Doped Stripes in Models for the Cuprates Emerging from the One-Hole Properties of the Insulator

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The extended and standard *t-J* models are computationally studied on ladders and planes, with emphasis on the small J/t region. At couplings compatible with photoemission results for undoped cuprates, half-doped stripes separating π-shifted antiferromagnetic (AF) domains are found, as in Tranquada's interpretation of neutron experiments. Our main result is that the elementary stripe "building block" resembles the properties of *one* hole at small J/t, with robust AF correlations across the hole induced by the local tendency of the charge to separate from the spin. This suggests that the seed of half-doped stripes already exists in the unusual properties of the insulating parent compound.

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The understanding of high temperature superconductors is among the most important open problems in strongly correlated electrons. A remarkable development in recent years is the accumulation of experimental evidence compatible with stripe formation in the normal state of underdoped cuprates [1]. This includes spin incommensurability (IC) in neutron experiments, results believed to be caused by stripes separating π-shifted antiferromagnetic (AF) domains [1]. More recently, it has been shown that the stripes are metallic [2], the result compatible with proposals of the normal state of $x = 1/8$ cuprates as made out of half-doped stripes [1]. Whether stripe formation is beneficial or detrimental to superconductivity is unclear, but it appears that stripes are an important ingredient of the normal state that cannot be ignored.

The theoretical explanation of stripe formation is much debated. Early work reported stripes in the *t-J* (at large J/t with $1/r$ repulsions) and Hubbard (Hartree-Fock) models [3,4]. However, these stripes were insulating with hole density $n_h \sim 1.0$, different from the experimental $n_h \sim 0.5$ stripes [5]. Recently, considerable progress was made when doped stripes were reported by White and Scalapino within the standard *t-J* model [6] (see also Ref. [7]). In Ref. [6] the analysis was performed at couplings where two holes form *d*-wave pairs, and the stripes are sometimes described as a condensation of these pairs into a stripe domain wall [8]. However, experiments are usually interpreted as holes moving freely along site-centered stripes [1]. In addition, the "extended" *t-J* model with hopping beyond neighboring sites, or the standard *t-J* model with very small J/t, is needed [9,10] to reproduce the insulator one-hole photoemission (PES) dispersion [11]. Thus, understanding metallic stripe formation requires further work and searching for stripes in the extended *t-J* model, particularly in regimes without hole binding and where the absence of phase separation (PS) is not controversial, is important to clarify the driving mechanism for these unusual complex structures.

Building upon previous investigations [6,7], in this Letter indications of $n_h \sim 0.5$ stripes compatible with experiments [1] are reported in the extended and standard *t-J* models on ladders and square clusters. These stripes do not seem composed of hole pairs (although pairs forming domain walls may be present at larger J/t than studied here [8]). They also exist in the t-J_z model [12] and using classical spins [7], implying that the details of the AF spin background are unimportant for its stabilization. Moreover, our most important result is that the basic stripe "building block" exists already in the *insulator* where one-hole wave functions have a complex spin structure with strong AF correlations across the hole, resembling the stripe spin correlations found here numerically. These results provide a rationalization for stripe formation built upon the *one*-hole properties, in regimes where spin and charge are almost separated [9].

The extended *t-J* model used here is defined as

$$H = J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) - \sum_{im} t_{im} (c_i^\dagger c_m + \text{H.c.}),$$

where t_{im} is $t(=1)$ for nearest neighbors (*NN*), t' for next *NN*, and t'' for next *NN* sites, and zero otherwise. The rest of the notation is standard. The t-J_z model is obtained by $J \to J_z$ and $\mathbf{S}_i \cdot \mathbf{S}_j \to S_i^z S_j^z$, and $t' < 0$ and $t'' > 0$ are relevant to explain PES data [9–11]. Here the density matrix renormalization group (DMRG) [6,13], Lanczos [14], and an algorithm using a small fraction of the ladder rung basis (optimized reduced-basis approximation, or ORBA [15]) are used. Results are presented in (i) the small J/t region with $t' = t'' = 0.0$, and (ii) small and intermediate J/t with nonzero t' and t'' [10]. These two regions have similar physics [9], and the extra hoppings are expected to avoid PS [5,16]. Intuitively, t', t'' increase hole mobility, as reducing J/t does, but also avoid ferromagnetism at small J/t [9]. Note also that no coupling fine-tuning is needed: the results below appear in a robust region of parameter space.

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In Fig. 1, DMRG and ORBA results for $4 \times N$ clusters are shown. In Fig. 1a the rung density for a 4×8 (4×12) cluster with four (two) holes at small J/t is presented. Cylindrical boundary conditions (CBC) are used, i.e., open boundary conditions (OBC) along legs and periodic boundary conditions (PBC) along rungs [6]. The four holes separate into two groups of two holes, a surprising result since for a square lattice $J_c = 0.2$ is the critical value for hole pair binding in the t-J_z model, and in the t-J model J_c is expected to be larger [17]. Similar results are found in the t-J_z model (Fig. 1a) and at intermediate J/t but with $t' \neq 0$, which increases the hole mobility: Fig. 1b with six holes shows the formation of three groups of two holes as in Fig. 1a. This is not spuriously caused by the OBC along legs, as shown in Fig. 1c with results using PBC in both directions. As ORBA starting configuration holes clustered (phase separated) or spread apart (free gas) were used, with PBC or CBC, and in both cases the results converged to the same "stripe" answer.

To study the two-hole state internal structure, in Fig. 1d the density distribution of one hole around the other is shown, for one of the two-hole regions of Fig. 1a. The largest density is at two lattice spacings along the rung, and the hole distribution does not resemble a tight d-wave bound state [14]. Similar conclusions were reached for the two holes of Fig. 1c. The result is actually compatible with the formation of a short site-centered stripe where the two holes form a closed loop with density 0.5 along a rung [18]. These stripes appear to occupy more than one rung in Figs. 1a–1c, and thus they could also be labeled as bond centered [6]. However, this effect seems to arise from stripe tunneling between neighboring rungs, as the one-hole projection suggests (Fig. 1d). Similar results regarding half-doped stripe formation were also found on 6×6 clusters, as exemplified in Fig. 2a where sets of three holes form individual $n_h \sim 0.5$ stripes. Overall the results are consistent with Tranquada's description of stripes [1]. They are also consistent with numerical reports for the standard t-J model [6], although our interpretation of the results (below) is different.

The half-doped stripes reported here also lead to spin IC. For example, in Fig. 1e the spin structure factor is shown for the cases of Figs. 1a and 1b. The peak deviation from (π,π) appears in a robust region of parameter space. The spin IC is understood calculating spin-spin correlations when two holes in, e.g., the cluster of Fig. 1c

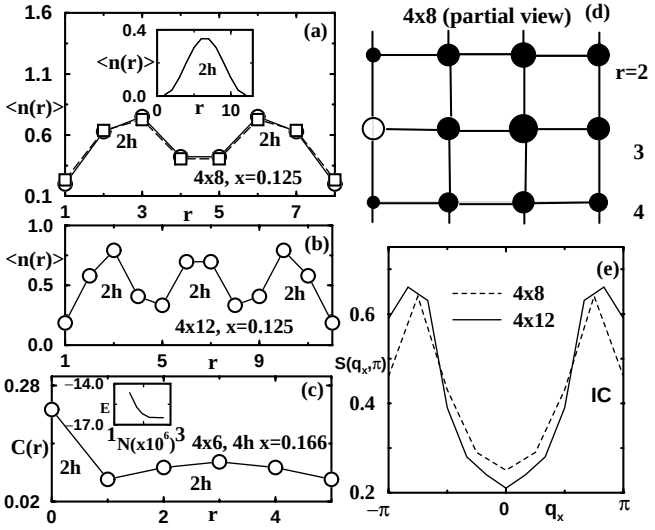

FIG. 1. (a),(b) Rung hole density $\langle n(r)\rangle$ vs rung index r using DMRG, with PBC along rungs and OBC along legs, to illustrate the $n_h \sim 0.5$ stripe formation. x is the overall hole density. (a) corresponds to a 4×8 cluster with four holes. Solid (dashed) lines are for the standard t-J (t-J_z) model with $J = 0.2$ ($J_z = 0.3$), $t' = t'' = 0.0$ (inset: same as solid lines but for 4×12 with two holes). (b) Same as (a) but for a 4×12 cluster with six holes, $J = 0.5$, $t' = -0.3$, and $t'' = 0.0$. (c) Hole density at rung r, defined now as $C(r) = \sum_{i \in r} \langle n_0 n_i \rangle$ where the sum is over sites belonging to rung r, 0 is an arbitrary site of rung $r = 0$, and $\langle n_0 n_i \rangle$ is the hole density-density ground-state correlation. The cluster is 4×6 with PBC in both directions, four holes, $J = 0.2$, $t' = -0.35$, and $t'' = 0.25$ (ORBA with $\sim 3 \times 10^6$ states). The inset shows ground-state energy vs the number of states. (d) Distribution of one hole around a second hole projected at the open circle position, for the case in (a) at the indicated rungs (running horizontally). Full circle areas are proportional to the hole density. (e) $S(q_x, \pi)$ vs q_x for the clusters, couplings, and densities of (a) and (b).

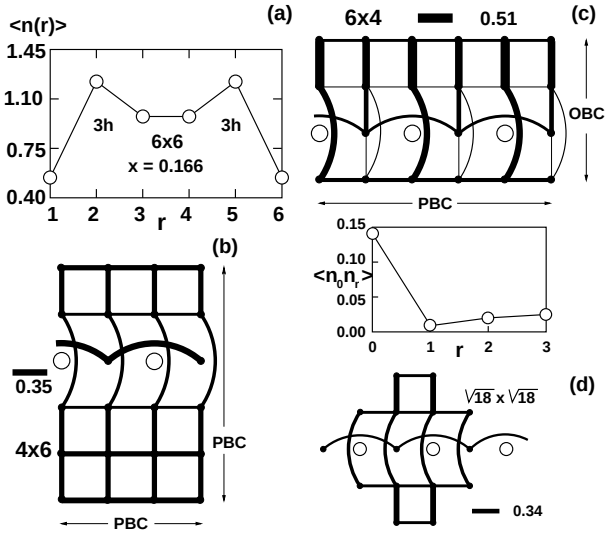

FIG. 2. (a) Rung hole density $\langle n(r)\rangle$ vs rung index r using DMRG on a 6×6 cluster with six holes, CBC (OBC along the direction shown with invariance under reflexions assumed), $J = 0.2$, and $t' = t'' = 0.0$ (800 states, eight sweeps). (b) Spin-spin correlations for two mobile holes projected at their most probable relative distance (circles) in the two-holes ORBA ground state of a 4×6 cluster, $J = 0.2$, $t' = -0.35$, and $t'' = 0.25$. Lines indicate AF correlations (thickness proportional to absolute value). (c) Same couplings, cluster, technique, and conventions as in (b) but using PBC (OBC) along legs (rungs), and three holes. Also shown are the hole density-density correlations along a center leg, showing that there is no charge order. (d) AF spin correlations for a large weight ground-state configuration of an exactly solved three hole, 18 site PBC cluster, $J = 0.4$, $t' = -0.20$ and $t'' = 0.14$.

are projected into their most probable location (Fig. 2b): a π shift across the stripe can be clearly observed. The across-the-stripe AF correlation strength increases reducing J/t and/or increasing $t' < 0$ and $t'' > 0$ in magnitude.

Results compatible with $n_h \sim 0.5$ stripes and associated π shifts appear in other clusters as well. On a cylindrical 6×4 cluster with PBC along the long direction, the three-holes ground state has characteristics compatible with a doped one-dimensional (1D) closed loop along the PBC direction, with π shifts across the stripe (see Fig. 2c, where one of the two degenerate most dominant ground-state hole configurations is shown). Stripe-fluctuation configurations are close in weight. A *h*-*s*-*h*-*s*-*h*-*s* loop (h = hole, s = spin) provides a pictorial representation of our results, but this configuration is not rigid neither along nor perpendicular to the loop. Density correlations along the stripe (Fig. 2c) are actually compatible with a 1D $n_h \sim 0.5$ system at large on-site U interactions [19], suggesting that the stripes described here are metallic. No indications of a charge density wave along the stripe were found. Note also that spin IC induced by antiferromagnetism across holes also exists *along the stripes*, with wave vector $\pi/2$ for a half-doped stripe. This spin IC appears also in half-doped 1D models [19]. For an isolated CuO plane, IC should be present in both directions, although with quite different wave vectors and intensities.

Similar results are found in small square clusters: in the two-holes 4×4 lattice with CBC, a two-hole stripe forms along the PBC direction [9]. With PBC in both directions, the ground state resembles a mixture of stripes along both axes and since nonzero $t' - t''$ avoids PS, our results are not expected to have the boundary effects recently discussed [16]. Indications of stripes are found even in tilted clusters: the PBC $\sqrt{18} \times \sqrt{18}$ lattice allows for $n_h \sim 0.5$ closed loops with three holes and such a structure has a large ground-state weight (Fig. 2d). Precursors of the spin structures in Figs. 1 and 2 appear on two- and three-leg ladders as well, e.g., in Fig. 3a the two-holes ground-state dominant hole configuration of a 3×6 cluster is shown, with its spin correlations. On two-leg ladders with many holes, π shifts appear at small J/t (Fig. 3b), and each hole is "confined" to a rung, precursor of a rung stripe as the leg number grows. Spin IC is here found both for the two-leg (Fig. 3c) and three-leg ladders.

The results thus far suggest that doped stripes can form in spin and hole models using realistic couplings. To gain insight into the mechanism driving this complex structure, consider now the *one*-hole problem. Figure 3d shows four-leg ladder spin correlations around a mobile hole for momentum (π,π). The AF correlations across the hole are similar to the correlations around the individual holes composing the stripes. The π-shift characteristic of the stripes exists in the one-hole state not only at (π,π) but at several momenta, such as $(0, \pi)$, and, in this sense, the spin IC exists already at the one-hole level, a remarkable result. Similar conclusions are reached for three- and two-leg ladders

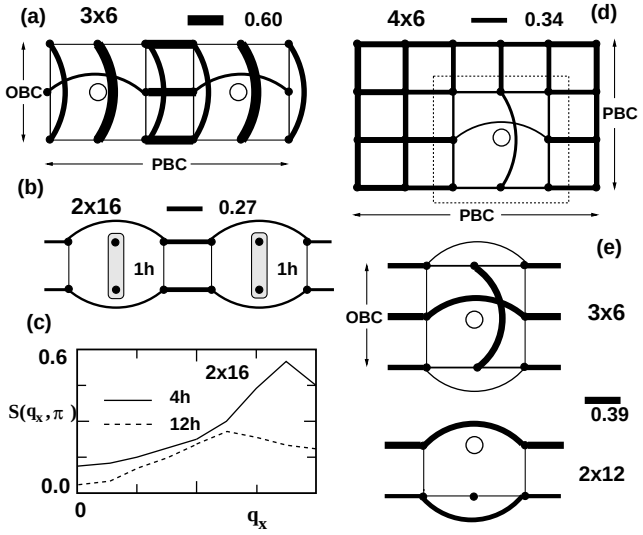

FIG. 3. (a) AF spin correlations for two holes on the 3×6 cluster solved exactly at $J = 0.2$, $t' = -0.35$, and $t'' = 0.25$, with holes projected at their most probable distance in the ground state. (b) AF spin correlations at the center of a 2×32 cluster with 12 holes (OBC—legs) using DMRG at $J = 0.2$, $t' = t'' = 0.0$. Shaded regions contain the holes. (c) $S(q_x, \pi)$ vs q_x for a DMRG 2×16 cluster with 12 and 4 holes and couplings ($J = 0.4$, $t' = -0.35$, $t'' = 0.25$) and ($J = 0.2$, $t' = t'' = 0.0$), respectively. (d) Exact AF spin correlations of the PBC 4×6 cluster with one hole and $\mathbf{q} = (\pi, \pi)$, $J = 0.2$, $t' = -0.35$, and $t'' = 0.25$. An elementary block conjectured to form a part of the stripes is framed. (e) Results for 1 hole as in (d) but for a 2×12 cluster at $J = 0.2$, and a 3×6 cluster at $J = 0.1$, both for $t' = -0.35$, $t'' = 0.25$, and $\mathbf{q} = (0, \pi)$.

(Fig. 3e). Also on small square clusters robust across-the-hole AF correlations exist for one hole. Although spin IC was found in early *t*-*J* model studies [14], and the nontrivial structures as in Fig. 3d were noticed before [6], it was only recently tentatively explained [9] as (local) spin-charge separation, similar to the 1D Hubbard model where spins across holes are antiparallel [19].

The results shown here lead us to believe that the observed doped stripes are made out of one-hole building blocks (Fig. 3d). In this respect the insulator limit already carries the essential information needed to build the stripes, providing an unexpected potential simple link between undoped and doped cuprates. This is compatible with the behavior of the large energy scale PES pseudogap which can be traced back to the one-hole dispersion of the insulator [11], suggesting a smooth evolution from the undoped to underdoped regimes.

However, further elaboration is needed since for one hole the lowest energy is found at $\mathbf{q} \sim (\pi/2, \pi/2)$ [10,14]. Naively, hole pockets at $(\pi/2, \pi/2)$ should appear at finite hole density. In addition, across-the-hole AF bonds are weaker at $(\pi/2, \pi/2)$ than at momenta such as $(\pi, 0)$ or (π,π) [9], although they are still present. To address this issue let us calculate $\langle n_{\mathbf{q}} \rangle = \langle c_{\mathbf{q}}^{\dagger} c_{\mathbf{q}} \rangle$, i.e., the ground-state hole number with a given momentum $\mathbf{q}$ (note that $\langle n_{\mathbf{q}} \rangle$ includes both coherent and incoherent weight).

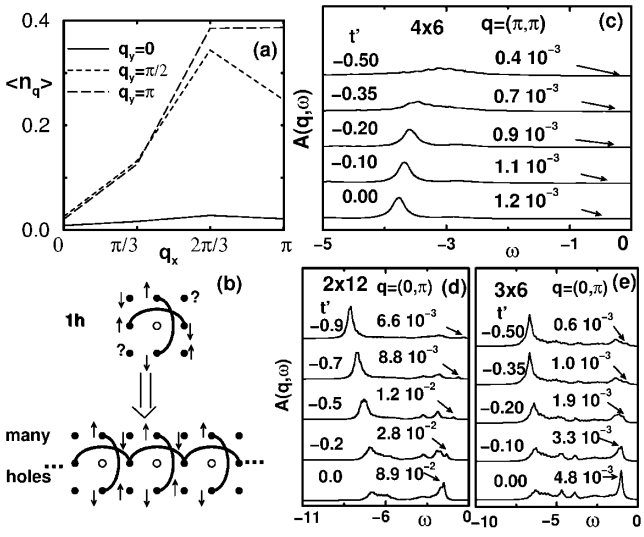

FIG. 4. (a) $\langle n_{\mathbf{q}} \rangle$ vs $\mathbf{q}$, for the two-hole ground state of the 4×6 cluster of Fig. 2b. (b) Qualitative representation of a one-hole state with strong AF correlations across the hole as the building block of $n_h \sim 0.5$ stripes. In the one-hole case the frustration effect is shown with question marks. (c) Exact spectral function $A(\mathbf{q}, \omega)$ for one hole on the 4×6 cluster with PBC in both directions, $J = 0.2$, $\mathbf{q} = (\pi, \pi)$, and $t'/t'' = -1.4$. Values of t' as well as the (small) weight in the first pole (and its location) are indicated. Note the accumulation of weight at large energies. (d) Same as (c) but for a 2×12 cluster with PBC along legs and $\mathbf{q} = (0, \pi)$. (e) Same as (c) but for a 3×6 cluster (PBC—leg; OBC—rung) at $\mathbf{q} = (0, \pi)$.

As an example, consider the two-hole problem on the 4×6 lattice of Fig. 2b. The interesting result in Fig. 4a is that the ground state carries dominant weight at momenta around (π, π), and the one-hole states with this momentum have robust AF correlations across the hole (Fig. 3d), compatible with our conjecture [20]. There are no indications of small hole pockets in our studies, and the Fermi surface appears open. In this framework the across-the-hole correlations of the, e.g., (π, π) or $(\pi, 0)$ holes can be "linked," as pictorially shown in Fig. 4b, improving the hole mobility since now they share a large region where they do not need to fight against the spin background to move. Creating a stripe loop also avoids the spin frustration intrinsic of the individual hole states when across-the-hole robust correlations are present (Fig. 4b). In addition, our results help to better understand the observed stripe density: for $n_h \sim 1$ the across-the-hole AF bonds in the stripe direction cannot form and holes do not improve their kinetic energy, while for a very hole diluted stripe the finite-size elementary blocks (Fig. 3d) do not touch and cannot have a common spin arrangement. For completeness, in Figs. 4c and 4d the one-hole spectral function is exactly calculated on four-, three-, and two-leg ladders at small J/t. Note the remarkable small quasiparticle weight, correlated with a robust across-the-hole AF correlation (see also [9]). The one-hole states contributing to stripes have exotic properties, including a tendency to spin-charge separation [9].

Summarizing, indications of $n_h \sim 0.5$ stripes were found in the extended t-J, t-J_z, and (at small J/t) in the standard t-J models. The gain of kinetic energy against the loss of AF energy appears enough to stabilize stripes, namely, the driving force is a one-hole process and the seed for stripes is already present in the insulator. Contrary to most approaches to stripe formation, here the *small* J/t regime was emphasized. The scenario reported here is a generalization of the 1D spin-charge separation involving individual holons, with the twist that stripes of holons are needed in 2D to avoid frustration. This result is compatible with Zaanen's picture of stripes as "holons in a row" [3]. Charge and spin could be separated in 2D in more subtle ways than anticipated.

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