.

Recently, a more detailed study of superconductivity near phase separation in the Emery-Varma model was discussed using exact diagonalization techniques[53–55] applied to the one-dimensional version of Eq. (21) (i.e., for the "two-band" Hubbard model). Part of the results of these studies (which go beyond the mean-field approxima-

tion) are summarized in Fig. 9. In this figure, the copper (oxygen) sites are represented by large (small) circles. The ground state at half-filling ($n_h=0$) is shown in the atomic limit $t_{pd}=0$ in Fig. 9(a) (where the direction of the spins is arbitrary). There is one hole per copper site. Figure 9(b) shows the ground state introducing two holes ($n_h=2$) and assuming $V<\Delta+\frac{3}{4}U_p$. In this case the holes populate the oxygen sites. However, if $V>\Delta+\frac{3}{4}U_p$, the ground state drastically changes to the one shown in Fig. 9(c), where in addition, it is assumed that $U_d>\frac{3}{2}(U_p+2\Delta)$, otherwise doped holes would prefer to be located in copper sites in the limit $V=\infty$. In this case, the electrons tend to occupy the oxygens depopulating the coppers.

In Fig. 9(c), the minimum energy is obtained by the formation of "biexcitons" (in the language of Ref. 53), and thus a charge-transfer instability from copper to oxygen ions occurs. This same phenomenon takes place in two dimensions as shown in Fig. 9(d) also for the case of $n_h=2$, and large V. When additional holes are added to the system, the region of doubly occupied oxygens increases in size. Then, the nearest-neighbor repulsion V leads to the formation of tight hole bound states at the oxygen sites. In turn, this leads to phase separation which occurs between a phase with a density of one particle per cell (with the charges on the copper sites), and a region of density of two particles per cell (with all the charge on oxygens). However, remember that the results summarized in Fig. 9 were obtained in the atomic limit. When $t_{pd}\neq 0$ the actual phase boundaries, and even the existence of phase separation, depends on the interplay between the kinetic energy and the Coulomb terms. In order to study this interplay, exact diagonalization techniques were recently applied[54,55] to finite chains for particular values of the parameters of the two-band model. Indications of superconductivity were observed in a special region of parameter space by studying the value of the parameter K_ρ used in conformal field theory, and by the analysis of the anomalous flux quantization in the presence of an external flux through the ring (i.e., closing the chain with periodic boundary conditions).

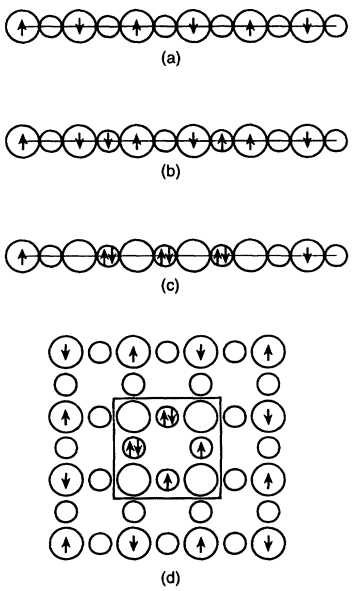

FIG. 9. Ground state of the two-band model for different densities and couplings in the atomic limit. (a)–(c) are in one dimension, while (d) is in two dimensions. (a) half-filling $n_h=0$; (b) $n_h=2$ and $V<\Delta+\frac{3}{4}U_p$; (c) $n_h=2$ and $V>\Delta+\frac{3}{4}U_p$; (d) $n_h=2$ and large V.

In this section, we also use Lanczos diagonalization techniques to obtain ground-state properties of the one-dimensional version of Eq. (21), and analyze further the interplay between superconductivity and phase separation, according to the ideas discussed in the introduction. Due to the rapid growth of the Hilbert space of the problem with the chain size, our analysis is limited to six cells (12 sites), periodic boundary conditions, and $n_h=2$, 4, and 6 holes. In order to work in the regime of hole pairing in oxygen sites, we select $U_d=7$, $U_p=0$, and $\Delta=1.5$, all in units of the hopping integral t_{pd}. The parameters satisfy the relation $U_d>\frac{3}{2}(U_p+2\Delta)$, and are similar to those used by Sudbo *et al.*[54] The parameter V is varied between 0 and 8, which is large enough to reach the phase-separated regime. A quantitative indication of the charge transfer from Cu to O sites, and eventually of phase separation, is given by the average occupation of oxygen sites. Alternatively, a more clear indicator of the crossover from the state shown in Figs. 9(b) and 9(c) is given by the susceptibility $\chi_{ps}=\langle n_O^2\rangle-\langle n_O\rangle^2$ (see Ref. 56). This quantity is maximized when a transfer of charge from copper to oxygen takes place, i.e., at the phase-separation transition, and then it slowly decays to zero at large V once phase separation has already occurred, since the fluctuations in the occupation number of the oxygens vanish in this limit. An independent determination of the crossover to the phase-separated regime is given by the short-wavelength component of the susceptibility associated with the correlations of pairs of holes in the oxygen sites.[57] This quantity (that we called X) is normalized such that it is equal to 1 for $V\rightarrow\infty$ if the phase-separated state Fig. 9(c) is reached in this limit. For details see Ref. 57.

The numerical results for the susceptibility χ_{ps} are shown in Fig. 10(a) for the case of two holes $n_h=2$, and hopping $t_{pd}=0.5$, and $t_{pd}=1$. In the atomic limit ($t_{pd}=0$), the crossover between the two states is sharp, and takes place at $V=\Delta=1.5$ (not shown in the figure). For a fixed Δ, the value of V at which the crossover occurs increases with $t_{\rm pd}$, and it is located between $2\leq V\leq 3$ for $t_{pd}=1$. The order parameter X has its maximum variation also in the same interval, making the results compatible among themselves and with the simple picture shown in Figs. 9(a)–9(d). On the other hand, the results corresponding to $n_h=4$ are very different. The order parameter X does not saturate to 1 at large V, and the occupation number of oxygen sites is maximized in this limit (i.e., apparently there is no occupancy of the copper sites). However, this result is a finite-size effect. To visualize this problem, simply add two more holes to the six cells chain shown in Fig. 9(c). In the atomic limit the possible states are five double-occupied oxygens or four

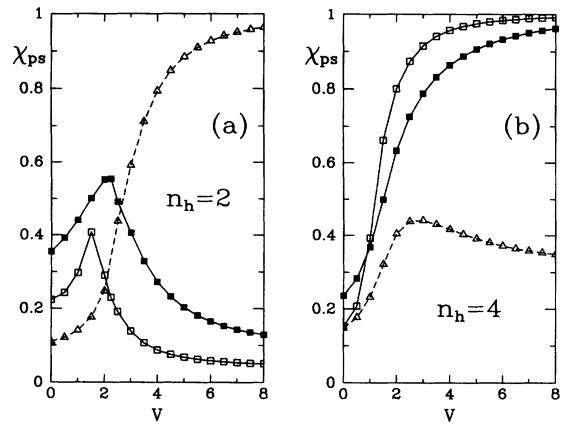

FIG. 10. (a) χ_{ps} (defined in the text) as a function of V, for $U_d=7$, $U_p=0$, and $\Delta=1.5$, on a six-cell cluster with eight holes (i.e., $n_h=2$). The open squares are results for $t_{pd}=0.5$, while the full squares correspond to $t_{pd}=1$. The triangles joined by dashed lines correspond to the order parameter X used in Ref. 57; (b) is the same as (a) but with 10 holes, i.e., $n_h=4$.

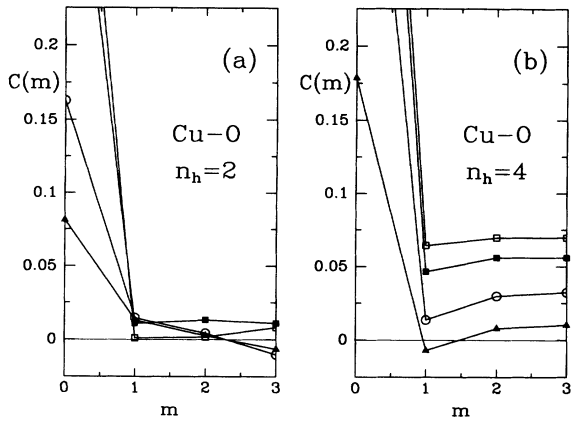

FIG. 11. (a) Pairing correlations $C(m)$ (defined in the text) as a function of distance for the one-dimensional Cu-O model with $n_h=2$ at $U_d=7$, $U_p=0$, $\Delta=1.5$, and $t_{pd}=1$. The full triangles, open circles, full squares, and open squares correspond to $V=0.0$, 2.0, 4.0, and 8.0, respectively; (b) same as (a) but for $n_h=4$.

double-occupied oxygens and two single-occupied oxygens, and thus strictly speaking the phase-separated regime defined before cannot be realized due to the particular size of the chain, and the five pairs of holes have a finite mobility (as in a doped attractive Hubbard chain). This effect does not occur on a larger chain (as an example consider 20 holes on a 12-cell chain which keeps the density constant). Then, the results of Fig. 10(b) should not be considered representative of the bulk limit, and they are shown here mainly as a warning to the reader that finite-size effects have to be carefully controlled in these numerical studies.

In order to study the existence of a superconducting phase arising from the mechanism of hole pairing at the oxygen sites, we studied the pairing correlation

$$C(m)=\frac{1}{N}\sum_j \langle \Delta_{j+m}^{\dagger}\Delta_j \rangle \ , \tag{22}$$

where the pairing operator is defined as $\Delta_j=c_{j\uparrow}c_{j\downarrow}$, and j denotes oxygen sites. The results for the pairing correlations corresponding to the chain of six cells, and the same values of parameters as used in Fig. 10(b), are shown in Fig. 11(a) for $n_h=2$, at several values of V. It can be seen that the pairing correlation at the largest distance slowly increases with V up to $V=4$ (measured with large steps in V of 2 in units of t_{pd}), i.e., approximately in the crossover to the phase-separated regime. At $V=6$, phase separation has been reached and the double-occupied oxygen sites are in contiguous sites forming a rigid structure with very low mobility. Consequently, the pairing correlations are suppressed at large V. Then, Fig. 11(a) shows a behavior qualitatively very similar to those reported before for the t-J model and the t-U-V model, i.e., the region where superconducting correlations exist in the vicinity of phase separation. However, note that the size of the tail in the pairing correlation is much smaller than that observed for the t-J model in one and two dimensions.[26,19] Actually, we measured the pairing correlations at the same parameters used before by Sudbo *et al.*,[54] and also in the superconducting region studied by Sano and Ono[55] in the $U_d=\infty$ limit. We observed that the tail in $C(m)$ is negligible in both cases (perhaps due to a competition with a charge-density-wave state), and thus only the conformal field theory parameter K_ρ is left for the analysis of pairing in this region (it is expected that K_ρ will present smaller finite-size effects than the actual correlations). This is unfortunate since to study other properties of the superconducting condensate (specially dynamical properties) it is important to have robust pairing correlations developed in the ground state of the clusters that can be studied numerically. Note also that the superfluid density does not exist in one dimension since for its definition a careful two-dimensional limit in the current correlations needs to be considered,[58] as mentioned briefly in Appendix A. One should be careful in not confusing the Drude weight and the superfluid density which are obtained from very similar current correlations.

In Fig. 11(b), the results corresponding to $n_h=4$ are shown, again for several values of V. The pairing correlations are clearly more robust than those shown at smaller hole doping in Fig. 11(a). However, this effect is unfortunately spurious and caused by the finite size of the chain as discussed before. The 10 holes prefer to be located on oxygen sites, with none on copper sites, and thus the oxygen pairs have enough mobility to induce a robust pairing signal. We are currently investigating the possibility of enlarging the range of the repulsive density-density interaction in order to stabilize the results of Fig. 11(b). Work is in progress. Finally, in the case $n_h=6$ all oxygen sites are doubly occupied in the large V limit, and we observed that $C(m)$ decays to zero rapidly with distance as expected.

In short, a numerical analysis of the two-band Hubbard model on a chain roughly shows a behavior similar to that of the t-J model in 1D and 2D, and of the t-U-V model, namely, the presence of superconducting correla-

tions near half-filling. A study of the same phenomenon for a three-band model in 2D would be important.

V. CONCLUSIONS

In this paper we have analyzed several models of correlated electrons using both numerical and analytical techniques. In particular, we search for superconducting phases as a function of couplings and densities. Our main result is that the two-dimensional t-J model has a region of $d_{x^2-y^2}$ superconductivity near phase separation centered at a density of quarter-filling $\langle n \rangle = \frac{1}{2}$. In addition, an interesting transition from d-wave to s-wave superconductivity was observed reducing the electronic fermionic density. Although the presence of the d-wave superconducting phase for realistic densities remains unclear, we argued that numerical studies in this region may be affected by the small number of pairs contributing to the signal. Then, we believe that the possibility of finding superconductivity in this model in the realistic region of small J/t and densities close to half-filling is still open. The most favorable channel in this region is clearly $d_{x^2-y^2}$. Now that superconductivity has been identified in the phase diagram, we believe that the most suitable procedure to follow is to describe the quarter-filling region with a variational wave function of condensed d-wave pairs, such that a good agreement with the numerical work is found, and then the variational calculation should be repeated at other densities on larger clusters.

In addition, in this paper we conjectured that the presence of superconductivity near phase separation observed for the t-J model may be a general feature of several models of correlated electrons. To explore this possibility we studied analytically the t-U-V model in two dimensions at half-filling. Indeed, we observed superconductivity near phase separation in the regime of attractive couplings. For large and negative U the condensate is s wave, while increasing U it becomes $d_{x^2-y^2}$, as for the t-J model. We also observed signals of superconductivity near phase separation for the one-dimensional two-band Hubbard model. In this case the analysis was done using numerical methods. As a rule of thumb, we believe that once an electronic model is proposed to describe a superconducting material, first it is convenient to search for indications of phase separation in the phase diagram, which is usually not very difficult, and then superconductivity should be analyzed in its boundary. This rule seems to work in all models of correlated electrons that we are aware of (at least those with finite-range interactions).

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APPENDIX A: STUDY OF THE SUPERFLUID DENSITY

For completeness, in this appendix we remind the reader of an alternative way to characterize a superconducting phase. In the bulk of this paper, we have used the existence of long-range order in the equal-time pairing correlation as an indication of superconductivity. However, there is another approach that does not involve the study of different symmetry sectors. This technique consists in the evaluation of the "superfluid density" D_s in the region of interest. It has been recently shown[58] that this quantity can be obtained on a finite cluster following steps similar to those necessary to calculate the Drude weight.[5] Actually, it can be shown that

$$\frac{D_s}{2\pi e^2} = \frac{\langle -T \rangle}{4N} - \frac{1}{N} \sum_{n \neq 0} \frac{1}{E_n - E_0} |\langle n | j_x(\mathbf{q}) | 0 \rangle|^2 , \tag{A1}$$

where e is the electric charge, the current operator in the x direction with momentum $\mathbf{q}$ is given by

$$j_x(\mathbf{q}) = \sum_{l,\sigma} e^{i\mathbf{q}\cdot l} (\bar{c}^{\dagger}_{l,\sigma} \bar{c}_{l+\hat{x},\sigma} - \bar{c}^{\dagger}_{l+\hat{x},\sigma} \bar{c}_{l,\sigma}) ,$$

$\langle -T \rangle$ is the mean value of the kinetic energy operator of the model under study, $|n\rangle$ are eigenstates of the Hamiltonian with energy E_n (where $n=0$ corresponds to the ground state), and the rest of the notation is standard. The momentum $\mathbf{q}=(q_x,q_y)$ of the current operator needs to be selected such that $q_x=0$ and $q_y \to 0$. The constraint of having a small but nonzero q_y is necessary to avoid a trivial cancellation of D_s due to rotational and gauge invariance.[58] On the 4×4 cluster, the minimum value of q_y is $\pi/2$, which unfortunately is not small. D_s given by Eq. (A1) can be evaluated numerically using a continued fraction expansion technique.[5]

Results for D_s have already been presented for the 2D t-J model close to phase separation in Ref. 19. The superfluid density has a clear peak in the same region where the pairing correlations are maximized. Thus, the results obtained with these quantities are consistent with each other, and they support the conclusion that a superconducting phase exists in the 2D t-J model. Note also that in Ref. 19 it was shown that the *Drude* peak is very large not only in the superconducting phase, but also for smaller values of J/t. This is to be expected since a small resistivity (actually zero in the bulk limit) does not uniquely mean that the system superconducts, since a perfect metal has also zero resistivity. For details see Refs. 19, 58, and 4.

It is interesting to remark that we have carried out a

study of D_s in the one-band Hubbard model with a repulsive interaction on a 4×4 cluster.[59] Unfortunately, we have not observed any indication of superfluidity in this model based on D_s. Since other groups may attempt such a study, it would be helpful for them to have some numerical results to compare with, and thus we provide them here: working at $U/t=8$ (which is the most realistic region of parameter space for the one-band Hubbard model as a model of high-T_c cuprates), and at the representative density of 14 (8) electrons, we found that $\langle -T\rangle/4N=0.26473$ (0.28028). The complicated second term on the rhs of Eq. (A1) evaluated at momentum $\mathbf{q}=(0,\pi/2)$ gives -0.33636 and -0.34836, for 14 and 8 electrons, respectively. Then, $D_s/(2\pi e^2)=-0.07163$ and -0.06808, again for 14 and 8 electrons, respectively. Note that a negative result for D_s is not impossible on a finite system, and similar problems have been observed in the analysis of the Drude peak near half-filling for the one-band Hubbard model.[60] Also in the t-J model, at *small* J/t, the superfluid density is negative on finite clusters. These results should be taken as indicative that there are *no* strong superconducting correlations in these regimes of parameter space.

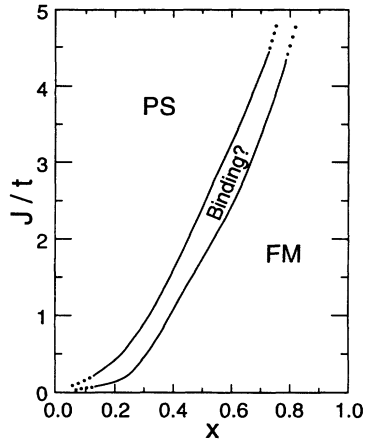

FIG. 12. Schematic phase diagram of the two-dimensional t-J model when the fermionic statistics of the particles is removed. FM denotes a ferromagnetic region, while PS is phase separation. In the narrow region between these two phases, "binding" (i.e., $\Delta_B<0$) is observed, but such a narrow strip may be a finite-size effect (and thus we included an interrogation mark in the figure).

APPENDIX B: HARD-CORE BOSONS IN THE t-J MODEL

In Sec. II, the phase diagram of the two-dimensional t-J model was analyzed, finding indications of superconductivity near phase separation. This result is qualitatively similar to that found in the one-dimensional version of the same model.[38] It is interesting to notice that in one dimension the *statistics* of the particles described by the t-J model is irrelevant since a pair of them cannot be interchanged due to the constraint of no double occupancy at every site.[61] In other words, fermions and hard-core bosons produce the same physics in this model. Other one-dimensional models have the same property. Then, a natural question arises: is the role of the statistics in two dimensions important for the qualitative features of the phase diagram? In order to study this problem we analyze the same t-J model defined in Sec. II but removing the fermionic statistics, i.e., considering hard-core bosons with spin $\frac{1}{2}$. This is an artificial model without physical realization (to the best of our knowledge) but mathematically well defined, and its analysis will teach us whether the signs coming from fermionic permutations are important for the phase diagram.[62] As an additional motivation note that sometimes the treatment of hard-core bosons is simpler than that of fermions. In particular, it may occur that Monte Carlo simulations without "sign problems" can be carried out for bosons and not for fermions. Then, it is important to know how drastic an approximation would be to neglect the statistics in the two-dimensional t-J model.

Using a 4×4 cluster and exact diagonalization techniques, we investigated the quantum numbers of the ground state, and the sign of

$$\Delta_B=E(n+2)+E(n)-2E(n+1)$$

as a criterium to analyze the presence of binding of particles in the system [where $E(m)$ is the ground-state energy in the subspace of m holes]. In an analogous way, we search for indications of phase separation studying the sign of

$$\Delta_{\rm PS}=E(n+4)+E(n)-2E(n+2)\ .$$

Although the actual results are somewhat erratic (probably due to finite-size effects), the analysis of these numbers shows a clear pattern which is schematically shown in Fig. 12. The region of phase separation is robust and not appreciably affected by the statistics of the particles. However, the metallic region of the phase diagram drastically changes replacing fermions for hard-core bosons. A large "ferromagnetic" region is observed at all densities. The total spin is maximized (fully polarized ferromagnet) for small J/t, and then it decreases until the boundaries of the phase are reached. It can be shown that even two particles in an otherwise empty lattice minimize their energy by forming an $S=1$ state, at least for J/t smaller than some finite number and on a finite cluster. Numerically we systematically observed a small window between the ferromagnetic and phase-separated regimes. In this regime, we found $\Delta_B<0$ suggesting the presence of pairing. However, it is not clear whether this small detail will survive the bulk limit increasing the lattice size. Then, we conclude that the phase diagram of the two-dimensional t-J model is strongly affected by the statistics of the particles, and approximations that do not handle this properly may produce incorrect results.

[1]J. Bednorz and K. Müller, Z. Phys. B **64**, 188 (1986); Rev. Mod. Phys. **60**, 585 (1988).

[2]B. Batlogg, Phys. Today **44** (6), 44 (1991); B. Batlogg, H. Takagi, H. L. Kao, and J. Kwo, in *Electronic Properties of High T_c Superconductors, the Normal and the Superconducting State,* edited by H. Kuzmany *et al.* (Springer-Verlag, Berlin, 1992).

[3]A. Schilling *et al.*, Nature **363**, 56 (1993); S. N. Putilin, E. V. Antipov, O. Chmaissem, and M. Marezio, *ibid.* **362**, 226 (1993).

[4]E. Dagotto, Rev. Mod. Phys. (to be published).

[5]E. Dagotto, A. Moreo, F. Ortolani, D. Poilblanc, and J. Riera, Phys. Rev. B **45**, 10 741 (1992).

[6]S. Uchida, T. Ido, H. Takagi, T. Arima, Y. Tokura, and S. Tajima, Phys. Rev. B **43**, 7942 (1991); D. B. Tanner, and T. Timusk, *Physical Properties of High-Temperature Superconductors III,* edited by Donald M. Ginsberg (World Scientific, Singapore, 1992), pp. 363–469.

[7]D. C. Johnston, Phys. Rev. Lett. **62**, 957 (1989).

[8]A. Moreo, Phys. Rev. B **48**, 3380 (1993); see also R. R. P. Singh and R. L. Glenister, *ibid.* **46**, 11 871 (1992).

[9]A. Fujimori, Jpn. J. Appl. Phys. **7**, 125 (1992); J. Phys. Chem. Solids **53**, 1595 (1992).

[10]E. Dagotto, A. Moreo, F. Ortolani, J. Riera, and D. J. Scalapino, Phys. Rev. Lett. **67**, 1918 (1991); T. Tohyama and S. Maekawa, Physica C **191**, 193 (1992); E. Dagotto, F. Ortolani, and D. Scalapino, Phys. Rev. B **46**, 3183 (1992); See also E. Dagotto, R. Joynt, A. Moreo, S. Bacci, and E. Gagliano, *ibid.* **41**, 9049 (1990).

[11]T. Tanamoto, H. Kohno, and H. Fukuyama, J. Phys. Soc. Jpn. **61**, 1886 (1992); **62**, 717 (1993); **62**, 1455 (1993).

[12]S.-W. Cheong *et al.*, Phys. Rev. Lett. **67**, 1791 (1991).

[13]A. Moreo, E. Dagotto, T. Jolicoeur, and J. Riera, Phys. Rev. B **42**, 6283 (1990).

[14]R. O. Anderson *et al.*, Phys. Rev. Lett. **70**, 3163 (1993).

[15]J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B **39**, 7074 (1989); J. Riera and A. P. Young, *ibid.* **39**, 9697 (1989); Y. Hasegawa and D. Poilblanc, *ibid.* **40**, 9035 (1989); E. Dagotto, J. Riera, and A. P. Young, *ibid.* **42**, 2347 (1990); M. Boninsegni and E. Manousakis, *ibid.* **47**, 11 897 (1993); D. Poilblanc, J. Riera, and E. Dagotto (unpublished).

[16]N. Bulut and D. Scalapino, Phys. Rev. Lett. **67**, 2898 (1991); P. Monthoux, A. Balatsky, and D. Pines, *ibid.* **67**, 3448 (1991).

[17]A. Moreo, Phys. Rev. B **45**, 5059 (1992), and references therein. See also M. Imada and Y. Hatsugai, J. Phys. Soc. Jpn. **58**, 3752 (1989); D. J. Scalapino, S. R. White, and S. C. Zhang, Phys. Rev. B **47**, 7995 (1993).

[18]R. T. Scalettar *et al.*, Phys. Rev. B **62**, 1407 (1989); A. Moreo and D. J. Scalapino, Phys. Rev. Lett. **66**, 946 (1991).

[19]E. Dagotto and J. Riera, Phys. Rev. Lett. **70**, 682 (1993).

[20]V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).

[21]In this respect the results presented here are similar in spirit to those obtained in the context of particle physics many years ago, when it was shown that quantum chromodynamics (QCD) confines at large bare couplings on a lattice [see J. Kogut, Rev. Mod. Phys. **51**, 659 (1979); **55**, 775 (1983)]. Although this is not at all the realistic regime, such a result was considered as an important progress towards showing that QCD confines. Actually, it was enough to carry out a Monte Carlo simulation of lattice QCD to show that the regime of strong coupling and weak coupling (i.e., the physically realistic regime due to asymptotic freedom) were analytically connected. We hope that a similar program will start also in the context of the 2D *t-J* model based on the results discussed in this paper.

[22]This result has also been noticed in the context of the three-band Hubbard model. See, for example, M. Grilli, R. Raimondi, C. Castellani, C. Di Castro, and G. Kotliar, Phys. Rev. Lett. **67**, 259 (1991); R. Raimondi, C. Castellani, M. Grilli, Y. Bang, and G. Kotliar, Phys. Rev. B **47**, 3331 (1993).

[23]V. J. Emery and S. A. Kivelson, Physica C **209**, 597 (1993).

[24]P. C. Hammel *et al.*, Phys. Rev. B **42**, 6781 (1990); Physica C **185**, 1095 (1991); P. C. Hammel, E. Ahrens, A. Reyes, J. Thompson, Z. Fisk, P. Canfield, J. Schirber, and D. MacLaughlin (unpublished).

[25]S. Kivelson, V. Emery, and H. Q. Lin, Phys. Rev. B **42**, 6523 (1990).

[26]E. Dagotto and J. Riera, Phys. Rev. B **46**, 12 084 (1992).

[27]M. Troyer, H. Tsunetsugu, T. M. Rice, J. Riera, and E. Dagotto, Phys. Rev. B **48**, 4002 (1993).

[28]A possible algorithm to use for the study of large clusters is the "many-body basis set reduction" discussed in J. Riera and E. Dagotto, Phys. Rev. B **47**, 15 346 (1993).

[29]The "square" lattices that can cover the bulk, and also hold a perfect Néel order with periodic boundary conditions are those satisfying $N=n^2+m^2$, where N is the number of sites, and n,m are integers, with $n+m$ even [see J. Oitmaa and D. Betts, Can. J. Phys. **56**, 897 (1978)].

[30]Note, however, that this cluster is not invariant under reflections.

[31]S. Maekawa (private communication); Y. Ohta, T. Shimozato, R. Eder, K. Tsutsui, and S. Maekawa (unpublished).

[32]H. Q. Lin, Phys. Rev. B **44**, 4674 (1991).

[33]Y. C. Chen and T. K. Lee (unpublished), also studied the low-density regime of the *t-J* model in two dimensions finding a region of *s*-wave pairing compatible with our results.

[34]R. Valenti and C. Gros, Phys. Rev. Lett. **68**, 2402 (1992).

[35]C. Gros, Phys. Rev. B **38**, 931 (1988); see also C. Gros, R. Joynt, and T. M. Rice, Z. Phys. B **68**, 425 (1987); G. J. Chen, R. Joynt, F. C. Zhang, and C. Cros, Phys. Rev. B **42**, 2662 (1990).

[36]T. Barnes, Int. J. Mod. Phys. C **2**, 659 (1991).

[37]D. van der Marel (unpublished). Here the RPA approximation is used to find the phase diagram of the *t-J* model. In excellent agreement with our results, a region of *d*-wave superconductivity is found near half-filling, with a transition to extended *s*-wave superconductivity at low electronic doping. The transition of pairing angular momentum as a function of density was also observed in ^{3}He. See V. J. Emery and A. M. Sessler, Phys. Rev. **119**, 43 (1960), and references therein.

[38]M. Ogata, M. Luchini, S. Sorella, and F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).

[39]A calculation along these lines has been reported by Valenti and Gros (Ref. 34). The position of the transition to phase separation at quarter-filling is in excellent agreement with the numerical results (i.e., $J/t\sim 3$, see their Fig. 1 including the density-density attraction in the Hamiltonian). However, their wave function does not show indications of superconductivity at this doping (only at low electronic densities). Then, the Valenti-Gros wave function does not seem accurate enough to describe the physics of the *t-J* model at quarter-filling, at least at large J/t.

[40]W. Putikka, M. Luchini, and T. M. Rice, Phys. Rev. Lett. **68**, 538 (1992).

[41]Y. C. Chen and T. K. Lee, Phys. Rev. B **47**, 11 548 (1993).

[42]C. S. Hellberg and E. J. Mele, Phys. Rev. B **48**, 646 (1993).

[43]Z.-X. Shen *et al.*, Phys. Rev. Lett. **70**, 1553 (1993); W. N. Har-

dy, D. A. Bonn, D. C. Morgan, R. Liang, and K. Zhang, Phys. Rev. Lett. **70**, 3999 (1993).

[44]A more complete study of this model including corrections to the mean-field approximation, and an extensive numerical analysis is planned.

[45]J. Inoue and S. Maekawa, Prog. Theor. Phys. Suppl. **108**, 313 (1992).

[46]J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang, Phys. Rev. B **39**, 11 663 (1989).

[47]For previous work on this phase using an attractive V term see V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).

[48]R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 114 (1990).

[49]However, it is fair to point out that in the case of the t-U-V model the attractive force that produces pairing (U term) is not strictly the same that induces phase separation (V term). However, we can think of them as forming part of a unique attractive force that decays with distance by moving in parameter space along straight lines $U \propto V$ in the quadrant where both U and V are negative.

[50]C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. **62**, 681 (1987).

[51]A study of the two-band Hubbard model including long-range interactions is planned.

[52]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[53]A. Sudbo, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **46**, 5548 (1992).

[54]A. Sudbo, C. M. Varma, T. Giamarchi, E. B. Stechel, and R. T. Scalettar, Phys. Rev. Lett. **70**, 978 (1993).

[55]K. Sano and Y. Ono, Physica C **205**, 170 (1993). See also W. Bardford and M. W. Long, J. Phys. Condens. Matter **5**, 199 (1993).

[56]R. T. Scalettar, D. J. Scalapino, R. L. Sugar, and S. R. White, Phys. Rev. B **44**, 770 (1991).

[57]F. F. Assaad and D. Wurtz, Phys. Rev. B **44**, 2681 (1991).

[58]D. J. Scalapino, S. R. White, and S. C. Zhang, Phys. Rev. Lett. **68**, 2830 (1992).

[59]For details on the technique used, we refer to G. Fano, F. Ortolani, and F. Semeria, Int. J. Mod. Phys. B **3**, 1845 (1990).

[60]R. Fye *et al.*, Phys. Rev. B **44**, 6909 (1991).

[61]In principle, working on a finite ring the statistics of the particles can be noticed through hopping processes that use the boundary. But in the bulk limit of the t-J model on a chain, the statistics should not affect the results.

[62]For a previous analysis changing the statistics of particles in the t-J model see M. W. Long and X. Zotos, Phys. Rev. B **45**, 9932 (1992).