# Hole pairing and clustering in the two-dimensional $t$-$J$ model

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Hole-density correlation functions in the $t$-$J$ model on lattices with square geometry are studied by the method of exact diagonalization for systems of various sizes with up to 26 sites. For the largest sizes we employ only a restricted basis, whereby for the extrapolation we introduce and test a scaling procedure. For two holes in an antiferromagnet our results confirm their binding for $J > J_c \sim 0.2t$. For four holes the two-point and four-point density correlations, calculated for $N = 18, 20$ sites, show clear evidence for hole-clustering instabilities for $J > J_s \sim 1.5t$; a first instability is likely to be towards a striped phase, with holes forming domain walls along the $(0,1)$ or $(1,0)$ direction. Signs for the phase separation into a hole-rich and a hole-free phase appear only at $J > J_s^* \sim 2.5t$. Results in the intermediate regime $0.4 < J/t < 1.2$ are consistent with the pairing picture, although there are also indications for a large weight of configurations representing domain walls along the $(1,1)$ direction.

## I. INTRODUCTION

Since the discovery of high-temperature superconductivity (SC) in copper oxides, the central theoretical question remains whether proposed models representing electrons in these substances as strongly correlated[1] allow also for a ground state with SC pairing. In particular, one would like to have a proper understanding of the phase diagram of the prototype models for correlated systems, such as the Hubbard model and the $t$-$J$ model.[2] There are numerous analytical approaches giving hope to SC in these models, in particular in the regimes representing weakly doped magnetic insulators. On the other hand the evidence for pairing from numerical studies,[3] at least for the Hubbard model (results obtained mainly by the quantum Monte Carlo method), is rather negative so far.

The phase diagram is controversial in the $t$-$J$ model as well.[2] Exact diagonalization studies on small systems indicate that two holes added to the reference antiferromagnetic (AFM) insulator form a bound state above the threshold $J > J_c \sim 0.15t$.[4,5] The latter effect has been interpreted by some authors as an instability towards a hole-spin phase separation (PS), appearing at all $J/t$ for small (vanishing) doping.[6] However, a recent high-temperature-expansion calculation,[7] as well as a variational approach,[8] supports the existence of phase separation only in the regime $J > J_s > 1.2t$. Still an explanation for such a critical $J_s$ is missing, since it is low as compared to simple phase separation estimates,[6] but too large to be connected with the onset of hole binding $J_c$.[4,9] Although at low doping the intermediate regime $J_c < J < J_s$ would be a candidate for enhanced SC correlations, a clear numerical evidence for the latter is not found in the most extensively studied $4 \times 4$ system.[10,3]

Insight into a possible pairing in the $t$-$J$ and Hubbard models has been recently gained by studying one-dimensional (1D) models in an external staggered magnetic field $h$.[11] This field simulates in 1D the effect of the AFM correlations as present in $D \geq 1$ and consequently the spin-string effect, mass enhancement, and some other phenomena found previously in 2D models. Within the $t$-$J$-$h$ model it has been shown that at low doping there exists a broad regime $J_c < J < J_s$ where one can clearly establish the existence of paired holes.

With the experience from the 1D $t$-$J$-$h$ model we revisit in this paper the 2D $t$-$J$ model. To avoid as much as possible finite size effects, which appear to be more pronounced when comparing results of systems with different quantum numbers such as the number of holes $N_h$ and the total spin $S$, we rely here mainly on the analysis of correlation functions within a given system. We use in particular the (two-point) hole-density correlation function $g(r)$ together with the following simple criteria: (a) The bound state for $N_h = 2$ holes should be characterized by a well pronounced maximum at $g(r = r_0)$ where $r_0 < L_0 = \sqrt{N/2}$, and $L_0$ is the largest distance in a square system with $N$ sites and periodic boundary conditions. (b) In the phase-separated regime $g(r)$ must fall off with $r$, at least for $r \gg N_h$. (c) For $N_h = 4$ the indication for pairing are two maxima in $g(r)$, one at the pair radius $r_0$ and another at the interpair distance $r = L_0$. For $N_h = 4$ an analogous, but more complete information, is contained also in the four-point hole correlation function $G$. Our investigations are complementary to recent exact diagonalization studies, where mainly energies have been calculated.[5] In this study we are moreover able to consider larger lattices by using only a restricted basis and appropriate scaling of the results.

The organization of the paper is as follows. In Sec. II we present the method with the restricted basis set and

the corresponding scaling for the extrapolation to the total basis. In Sec. III results for the binding of two holes are discussed. Section IV is devoted to the analysis of $g(r)$ correlations for four holes. In Sec. V the latter information is supplemented by four-point correlations $G$ in order to establish the character of the $N_h = 4$ ground state in the (possible) pairing regime. Numerical and analytical arguments are also presented that at low doping the first PS instability is not towards hole-rich and spin-rich phases but rather to a striped phase with holes forming (soliton) lines [incommensurate charge-density-wave (CDW) and spin-density-wave (SDW) structure].

## II. METHOD

We study in the following the 2D $t$-$J$ model[1,2]

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

where $c_{i,s}(c^{\dagger}_{i,s})$ are projected fermionic operators, taking into account that double occupancy of sites is not allowed. $n_i$ and $\mathbf{S}_i$ are the corresponding local fermion number and spin operators, respectively.

Our aim is to obtain results for $N$-site systems with square geometry and periodic boundary conditions which satisfy the condition $N = l^2 + m^2$, $l, m$ integers.[12] Restricting ourselves to even $N$, we consider the sizes $N = 18, 20, 26$, while the $N = 16$ system has been studied quite extensively before.[4,13,10,3] Becuase of computer storage and time restrictions, we are able to perform the full exact diagonalization of the model at most for $N = 20, N_h = 2$ where the total number of basis states, $N_{\text{tot}} = 462402$, and $N = 18, N_h = 4$, with $N_{\text{tot}} = 583696$. In both cases the numbers are for the sector with total spin projection $S_z = 0$ and wave vector $q = 0$, where the ground states belong.

For the next larger lattices (with the square geometry) the full diagonalization is not yet feasible; e.g., for $N = 26, N_h = 2$ the total basis would be $N_{\text{tot}} > 3 \times 10^7$, while for $N = 20, N_h = 4$, $N_{\text{tot}} > 3 \times 10^6$ within the same sector. We can show, however, that one can obtain, even for these systems, some sensible results by working within a restricted basis set with $N_{\text{st}}$ states and then perform the appropriate scaling towards $N_{\text{tot}}$. The choice of the restricted basis certainly depends on the problem, but in general it has to satisfy two criteria: (a) The hierarchy of restricted states should roughly reflect the hierarchy of the basis states as represented in the ground state wave function, and (b) the basis set must be easy to use, i.e., easy to index, etc. Since we are interested in the $t$-$J$ model (1) in the regime of pronounced AFM correlation, the natural lowest-order basis states are those with the different hole configurations in the background spin Néel state. Starting from these $N_0$ configurations we then build configurations with a finite number $N_r$ of reversed spins. The maximum number of reversed spins is $N_{r\max} = N - N_h$, while the results essentially saturate at $N_{r2} = N_{r\max}/2$. Still we are not able to reach $N_{r2}$ in general, but rather smaller values. E.g., for $N = 26, N_h = 2$ we reach $N_r = 6$ with $N_{\text{st}} = 443612$, while for $N = 20, N_h = 4$, $N_r = 6$, with $N_{\text{st}} = 729171$, again considering the $S_z = 0$ and $q = 0$ sector.

Since we are, in the latter cases, still well below $N_{r2}$, it is essential to perform an extrapolation of the results. We present here the basic scaling idea on the example of the ground state energy $E_0$. Let us suppose that the Hamiltonian can be separated in an unperturbed part and a perturbation, i.e., $H = H_0 + \eta H'$. E.g., in Eq. (1) one can consider as perturbation the hopping $\eta = t/J$ and (or) the spin flip term $\eta = J_{\perp}/J_{\parallel}$. Formally the total energy can be written in terms of the perturbation power series

$$E_0 = \epsilon_0 + \eta^2 \epsilon_2 + \cdots + \eta^{2k_0} \epsilon_{2k_0} + \cdots, \tag{2}$$

where for simplicity only even powers have been considered (as they emerge from the hopping term). Assuming that $\eta = 1$ is the radius of convergence of the series, then $\epsilon_{2k}$ must all be extensive and of the same order of magnitude. Because of the hierarchical structure of the excited states as they become involved in the perturbation expansion, one needs for the evaluation of a particular term in the series approximately $N_{\text{st}} = N_0, N_0 M, N_0 M^2, \ldots, N_0 M^{k_0}$ states, respectively, where $M \gg 1$ reflects the connectivity of the model Hamiltonian. For $\eta < 1$ the error by truncating the series at the order $2k_0 - 2$ is

$$\Delta E_0 \propto \frac{\eta^{2k_0}}{1-\eta^2} \propto \eta^{2\ln \frac{N_{\text{st}}}{N_0}/\ln M} = \left(\frac{N_{\text{st}}}{N_0}\right)^{2\ln\eta/\ln M}. \tag{3}$$

If $\eta \ll 1$, one obtains from Eq. (3) the power law behavior

$$\Delta E_0 \propto N_{\text{st}}^{-p}, \quad p = -2\frac{\ln\eta}{\ln M} > 0. \tag{4}$$

On the other hand, if $\eta \lesssim 1$, we get

$$\Delta E_0 \propto \ln \frac{N_{\text{tot}}}{N_{\text{st}}}, \tag{5}$$

where we have already taken into account that $\Delta E_0 = 0$ at $N_{\text{st}} = N_{\text{tot}}$ .

The scaling arguments presented above cannot be considered as derivations, but rather as a rough classification of quantum systems into the perturbative Eq. (4) and the unperturbative one Eq. (5), at least from the standpoint of the numerical diagonalization of finite (small) systems. It is clear that the behavior can depend on the particular choice of the representation used for the basis states. Nevertheless it seems that near half-filling the $t$-$J$ model, both the undoped (the Heisenberg model) and the doped one, belong to the latter class within the regime of strong AFM correlations, irrespective of the basis representation employed. On the other hand, the Hubbard model at modest $U/t > 1$ can well fall within the perturbative class, Eq. (4), for finite systems. This can explain the remarkable accurate energies for the 2D Hubbard model obtained recently by the Monte Carlo diagonalization method within a restricted basis.[14] We can note here that if the restricted basis set is chosen

using the stochastic algorithm, as has been suggested in Ref. 14, the difference $\Delta E_0$ is reduced for a fixed site of the basis set, nevertheless the scaling behavior is expected to remain qualitatively unchanged.

Arguments, shown on the example of the ground state energy, should apply to correlation functions as well, at least for $k_0 \gg 1$ or $N_{\rm st} \gg N_0$. We consider the hole-density correlations, defined for the ground state $|\Psi_0\rangle$,

$$g(\mathbf{r}) = N\langle\Psi_0|n_h(\mathbf{r}_1)n_h(\mathbf{r}_1+\mathbf{r})|\Psi_0\rangle, \tag{6}$$

where $n_h(\mathbf{r}_i) = 1 - n_i$. We employ here as a test the $N = 20$ system with $N_h = 2$ holes and $J/t = 0.4$. In Fig. 1(a) we present results for $g(r)$ for nonequivalent

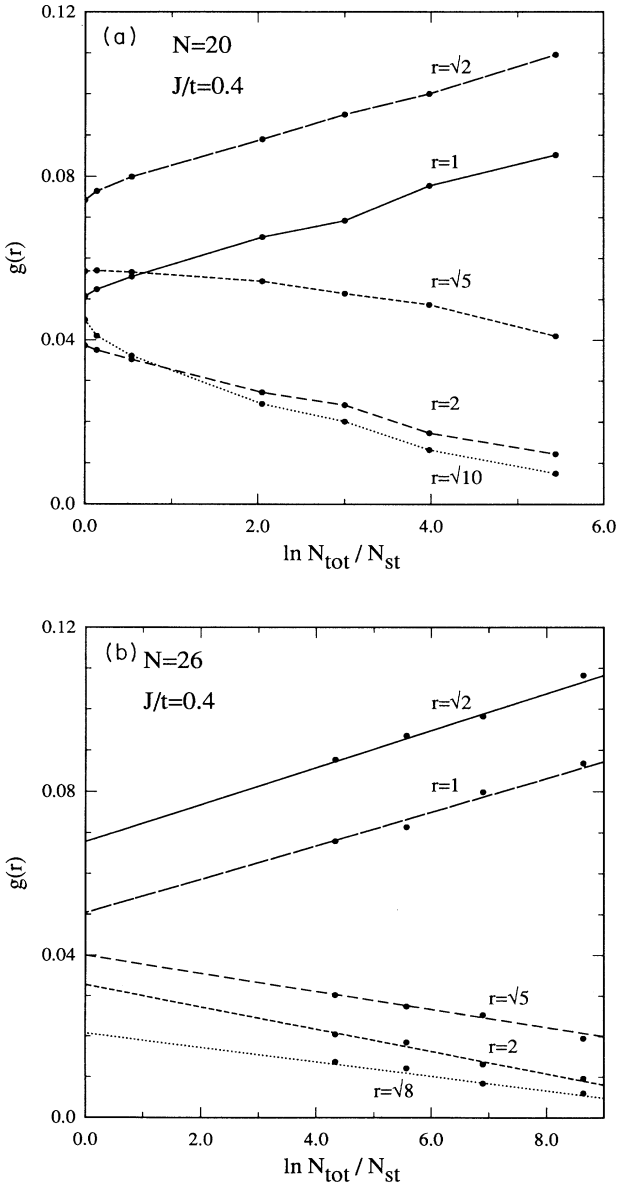



FIG. 1. Hole-density correlations $g(r)$ for $N_h = 2$, different $r$, and different number of reversed spins $N_r$ (dots) scaled vs $N_{\rm tot}/N_{\rm st}$: (a) for $N = 20$ lattice and $N_r = 3, 4, 5, 6, 9, 11, 18$ and (b) for $N = 26$ lattice and $N_r = 3, 4, 5, 6$.

distances $r$, whereby the values correspond to different number of reversed spins $N_r = 3, 4, \ldots, 10, 18$. Results follow very well the scaling ansatz, Eq. (5). Some deviations from the general trend appear on approaching the total basis at $N_r > N_{r2}$, where both degenerate Néel subspaces of basis states begin to couple. This effect is anyhow more pronounced only for the most sensitive largest distance $r = \sqrt{10}$. For $N = 26, N_h = 2$ the full diagonalization cannot be performed, but the analogous results for $g(r)$, as presented in Fig. 1(b) for $J/t = 0.4$, seem to justify the use of the scaling equation (5) for extrapolating the results to $N_{\rm st} = N_{\rm tot}$. It should, however, be noted, that in practice the extrapolation can be meaningfully performed only for systems which do not show qualitative changes in the ground state wave function $|\Psi_0\rangle$, when increasing $N_{\rm st}$. Some opposite examples will be mentioned further on when we discuss results for $N_h = 2$ and $N_h = 4$.

## III. A PAIR OF HOLES

The ground state of two holes in an AFM insulator have been so far investigated numerically in most detail for the square $4 \times 4$ lattice with periodic boundary conditions.[4] The disadvantage of this lattice is that it has a degenerate ground state due to a particularly large lattice symmetry, as well as quite pronounced finite size effects on the pair binding energy $\epsilon_b$.[9] Nevertheless, more recent calculations of $\epsilon_b$, performed for the larger lattice with $N = 18, N = 20$ (Ref. 5) where the ground state is nondegenerate with momentum $q = 0$, confirmed the qualitative behavior of the $N = 16$ results.

We add to the above results the evaluation of the correlation function $g(r)$ for $N = 18, 20, 26$. In Fig. 2(a) we present the $g(r)$ values for $N = 20$ obtained within the total basis, while the results for $N = 18$ are very similar to those for $N = 20$. In Fig. 3, for ease of comparison, we also show $g(r)$ as a function of the distance $r$ for a few values of $J/t$ characteristic of different regimes. In Fig. 2(b) the extrapolated values for $N = 26$ are shown. Here we note that the scaling to $N_{\rm tot}$ becomes unreliable for $J/t \leq 0.2$. The reason is twofold: There are abrupt transitions appearing on varying $N_r$, which indicate on changes in the ground state character (bound versus unbound pair) and prevent a meaningful extrapolation. Also at $J/t < 0.1$ the spin correlations change from AFM to ferromagnetic ones around each hole (although the total spin remains $S = 0$) and our basic choice of the hierarchy of basis states becomes questionable. We should also mention that for the larger lattices, due to the periodic boundary conditions, the distance between far points is not uniquely defined, depending on the connecting path chosen. The hole correlations though are not very sensitive to the chosen definition.

When comparing the $N = 20$ and $N = 26$ results, we note the qualitative agreement in the variation of $g(r)$ with $J/t$. The agreement is even quantitative for the largest correlations, in particular for $r = \sqrt{2}$ and somewhat less for $r = 1$, this being an alternative sign of a pronounced binding independent of the system size. Both sizes confirm surprisingly small $g$ ($r = 2$), while there are

clear differences for the largest distances, e.g., $r = \sqrt{5}$, where the influence of finite size effects is likely to be more pronounced for the $N = 20$ system.

To interpret our results in terms of a transition from a bound to an unbound hole pair, we should recall analogous results for the 1D $t$-$J$-$h$ model. There the binding-unbinding transition at $J_c(h)$ is well characterized with (a) $g(r)$ having the maximum at $r_0 = N/2$ at $J < J_c$, while $r_0 = \zeta_0 \ll N/2$ for $J > J_c$, and (b) decaying $g(r)$ for $r \gg \zeta_0$ at $J > J_c$. Such a transition can be naively simulated in 1D by a variable attractive potential of a fixed range $\zeta_0 \propto (t/h)^{1/3}$. If we would apply the same idea directly to 2D, we should use $h \sim 0.6J$.

Using criterion (a) also for the present 2D results,

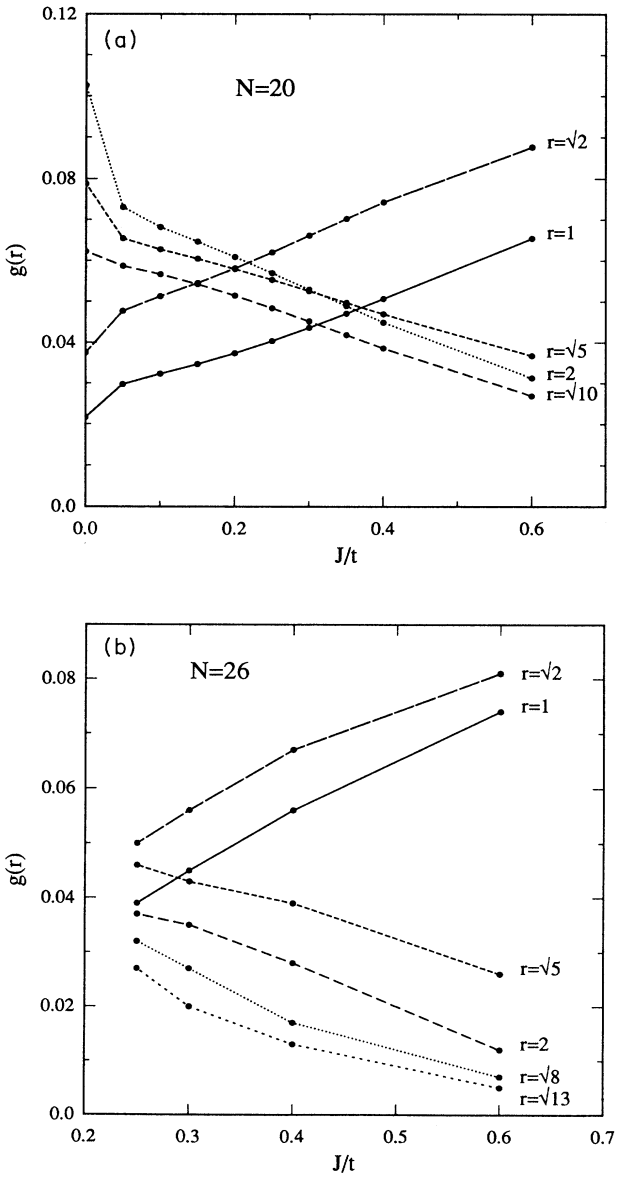



FIG. 2. $g(r)$ vs $J/t$ for $N_h = 2$, different $r$, and (a) $N = 20$ and (b) $N = 26$ lattice.

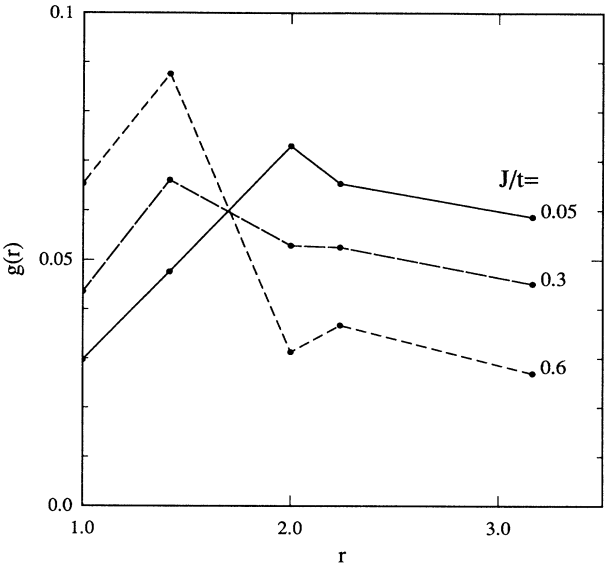



FIG. 3. $g(r)$ vs $r$ for $N_h = 2$, $N = 20$, and different $J/t$.

we would establish the binding threshold at $J_c \sim 0.2t$, which is also consistent with the value of the extrapolation breakdown as well as with the convergence of values of different $g(r)$ for $N = 26$. On the other hand it is still surprising that $g(r)$ curves for $N = 20$ in Fig. 2(a) vary rather smoothly through $J_c/t$ down to $J/t = 0.05$, where a more abrupt transition to predominant ferromagnetic correlations happens. This smooth transition can be an indication for possible more profound differences with the 1D $t$-$J$-$h$ model.

## IV. FOUR HOLES IN A SPIN BACKGROUND

The ground state wave function of four holes in a sufficiently large system should already contain the information, which of the three main possibilities is realized at low-doping in the regime where real space pairs are stable for two holes: (a) the phase separation where holes should exhibit the tendency to form droplets, (b) the pairing where two well separated pairs without a pronounced interaction should be established, and (c) the charge-density-wave instability where holes should exhibit a tendency to form a periodic structure.

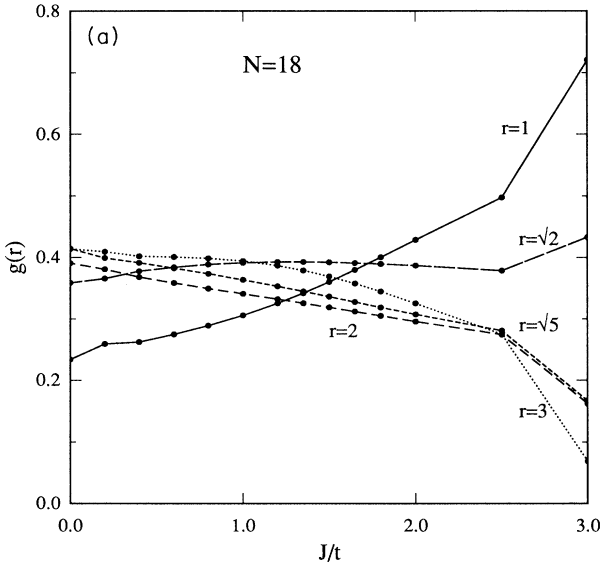
Again the comparison with the 1D $t$-$J$-$h$ model is instructive.[11] At large $J > J_s > t$ the PS is found for the $N_h = 4$ ground state using two independent criteria: (a) The hole-density correlations $g(r)$ are falling off monotonously with $r$, at least for large $r$, $N_h \ll r < N/2$, and (b) the clustering energy

$$\Delta = E_4 - 2E_2 + E_0, \tag{7}$$

being proportional to the inverse compressibility, is negative. It is characteristic that both criteria for $J_s$, i.e., for the onset of the PS, do not coincide for small 1D systems.[11] Generally $\Delta = 0$ seems to give a lower bound for $J_s$, while decaying $g(r)$ yields an upper bound. This

is not surprising in view of the strong perturbing effect of the finite doping concentration on the background spin configuration, as appears in particular for $N_h = 4$ for the available small systems.

In view of above results for 1D we reinvestigate the 2D $t$-$J$ model. Since we are interested here in the ground state with $N_h = 4$ while increasing $N$ as much as possible, systems with $N = 18, 20$ seem to present a substantial improvement over the most extensively studied $N = 4 \times 4$ lattice.[13,10,3] Namely, in the latter system with periodic boundary conditions the $N_h = 4$ ground state is again triply degenerate in $\mathbf{q}$. Moreover at large $J/t > 1$ these degenerate states reveal quite different forms of hole clusters, being an indication for a strong influence of finite size and boundary effects.



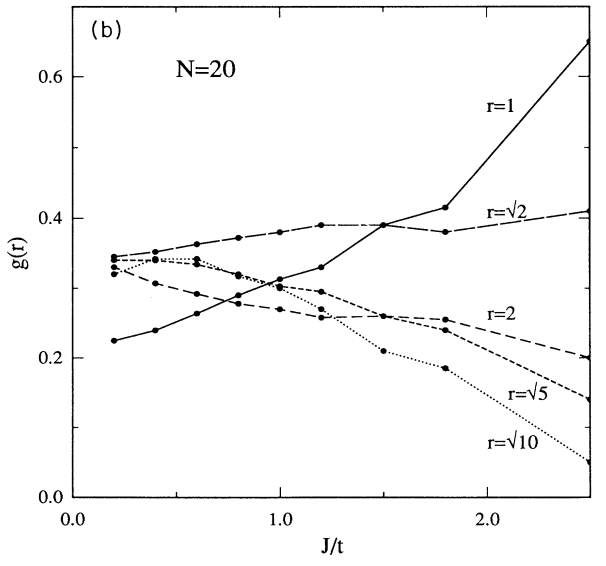




FIG. 4. $g(r)$ vs $J/t$ for $N_h = 4$, different $r$, and (a) $N = 18$ and (b) $N = 20$ lattice.

We present here results for $N = 18, 20$ lattices, where in both cases the ground state is $S = 0$ (for $N = 20$ we can establish this only approximately) and $q = 0$, at least for the most interesting regime $J/t > 0.1$. Results for $N = 20$ are again obtained by the extrapolation of data from the restricted basis, where we reached $N_r = 6$ reversed spins relative to the Néel spin configuration. It should be mentioned that the extrapolation is (compared to $N_h = 2$) somewhat more problematic in certain regimes, as discussed later.

Let us first comment on the behavior of hole-density correlations. In Fig. 4(a) we present $g(r)$ as a function of $J/t$ for $N = 18$ and in Fig. 5 we present $g(r)$ as a function of $r$ for different $J/t$ regimes. In comparison with $N_h = 2$ the values of $g(r)$ are much more uniform, except in the extreme PS regime at $J/t > 2$. As a reference, in a broad intermediate regime of $J/t$, one should consider here the result for free electrons, where $g(r)$ would be rather uniform with a reduced value at $r \sim 1$ due to the Fermi hole effect. It should be, however, stressed that the actual $r$ dependence, i.e., the hierarchy of $g(r)$ values in Fig. 4(a), is not reproduced by the free fermion $g(r)$ in any regime.

In Fig. 4(a) we can roughly distinguish three different regimes: (a) For $J/t < 0.2$, $g(r)$ increases monotonously with $r$, and so it is close to the behavior of four spinless fermions, or even more to four hard-core bosons. (b) At large $J/t > 2$, the $g(r)$ is falling off with $r$, being consistent with the clustering or the PS. An abrupt (crossover) transition to even stronger clustering is appearing at $J/t > 2.5$. (c) In the intermediate regime $0.5 < J/t < 1.5$, the largest correlations are for $r_0 = \sqrt{2}$ and $r_0 = L_0 = 3$. Since the maximum at $g(r = \sqrt{2})$ is characteristic for a single hole pair ($N_h = 2$), the behavior in this regime is consistent with the pairing picture, i.e., with the existence of two independent hole pairs.

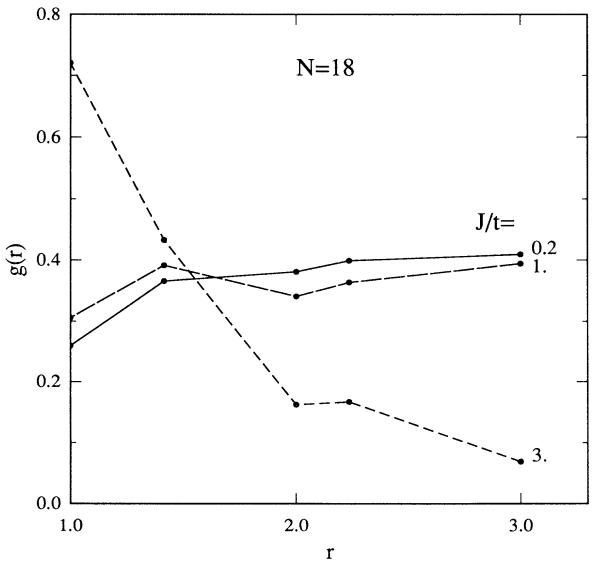



FIG. 5. $g(r)$ vs $r$ for $N_h = 4$, $N = 18$, and different $J/t$.

The same picture is also supported by the extrapolated results for $N = 20$, as presented in Fig. 4(b). Several comments to Fig. 4(b) are in order. Values for $r = L_0 = \sqrt{10}$ are probably underestimated in general, being most sensitive to large $N_r \geq N_{r2}$, as is also the case for $N_h = 2$ and $N = 20$ in Fig. 2(a). There are two crossover transitions, one at $J_s \sim 1.2\ t$ and another at $J_s^* \lesssim 2.5\ t$. These transitions appear in $|\Psi_0\rangle$ also on increasing $N_r$ and therefore prevent a reliable extrapolation around these points. While the transition at $J_s$ indicates the onset of some kind of hole clustering, the crossover at $J_s^*$ requires an essential change in the cluster form. Still the intermediate pairinglike phase $0.4 < J/t < 1.2$ is well pronounced for $N = 20$ in Fig. 4(b), moreover taking into account that values for $r = L_0$ are likely to be underestimated.

It is still not straightforward to fix the value for the instability $J_s/t$ (at small doping), which would limit the presumable pairing regime. The $N = 20$ results in Fig. 4(b) would indicate $J_s \geq 1.5\ t$, as it follows from decaying $g(r)$ as well as from the discontinuous variation of $g$ with $N_r$. In the same regime $J \geq J_s$ correlations for $N = 18$, as shown in Fig. 4(a), still do not satisfy the hierarchy expected for clustering, in particular $g(r = L_0) > g(r = 2), g(r = \sqrt{5})$. While this could indicate an even larger $J_s$, it can also be attributed to finite size effects, but as well to specific hole configurations discussed in the following paragraph. It should, however, be noted that the application of the alternative criterion $\Delta = 0$, Eq. (7), gives for $N = 18$ much smaller critical value $J_s \gtrsim 0.6t$,[5] which is not supported by $g(r)$ presented here. It is, however, plausible that due to the strong doping dependence of the AFM correlation of the spin background, $J_s^*$ represents only the lower bound as found also in the 1D $t$-$J$-$h$ model. In the same manner our $J_s$ values are likely to be upper bounds, so that the recently proposed marginal value $J_s/t \sim 1.2$ (Ref. 7) is not necessarily inconsistent with our analysis.

## V. DOMAIN WALLS VERSUS HOLE DROPLETS

It is important to establish the character of the instabilities appearing at $J_s > t$ and $J_s^* \gg t$. It should be reminded that in contrast to the numerical results, all simple estimates[6] of stable hole clusters (as relevant for small doping) would yield much larger $J_s > 2\ t$. We investigate this problem by calculating for $N_h = 4$ also the four-point hole density correlations

$$G_{ijkl} = N\langle\Psi_0|n_h(\mathbf{r}_i)n_h(\mathbf{r}_j)n_h(\mathbf{r}_k)n_h(\mathbf{r}_l)|\Psi_0\rangle, \qquad (8)$$

depending on the hole configuration $(ijkl)$. The variation of different $G$ with $J/t$ has been already studied for $N = 16$,[13] where the interpretation is more problematic due to the ground state degeneracy. To present results for the correlations $G$, corresponding to different configuration, we present in Fig. 6 our enumeration of sites in the $N = 18$ and $N = 20$ lattices.

In Fig. 7(a) we present $G$ for $N = 18$ and four characteristic configurations, dominating different regimes: (a) configuration (3 5 9 12), holes being as far apart as pos-

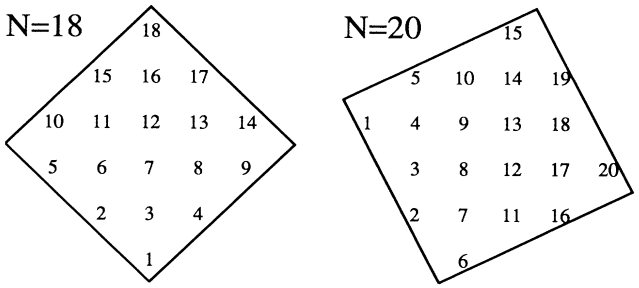



FIG. 6. Enumeration of sites in $N = 18$ and $N = 20$ lattices.

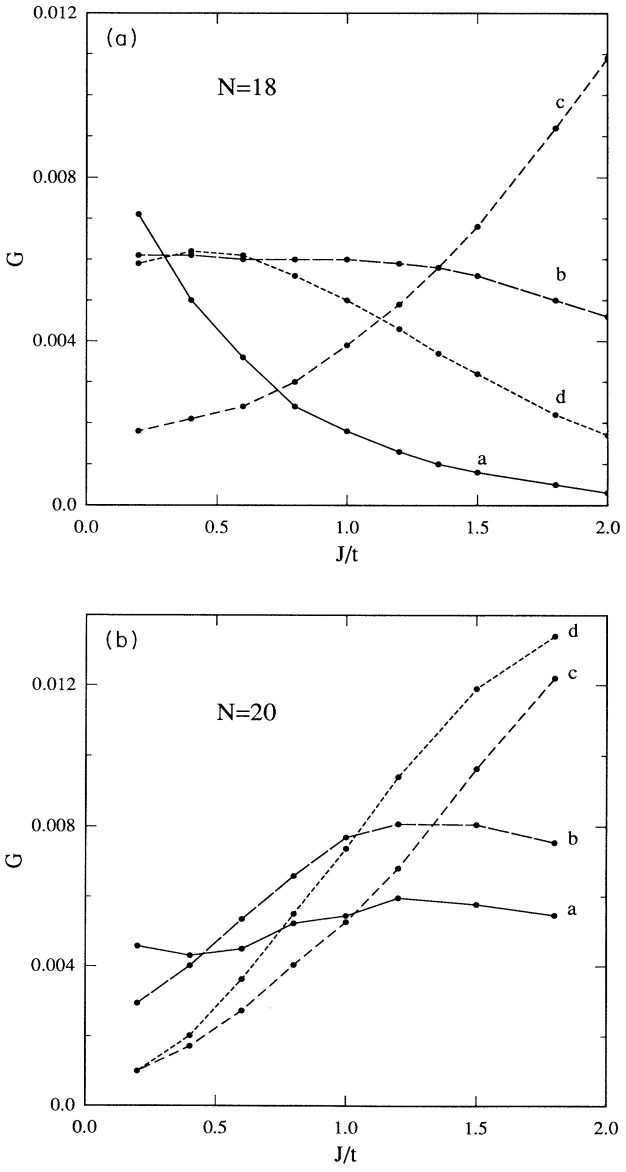



FIG. 7. Four-point hole-density correlations $G$ vs $J/t$ for $N_h = 4$ and four different configurations as presented in the text: (a) for $N = 18$ and (b) for $N = 20$.

sible in a $N = 18$ lattice, (b) (1 4 6 12), holes forming two separate pairs, with the intrapair distance $\sqrt{2}$, (c) (5 6 7 8) with holes forming a line (stripe) along the $(1,0)$ direction, and (d) (1 4 6 9) with three holes forming a domain wall (DW) along $(1,1)$. For $J/t < 0.3$ the largest is $G_a$, being consistent with the absence of binding and the character close to spinless fermions. In the intermediate regime $0.4 < J/t < 1.2$ pair contributions as, e.g., $G_b$ are dominating. It should be, however, stressed that there exists in both regimes a broad spectrum of other configurations with somewhat smaller $G$, consistent with the quite extended nature of the wave function. Also surprisingly large is the intermediate regime $G_d$, which indicates a quite stable diagonal DW. For $J/t > 1.2$ the hole-line configuration $G_c$ takes over steadily, with an increasing gap to the other configurations.

Similar conclusions can be drawn from the results for $N = 20$, as shown in Fig. 7(b). Again presented values are obtained by the extrapolation, so that they are subject to small uncertainty . Also we expect that the values for configurations with well separated holes or hole pairs could be underestimated. We show $G$ for four characteristic and dominant configurations: (a) (3 7 13 17) representing two separated hole pairs, (b) (2 8 13 19), with holes forming a line along the $(1,1)$ direction, (c) (3 8 12 17), with holes along the $(1,0)$ line, and (d) (1 2 3 6), holes representing a DW stretching over the system with periodic boundary conditions

Conclusions could be similar to the $N = 18$ case, with some differences clearly indicating on the size and even more shape effects. While separate pairs and $G_a$ dominate for $0.2 < J/t < 0.5$, a $(1,1)$ line formation $G_b$ becomes even more pronounced in the regime $0.5 < J/t < 1.2$. It is clear that for $N_h = 4$ such a line configuration is first possible for $N \geq 20$. Again the contribution $G_c$ of the ordering along $(1,0)$ is steeply increasing with $J/t$ and takes over the former contributions at $J > 1.5\ t$. Nevertheless, $G_d > G_c$, whereby the enhancement of $G_d$ can be attributed to a specific $N = 20$ shape effect, since the holes profit from closing the DW due to lattice periodicity.

The configuration $G_e$ with holes forming a droplet, e.g., (2 3 6 7) for $N = 18$ and (2 3 7 8) for $N = 20$, has a negligible contribution in the regime $J/t < 2$, both for the $N = 18$ and $N = 20$ lattices. Since this would be naively expected as the dominant configuration in the PS regime, its absence is the sign of an essentially different hole configuration in the regime $1.5 < J/t < 2.5$. On the other hand the abrupt transition at $J = J_s^* \sim 2.5\ t$, as seen also in Fig. 4(a), is accompanied by a dramatic change in the hole configuration. Namely, $G_e$ exhausts for $J > J_s^*$ to a large extent the whole weight of the wave function, while other contributions become negligible.

Our results are thus not consistent with the usual phase diagram with a single PS line, but rather with two essentially different phases for $J > J_s$. While for $J > J_s^*$ the instability is towards a hole-rich and a hole-free phase, in the intermediate regime $J_s < J < J_s^*$ the formation of hole DW's (stripes) is preferred. At finite hole concentrations this phase represents a CDW, and at the same time a spin-density-wave (incommensurate AFM) structure.

Assuming that at finite doping the first instability is towards the striped (CDW) phase, it would be helpful to establish in an alternative way the stability of a single line of holes, forming also a DW (soliton line) in an AFM structure. It should be noted that such DW-like inhomogeneous solutions have also been found within the Hartree-Fock approximation to the Hubbard model, although the stable direction was rather $(1,1)$ for large $U/t$.[15,16]

A possible approach is via the perturbation expansion in $t/J$ and in the exchange anisotropy $\gamma = J_\perp/J_\parallel$.[9] Since we are interested in the regime $J > t$, the limit $J \gg t$ can serve here as a valid starting point. In this regime bound hole pairs are more stable than separate holes, and so we need for comparison the hole pair energy $\epsilon_2 = E_2 - E_0$, expressed to the lowest orders in $t/J$ and $\gamma$ as[9]

$$\epsilon_2 = \frac{7}{2}J - \frac{16}{3}\frac{t^2}{J} - \frac{8}{3}\gamma\frac{t^2}{J} + 3.31\frac{t^4}{J^3}. \tag{9}$$

The energy of an infinite DW along the $(1,0)$ direction (per hole) $\tilde{\epsilon} = \epsilon/N_h$ can be expressed in the same way. For the DW surface energy (per hole) $\delta = \tilde{\epsilon} - \frac{1}{2}\epsilon_2$ we obtain

$$\delta = -\frac{1}{4}J + \frac{2}{3}\frac{t^2}{J} + \frac{4}{3}\gamma\frac{t^2}{J} - 6.7\frac{t^4}{J^3}. \tag{10}$$

This should be compared to the cohesion energy of the simple hole droplet $\tilde{\delta} = \Delta/4$, with $\Delta$ defined in Eq. (7),

$$\tilde{\delta} = -\frac{1}{4}J + \frac{4}{3}\frac{t^2}{J} + \frac{4}{3}\gamma\frac{t^2}{J} - 5.29\frac{t^4}{J^3}. \tag{11}$$

It is evident that always $\tilde{\delta} > \delta$. The origin of larger DW stability is in easy transverse fluctuations. Namely, predominantly 1D hole motion creates spin strings which are weaker since the DW is a boundary of two AFM domains with opposite staggered magnetization. For $N_h \gg 4$ and $J/t \gg 1$ hole droplets become, however, more stable since $\delta \gtrsim -\frac{3}{4}J$. Such droplets are highly unfavorable with respect to the kinetic energy, i.e., to the $t/J$ corrections, and hence a transition to the separation into a hole-rich and a hole-free phase is expected only at $J/t \gg 1$, as found in our numerical studies.

Equation (10) can be used also to estimate $J_s$ for the DW stability. From $\delta = 0$ it would follow that $J_s = 1.63t$ for $\gamma = 0$, while for $\gamma = 1$, $J_s > 2.5t$ is too high, indicating that the perturbation series are poorly convergent, consistent with large quantum fluctuations of the DW.

## VI. CONCLUSIONS

In this paper we investigated the possibility of pairing and clustering in the 2D $t$-$J$ model by finding numerically the ground state of finite systems representing the antiferromagnet doped with few mobile holes; in particular, results for $N_h = 2$ and $N_h = 4$ were presented. For $N_h = 2$ the hole-density correlations $g(r)$ in $N = 20$ and $N = 26$ lattices reconfirm the existence of real space pairs in a broad range of parameters $J > J_c \sim 0.2t$. So the proper understanding of the $N_h = 4$ system is crucial

to establish the phase diagram of the $t$-$J$ model at finite but small doping. Since in systems $N \leq 20$ available for the method of the (restricted) exact diagonalization and studied in this paper, $N_h = 4$ represents already a considerable doping concentration, results should be interpreted and generalized with care. This becomes evident also for four-point $G$ correlations when comparing $N = 18$ and $N = 20$ results. Namely, $N = 18$ does not allow for a formation of a $N_h = 4$ line of holes along the $(1,1)$ direction, so that the latter becomes more pronounced in the $N = 20$ lattice. On the other hand, for $N = 20$ the line of holes along $(1,0)$ is too close to a DW stretching through the system due to the specific lattice shape and periodic boundary conditions, so that the latter configuration obtains too large weight and dominates over the former for $J/t > 1$.

Taking into account the above finite lattice effects, our results, both for the two-point correlations $g(r)$ and four-point hole correlations $G$, are consistent with the picture of an instability towards the inhomogeneous hole distribution appearing at $J > J_s \sim 1.5t$. In contrast to earlier works[6–8] where only the instability towards the PS into a hole-rich and spin-rich phase has been considered for the $t$-$J$ model, we find clear evidence for the formation of hole (soliton) lines along the $(1,0)$ direction in this regime, which in a macroscopic system with a finite but low hole doping imposes the stability of hole DW and consequently the existence of the striped phase, being an incommensurate CDW and SDW structure. The transition to usual PS and clustering is very pronounced and abrupt only at $J_s^* \sim 2.5t$.

Quantum fluctuations due to hole hopping destroy the stability of $(1,0)$ hole DW's at $J < J_s$. The intermediate regime $0.4\ t < J < J_s$ at low doping is an evident candidate for the phase with paired (but separate) holes. We find the confirmation of the latter in $g(r)$, exhibiting two maxima, and in the dominant hole configurations as revealed by $G$. It should, however, be acknowledged that for larger lattices ($N = 20$) configurations representing $(1,1)$ hole DW's become also well pronounced, being consistent with the Hartree-Fock results within the Hubbard model at $U/t \gg 1$.[16,15] The latter contributions are, however, only slightly above (for $N = 20$) a large number of other pairing configurations. So the appropriate interpretation would not be in terms of another stable CDW structure, but rather in a $(1,1)$ DW structure destroyed by quantum fluctuations and thus allowing for a possible hole pairing.

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