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

G. B. Martins¹, C. Gazza², J. C. Xavier¹, A. Feiguin¹, and E. Dagotto¹

¹ National High Magnetic Field Lab and Department of Physics, Florida State University, Tallahassee, FL 32306, USA
² Instituto de Física Rosario (CONICET) and Univ. Nac. de Rosario, Bs. 27 de Febrero 210 bis, 2000 Rosario, Argentina

(November 19, 2018)

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 (G. Martins et al., Phys. Rev. B 60, R3716 (1999)). This suggests that the seed of half-doped stripes already exists in the unusual properties of the insulating parent compound.

PACS numbers: 74.20.-z, 74.20.Mn, 75.25.Dw

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. This includes spin-incommensurability (IC) in neutron experiments, results believed to be caused by stripes separating π-shifted AF domains. More recently, it has been shown that the stripes are metallic, result compatible with proposals of the normal state of x=1/8 cuprates as made out of half-doped stripes. Whether stripe formation is detrimental or 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. However, these stripes were insulating with hole density n_h≈1.0, different from the experimental n_h≈0.5 stripes. Recently, considerable progress was made when doped stripes were reported by White and Scalapino within the standard t-J model (see also Ref. [4]). In Ref. [1] 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. However, experiments are usually interpreted as holes moving freely along site-centered stripes. In addition, the “extended” t-J model with hopping near neighboring sites, or the standard t-J model with very small J/t, are needed to reproduce the insulator one-hole photoemission (PES) dispersion. 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 in this Letter indications of n_h≈0.5 stripes compatible with experiments 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). They also exist in the t-J$_z$ model and using classical spins, 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.

The extended t-J model used here is defined as

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

where t_{im} is t=(1) for nearest-neighbors (NN), t’ for next NN, and t’’ for next next NN sites, and zero otherwise. The rest of the notation is standard. The t-J$_z$ model is obtained by J→J$_z$ and $\mathbf{S}_i \cdot \mathbf{S}_j$→$\mathbf{S}_i^z \mathbf{S}_j^z$, and t’<0 and t’’>0 are relevant to explain PES data. Here the Density Matrix Renormalization Group (DMRG) and Lanczos, and an algorithm using a small fraction of the ladder rung-basis (optimized reduced-basis approximation, or ORBA) are used. Results are presented in (i) the small J/t region with t’’=0.0, and (ii) small and intermediate J/t with nonzero t’ and t’’ $\sim 0.5$. These two regions have similar physics, and the extra hoppings are expected to avoid PS. Intuitively, t’,t’’ increase hole mobility, as reducing J/t does, but also avoid ferromagnetism at small J/t. Note also that no coupling fine-tuning is needed: the results below appear in a ro-
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 \( n_0 \sim 0.5 \) stripe formation. \( x \) is the overall hole density. (a) corresponds to a \( 4 \times 8 \) cluster with 4 holes. Solid (dashed) lines are for the standard t-J (t-J\(_2\)) model with \( J=0.2, \ t'=-0.3 \) (inset: same as solid lines but for \( 4 \times 12 \) with 2 holes). (b) Same as (a) but for a \( 4 \times 12 \) cluster with 6 holes, \( J=0.5, \ t'=0.3 \), and \( t''=0.0 \). (c) Hole density at rung \( r \), defined now as \( C(r)=\sum_{i,j} \langle n_{i,j} \rangle \) where the sum is over sites belonging to rung \( r \), \( 0 \) is an arbitrary site of rung \( r=0 \), and \( \langle n_{i,j} \rangle \) is the hole density-density ground-state correlation. The cluster is \( 4 \times 6 \) with PBC in both directions, 4 holes, \( J=0.1, t'=-0.35, \) and \( t''=0.25 \) (ORBA with \( \sim 3 \times 10^6 \) states). The inset shows ground-state energy vs number of states. (d) Distribution of one-hole around the open circle position, for the case in (a) at the indicated rungs (running horizontally). Full circles 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).

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 4 (2) 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. The four holes separate into two groups of two holes, surprising result since for a square lattice \( J_c=0.2 \) is the critical value for hole pair binding in the t-J\(_1\) model, and in the t-J\(_2\) model \( J_c \) is expected to be larger [7]. Similar results are found in the t-J\(_2\) model (Fig.1a) and at intermediate \( J/t \) but with \( t''\neq0 \), which increases the hole mobility: Fig.1b with six holes show 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 2-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 [4]. 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 [3]. These stripes appear to occupy more than one rung in Figs.1a-c, and thus they could also be labeled as bond-centered [8]. 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 3 holes form individual \( n_0 \sim 0.5 \) stripes (invariance under reflexions was assumed along the legs). Overall the results are consistent with Tranquada’s description of stripes [9]. They are also consistent with numerical reports for the standard t-J model [10], although our interpretation of the results (below) is different.

FIG. 2. (a) Rung hole density \( \langle n(r) \rangle \) vs rung index \( r \) using DMRG on a \( 6 \times 6 \) cluster with 6 holes, CBC (OBC along the direction shown with invariance under reflexions assumed), \( J=0.2, \ t'=-0.35, \) and \( t''=0.25 \) (ORBA with \( \sim 3 \times 10^6 \) states). The inset shows ground-state energy vs number of states. (b) Spin-spin correlations for 2 mobile holes projected at their most probable relative distance (circles) in the 2 holes ORBA ground state of a \( 4 \times 6 \) 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 3 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 3 hole, 18 site PBC cluster, \( J=0.4, \ t'=-0.20 \) and \( t''=0.14 \).

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,b. The peak deviation from \( (\pi,\pi) \) appears in a robust region of parameter space. The spin IC is understood calculating spin-spin correla-
tions when two holes in, e.g., the cluster of Fig.1c 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 nh=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 3-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). A 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 nh=0.5 system at large on-site U interactions [11], 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 exist along the stripes, with wavevector π/2 for a half-doped stripe. This spin IC appears also in half-doped 1D models [12]. For an isolated CuO plane, IC should be present in both directions, although with quite different wavevectors and intensities.

Similar results are found in small square clusters: in the 2-holes 4×4 lattice with CBC, a 2-hole stripe forms along the PBC direction [13]. 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 [14]. Tendency to stripe formation is found even in tilted clusters: the PBC \(\sqrt{18}\times\sqrt{18}\) lattice allows for nh=0.5 closed loops with 3 holes and such structure has a large ground-state weight (Fig.2d) [13]. Precursors of the spin structures in Figs.1,2 appear on 2- and 3-leg ladders as well, e.g. in Fig.3a the 2 holes ground-state dominant hole configuration of a 3×6 cluster is shown, with its spin correlations. On 2-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 2-leg (Fig.3c) and 3-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. Fig.3d shows 4-leg ladder spin correlations around a mobile hole for momentum (π,π). The AF correlations across-the-hole are clearly 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, and, in this sense, the spin IC exists already at the one-hole level, a remarkable result. Similar conclusions are reached for 3- and 2-leg ladders (Fig.3e), and other momenta such as (0,π). Also on small square clusters robust across-the-hole AF correlations exist for one hole. Although spin IC was found in early studies of the t-J model [14], and the nontrivial structures as in Fig.3d were noticed before [11,12], it was only recently tentatively explained [15] as (local) spin-charge separation, similar to the 1D Hubbard model where spins across holes are antiparallel [19].

![FIG. 3.](image_url) (a) AF spin correlations for 2 holes on the 3×6 cluster solved exactly at J=0.2, t′=-0.35, 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,π) vs q, for a DMRG 2×16 cluster with 12 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 q=(π,π), J=0.2, t′=t″=0.35, and t″′=0.25. An elementary block conjectured to form part of 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 q=(π,0,π).

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=(π/2,π/2) [10,13]. Naively, hole pockets at (π/2,π/2) should appear at finite hole density. In addition, across-the-hole AF bonds are weaker at (π/2,π/2) than at momenta such as (π,0) or (π,π) [12], although they are still present. To address this issue let us calculate \(\langle n_q\rangle=\langle c_{q\uparrow}c_{q\downarrow}\rangle\), i.e. the ground-state hole number with a given momentum q (note that \(\langle n_q\rangle\) includes both coherent and incoherent weight). As example, consider the two-hole problem on the 4×6 lattice of Fig.2b. The interesting result in Fig.4a is that...
FIG. 4. (a) \( n_h \) vs \( q \), for the 2 hole ground-state of the \( 4 \times 6 \) 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 1 hole case the frustration effect is shown with question marks. (c) Exact spectral function \( A(q, \omega) \) for one-hole on the \( 4 \times 6 \) cluster with PBC in both directions, \( J=0.2 \), \( q=(\pi, \pi) \) 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 \( 2 \times 12 \) cluster with PBC along legs and \( q=(0, \pi) \); (e) Same as (c) but for a \( 3 \times 6 \) cluster (PBC-leg, OBC-rung) at \( q=(0, \pi) \).

The ground state carries dominant weight at momenta around \( (\pi, \pi) \), and the one-hole states with this momentum have robust AF correlations across-the-hole (Fig.3d), compatible with our conjecture [21]. 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., \( (\pi, \pi) \) 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 understanding better 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,d the one-hole spectral function is exactly calculated on 4-, 3- and 2-leg ladders at small \( J/t \). Note the remarkable small quasiparticle weight, correlated with a robust across-the-hole AF correlation (see also [3]). The one-hole states contributing to stripes have exotic properties, including a tendency to spin-charge separation [3].

Summarizing, indications of \( n_h \sim 0.5 \) stripes were found in the extended t-J, t-J\(_2\), 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 Zaenen’s picture of stripes as “holons in a row” [3]. Charge and spin could be separated in 2D in more subtle ways than anticipated.

The authors thank R. Eder, S. White and J. Zaenen for useful comments and NSF (DMR-9814350), FAPESP-Brazil, and Fundación Antorchas for support.

[1] J. M. Tranquada et al., Nature 375, 561 (1995); P. Dai et al., Phys. Rev. Lett. 80, 1738 (1998).
[2] N. Ichikawa et al., cond-mat/9910037.
[3] J. Zaenen, J. Phys. Chem. Solids 59, 1769 (1998).
[4] V. Emery et al., Phys. Rev. B56, 6120 (1997); J. Zaenen and O. Gunnarsson, Phys. Rev. B40, 7391 (1989); B. Stojkovic et al., Phys. Rev. Lett. 82, 4679 (1999).
[5] \( n_h \sim 1.0 \) stripes are unstable for realistic couplings (T. Toyota et al., Phys. Rev. B59, R11649 (1999))
[6] S. White and D. Scalapino, Phys. Rev. Lett. 80, 1272 (1998); Phys. Rev. B55, 6504 (1997); cond-mat/9907301.
[7] C. Buhler, S. Yunoki and A. Moreo, Phys. Rev. Lett. 84, 2690 (2000).
[8] S. White and D. Scalapino, cond-mat/9610104.
[9] G. Martins et al., Phys. Rev. B60, R3716 (1999).
[10] A. Nazarenko et al., Phys. Rev. B 51, 8676 (1995); V. I. Belinicher et al., Phys. Rev. B 54, 14914 (1996); R. Eder et al., Phys. Rev. B55, R3414 (1997); F. Lema and A. Aligia, Phys. Rev. B55, 14092 (1997); C. Kim et al., Phys. Rev. Lett. 80, 4245 (1998).
[11] F. Ronning et al., Science 282, 2067 (1998). See also R. Laughlin, Phys. Rev. Lett. 79, 1726 (1997).
[12] In agreement with retraceable-path calculations by A. Chernyshev, A. Castro Neto and A. Bishop, cond-mat/9909128.
[13] Truncation error was \( \sim 10^{-5} \) (600 states).
[14] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).
[15] E. Dagotto et al., Phys. Rev. B58, 12063 (1998).
[16] PS in the t-J model (small \( J/t \)) is still debated: C. Helmberg and E. Manousakis, Phys. Rev. Lett. 83, 132 (1999); S. White and D. Scalapino, ibid. 84, 3021 (2000); M. Candlandra and S. Sorella, cond-mat/9911478.
[17] J. Riera and E. Dagotto, Phys. Rev. B47, 15346 (1993); D. Poilblanc et al., Phys. Rev. B49, 12318 (1994).
[18] Stripes are like many-holes bound states, but different from the d-wave pairs of the square lattice.
[19] M. Ogata and H. Shiba, Phys. Rev. B 41, 2326 (1990).
[20] For the N=18 cluster, “diagonal” 3-hole loops can also be formed. They carry across-the-stripe \( \pi \)-shifts and substantial ground-state weight.
[21] It appears that the small energy difference \( J \) in favor of \( \pi/2, \pi/2 \) in the one-hole problem [3] is not sufficient to prevent the linear stripe formation along an axis. This may be related with the instability toward a spiral state (T. Dombre, J. Phys. France 51, 847 (1990)).