Stripes in the Ising limit of models for the cuprates

G. B. Martins,1 C. Gazza,2 and E. Dagotto1

1National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, Florida 32306
2Instituto de Física Rosario (CONICET) and Universidad Nacional de Rosario, 2000 Rosario, Argentina

(Received 19 June 2000)

The hole-doped standard and extended $t$-$J$ models on ladders with anisotropic Heisenberg interactions are studied computationally in the interval $0.0 \leq \lambda \leq 1.0$ ($\lambda = 0$, Ising; $\lambda = 1$, Heisenberg) at small $J/t$. It is shown that the approximately half-doped stripes recently discussed at $\lambda = 1$ survive in the anisotropic case ($\lambda < 1.0$), particularly in the “extended” model. Due to the absence of spin fluctuations in the Ising limit and working in the rung basis, a simple picture emerges in which the stripe structure can be mostly constructed from the solution of the $t$-$J$ model on chains. A comparison of results in the range $0.0 \leq \lambda \leq 1.0$ suggests that this picture is valid up to the Heisenberg limit.

In recent years, evidence has been accumulating that at least in one family of high-temperature superconducting compounds (La$_{2-x}$Sr$_x$CuO$_4$) one-dimensional (1D) charged stripes are formed upon hole doping of the insulating parent material.1 Although the presence of stripes in other compounds such as YBa$_2$Cu$_3$O$_{6+x}$ is still controversial,2 a large theoretical effort has been focused on the search for stripes in models for the cuprates. Early results reported stripes in Hartree-Fock treatments of the Hubbard model and also in the phase-separated regime of the $t$-$J$ model upon the introduction of long-range Coulomb interactions.3,4 However, these stripes have a hole density $n_h = 1.0$ in contradiction with the $n_h = 0.5$ density found experimentally.1,5 Improving upon this situation, recent studies of the $t$-$J$ model6,7 reported stripes with $n_h < 1.0$ at intermediate values of $J/t$, sometimes described as a condensation of $d$-wave pairs.8 However, the mechanism leading to $n_h < 1.0$ stripes, and even the presence of a striped ground state in the $t$-$J$ model at intermediate couplings, is still under discussion.9 In addition, evidence is accumulating that the pure $t$-$J$ model is not sufficient for the cuprates, and its “extended” version with hopping beyond nearest-neighbor sites10,11 is needed to explain photoemission spectroscopy (PES) results for the insulators.12

Very recently, indications of half-doped stripes have been found by Martins et al. in the extended $t$-$J$ model.13 They were also observed at small $J/t$ in the standard $t$-$J$ model, in both cases in regimes where two holes do not form bound states. This led to a novel rationalization of stripes as the natural way in which spin-charge separation is achieved in two-dimensional systems,13 similarly as in the phenomenological “holons in a row” picture.3 Moreover, stripes appear to emerge directly from the one-hole properties of the insulator,13 where holes have strong “across the hole” antiferromagnetic (AF) correlations11,14 in their (frustrated) effort to achieve spin-charge separation, similarly as it occurs in 1D systems.15

In spite of this progress, more work is needed to understand these complex striped states. An important issue is the role played by fluctuations in the spin sector. While the presence of a spin tendency to form an AF background is crucial for stripe formation, it is unknown whether the fine details of the spin sector (such as the presence of low-energy excitations) are important for its stabilization. To address this question, here a computational study is reported where the spin interaction contains an Ising anisotropy. Our main result is that stripes survive the introduction of this anisotropy, and a fully SU(2)-symmetric interaction is not needed for stripe formation. This result is in agreement with recent retraceable-path calculations for the $t$-$J$ model.16

The anisotropic extended $t$-$J$ model is defined as

\[
H = J \sum_{\langle ij \rangle} \left[ S_i^+ S_j^- + \frac{\lambda}{2} (S_i^+ S_j^- - S_i^- S_j^+) - \frac{1}{4} n_i n_j \right] - \sum_{im} t_{im} (c_i^+ c_m + H.c.),
\]

where $t_{im}$ is $t = 1$ for nearest-neighbors (NN) hopping between sites $i$ and $m$, $t'$ for next NN, $t''$ for next-next NN, and zero otherwise. The anisotropy in the spin sector is controlled by $\lambda$ ($\lambda = 0$, Ising; $\lambda = 1$, Heisenberg). The rest of the notation is standard. $t' = -0.35$ and $t'' = 0.25$ are believed to be relevant to explain PES data.10–12 The computational work is carried out using the density matrix renormalization group (DMRG) and Lanczos techniques, as well as an algorithm using a small fraction of the ladder rung basis [optimized reduced-basis approximation (ORBA)].

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 $t''$, in both cases working at $\lambda = 0.0$, 0.25, 0.50, and 1.00. These two regions (i) and (ii) have similar physics,11 and the extra hoppings are expected to avoid phase separation.9,20

To start our investigation, let us analyze the one-hole properties of the model, Eq. (1). Previous studies found a robust AF correlation between spins across the hole ($C_{AH}$),11,14 namely, between the spins separated by two lattice spacings located on both sides of a hole (working in the reference frame of the latter). This curious feature was interpreted as a short-distance tendency toward spin-charge separation,11 and it is believed to be crucial for stripe formation.13 It is important to clarify if similar correlations are still present in the anisotropic case. For this purpose, here 4×4 and 4×6 clusters were used with periodic boundary conditions (PBC), as well as cylindrical boundary cond-
are reached in the spin-polarized background. Calculating the NN correlations is dangerous for the stripe formation, which will not support this interpretation. Fortunately, the results are also in agreement with an early analysis by Barnes et al. that reported a reduction in the FM tendency upon an increase of spin correlations for values of $\lambda$ where the one-hole system did not have a robust AF $C_{AH}$. For the standard $t$-$J$ model at $J=0.2$, $t'=t''=0.0$, also shown in Fig. 2, the situation is less clear and in some cases the correlations become FM at $\lambda=0.0$, but in most situations they remain AF. In the extended $t$-$J$ model the stripe tendency is clearly stronger than in its standard version. Previous studies at $\lambda=1.0$ showed the coexistence of two or more $n_h=0.5$ stripes at hole density $x=1/8$ on four-leg ladders as the number of holes increases in a CBC cluster. It is important to show that this stripe phase survives the decrease of the spin fluctuations. That this is the case can be observed in Fig. 3 where DMRG results for the rung density $\langle n(r) \rangle$ vs the rung label $r$ are presented for a $4 \times 8$ cluster.
with four holes \((J = 0.3, t' = t'' = 0.0; \text{CBC})\). Figure 3 shows that from \(\lambda = 1.0\) down to \(\lambda = 0.25\) the two \(n_h = 0.5\) stripes are virtually unaltered. On the other hand, at \(\lambda = 0.0\) the FM tendency already discussed in the two-hole case of Fig. 2 prevents the formation of stripes in the standard \(t-J\) model. This problem does not occur in the extended version with \(t' < 0\) and \(t'' > 0\).

Let us now analyze the spin structure around the stripe once the spin fluctuations are fully turned off \((\lambda = 0.0)\). In Fig. 4(a), a stripe configuration with a clear \(\pi\) shift across the stripe is shown for a CBC \(4 \times 6\) cluster with two holes at \(\lambda = 0.0\). This dominant hole configuration was projected out of the ground state of an ORBA calculation where \(\approx 10^6\) states were kept in the rung basis. The couplings \((J = 0.2, t' = 0.0, t'' = 0.25)\) differ slightly from those in Fig. 2, but the results are representative and they are similar to those found at \(\lambda = 1.0\).\(^{25}\)

It is expected that the suppression of spin fluctuations would simplify the description of a ground state like the one in Fig. 4(a), either in the rung or \(S_z\) basis, since fewer states are needed to represent the spin background. Indeed the combination of CBC with the use of a rung basis (along the PBC direction) leads to a fairly simple description of such a state.

This can be observed in Fig. 4(b), where the spin correlations were calculated on a CBC \(4 \times 4\) cluster with two holes [same coupling as in Fig. 4(a)] using only the eight highest-weight rung-basis states out of the full ground state of the system, which has a total of \(102,960\) states. The results are very similar to those found with the full ground state and they capture the basic physics contained in the full calculation. The picture that emerges is the following: the spin correlations along the stripe are maximized — i.e., the two spins on it are locked in a singlet — implying that their correlations with the rest of the spins vanish. This means that in the “snapshot” of the ground state [Fig. 4(b)] the stripe is disconnected from the rest of the cluster, emphasizing its 1D character. In fact the only rung state that contains holes in the eight most dominant states kept in Fig. 4(b) is the ground state of the two-hole sector of a simple four-site ring calculation. This establishes a strikingly simple connection of the stripe problem with a truly 1D calculation. The “recipe” to construct a good representation of the stripe state is to consider the solution of half-doped 1D chains as a stripe, and antiferromagnetically couple the rest of the spins of the plane simply as if those stripes would be absent (thus generating the \(\pi\) shift across the stripes). This is a natural generalization to two dimensions of the 1D spin-charge separation concept, as emphasized in Ref. 13, where the spin portion of the wave function is constructed simply ignoring the holes.\(^{15}\) In 2D now it is the stripes that are ignored by the spins not belonging to them in their wave function. It is also important to notice that this picture appears to hold, in its main aspects, even at \(\lambda = 1.0\).

For completeness, in Fig. 5(a), ORBA results (with \(\approx 2 \times 10^6\) states kept in the rung basis) are presented for \(\langle n(r)\rangle\) vs \(r\), showing two \(n_h = 0.5\) stripes with two holes each. The calculation was performed with CBC. In Fig. 5(b) details of the spin correlations are shown, with the most probable hole configuration projected out of the ORBA ground state. At \(\lambda = 0.0\) a very good convergence in the ORBA method can be achieved: starting with initial states where the holes are uniformly distributed or phase separated, a fast convergence leads to the stripe results of Fig. 5(b).

FIG. 3. Rung hole density \(\langle n(r)\rangle\) vs rung index \(r\) calculated using the DMRG technique (243 states) on a \(4 \times 8\) cluster with four holes, CBC (OBC along the direction shown, with invariance under reflections assumed).

FIG. 4. (a) Spin-spin correlations for two mobile holes projected at their most probable configuration (circles) in the two-hole ORBA ground state of a \(4 \times 6\) cluster using CBC \((k_s = 0)\), \(J = 0.2, t' = 0.0, t'' = 0.25, \text{ and } \lambda = 0.0\). Solid lines indicate AF correlations (thickness proportional to absolute value); dashed lines indicate ferromagnetic correlations. (b) AF spin-spin correlations of the CBC \(4 \times 4\) cluster with two holes projected at their most probable distance. This result was obtained keeping just the eight-rung-basis states with the highest weight in the ground state (out of a full Hilbert space with 102,960 states). Same couplings and momentum as in (a). This approximation emphasizes the 1D character of the stripe; note also that the stripe formed by this procedure is completely decoupled from the rest of the cluster.

FIG. 5. (a) Rung hole density \(\langle n(r)\rangle\) vs rung index \(r\) calculated using the ORBA on a \(4 \times 6\) cluster with four holes, \(J = 0.2, t' = 0.0, t'' = 0.25, \text{ and } \lambda = 0.0\), using CBC with \(k_s = 0\). (b) Spin-spin correlations for four mobile holes at their most probable configuration in the four holes ORBA ground state of (a).
Summarizing, it has been shown that the striped states recently identified in models for the cuprates survive the introduction of an Ising anisotropy, particularly in the extended $t$-$J$ model. The important physics that stabilizes stripes appears to be the competition between spins that order antiferromagnetically and holes that need to modify the spin environment to improve their movement, leading to an interesting potential extension into 2D of the familiar 1D spin-charge separation ideas. The approach discussed here focuses on the small-$J/t$ limit, and it appears unrelated with others based on the large-$J/t$ phase-separated region. The fine details of the spin background do not seem important, and as a consequence doped stripes should be a general phenomenon in correlated electronic systems.

The authors thank NSF (DMR-9814350), the NHMFL (In-house Research Program), Fundacion Antorchas and MARTECH for partial support.

---

14. These correlations were also noticed in S.R. White and D.J. Scalapino, Phys. Rev. B 55, 6504 (1997).
17. Truncation error was $\sim 10^{-5}$ (800 states).
21. Fortunately, there is a weak dependence on boundary conditions: the results for CBC calculations, with correlations measured along the PBC direction, are qualitatively the same as for the PBC calculations for all couplings studied. The results along the OBC direction, although not very different, show some variation when compared to the results along the PBC direction: on average $C_{HH}$ is more AF in the OBC direction and its dependence with $\lambda$ is less monotonic than in the PBC direction.
23. As it occurs in the Nagaoka state of the one-hole sector of the $t$-$J$ model, which as the cluster grows is stabilized at smaller $J/t$, reaching the $J/t=0.0$ limit in the bulk (Ref. 18).
24. The results thus far are not in contradiction with our recent interpretation of stripe formation as related to the one-hole properties (Ref. 13), since this simple argument holds as long as the overall tendency in the spin sector is toward an AF state. Once ferromagnetism competes for one hole, the state that induces stripes upon further doping is now an excited state.
25. Note that in average all AF correlations (across holes and between NN spins) uniformly decrease with $\lambda$. The maximum AF correlation at zero doping for $\lambda=0.0$ is $-0.25$ and for $\lambda=1.0$ is $\approx -0.35$.
26. In the intermediate $J/t$ region it is still unclear whether stripes or a hole-paired state is stable.