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 $\pi$-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.

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 $\pi$-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.

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 $t$-$J$, 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

$$H = J \sum_{ij} \left(S_i \cdot S_j - \frac{1}{4} n_i n_j \right) - \sum_{im} t_{im} \left( c_i^+ c_m + H.c. \right) ,$$

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 $J \rightarrow J_z$ and $S_i \cdot S_j \rightarrow S_i^z S_j^z$, 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.
In Fig. 1, DMRG and ORBA results for $4 \times N$ clusters are shown. In Fig. 1a the rung density for a $4 \times 8$ ($4 \times 12$) 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 $t$-$J$ model, and in the $t$-$J$ model $J_c$ is expected to be larger [17]. Similar results are found in the $t$-$J$ 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 $6 \times 6$ 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 $(\pi, \pi)$ 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
are projected into their most probable location (Fig. 2b): a \( \pi \) 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 \( \pi \) shifts appear in other clusters as well. On a cylindrical \( 6 \times 4 \) cluster with PBC along the long direction, the three-hole ground state has characteristics compatible with a doped one-dimensional (1D) closed loop along the PBC direction, with \( \pi \) 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 \( 4 \times 4 \) 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 \( 3 \times 6 \) cluster is shown, with its spin correlations. On two-leg ladders with many holes, \( \pi \) 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 momenta \((\pi, \pi)\). The AF correlations across the hole are similar to the correlations around the individual holes composing the stripes. The \( \pi \)-shift characteristic of the stripes exists in the one-hole state not only at \((\pi, \pi)\) 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. 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 \( q \sim (\pi/2, \pi/2) \) [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 \((\pi, \pi)\) [9], although they are still present. To address this issue let us calculate \( \langle n_q \rangle = \langle c_q^\dagger c_q \rangle \), i.e., the ground-state hole number with a given momentum \( q \) (note that \( \langle n_q \rangle \) includes both coherent and incoherent weight).
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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[13] Truncation error was \( 10^{-5} \) (600 states).
[18] Stripes are like many-holes bound states, but different from the \( d \)-wave pairs of the square lattice.
[20] It appears that the small energy difference \( J \) in favor of \( \pi/2, \pi/2 \) in the one-hole problem [9,14] is not sufficient to prevent the linear stripe formation along an axis. This may be related to the instability toward a spiral state {T. Dombre, J. Phys. (Paris) 51, 847 (1990)].