Stripes in the Ising limit of models for the cuprates

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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 ($La_{2-x}Sr_xCuO_4$) 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 $YBa_2Cu_3O_{6+\delta}$ 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 model[6,7] 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 sites[10,11] 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) correlations[11,14] 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 excita-

tions) 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_z model.[16]

The anisotropic extended t-J model is defined as

$$H = J \sum_{\langle \mathbf{ij} \rangle} \left[S^z_{\mathbf{i}} S^z_{\mathbf{j}} + \frac{\lambda}{2}(S^+_{\mathbf{i}} S^-_{\mathbf{j}} + S^-_{\mathbf{i}} S^+_{\mathbf{j}}) - \frac{1}{4} n_{\mathbf{i}} n_{\mathbf{j}} \right]$$
$$- \sum_{\mathbf{im}} t_{\mathbf{im}}(c^\dagger_{\mathbf{i}} c_{\mathbf{m}} + \text{H.c.}), \qquad (1)$$

where $t_{\mathbf{im}}$ is $t(=1)$ for nearest-neighbors (NN) hopping between sites $\mathbf{i}$ and $\mathbf{m}$, t' for next NN, t'' for next-next NN, and zero otherwise. The anisotropy in the spin sector is controlled by λ ($\lambda = 0$, 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[6,17] (DMRG) and Lanczos[18] techniques, as well as an algorithm using a small fraction of the ladder rung basis [optimized reduced-basis approximation[19] (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 cilindrical boundary condi-
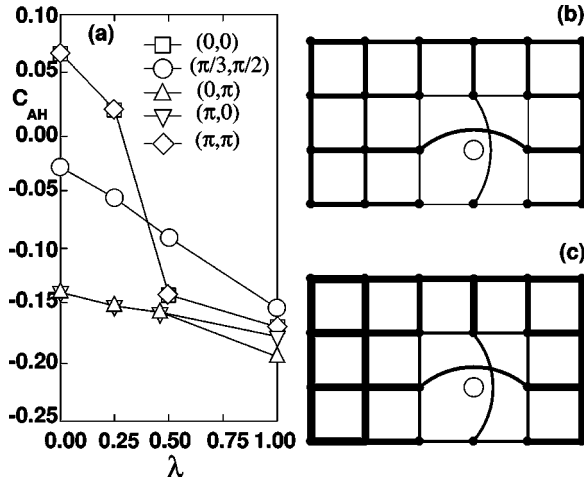
FIG. 1. (a) Exact diagonalization calculations of across-the-hole spin-spin correlations (C_{AH}) vs λ for several momenta on a 4×6 cluster with one hole, PBC, $J=0.2$, $t'=-0.35$, and $t''=0.25$. The results shown are for the long direction. (b) AF spin-spin correlations for (a) at $(\pi,0)$ and $\lambda=0.0$. (c) AF spin-spin correlations for (a) at (π,π) and $\lambda=0.5$. In (b) and (c) the hole is projected from the ground state to the site shown, and the dark lines represent AF spin-spin correlations with a thickness proportional to its absolute value.

tions (CBC) [open boundary conditions (OBC) along legs and PBC along rungs[6]], for several different couplings.[21] The results for C_{AH} in the one-hole lowest-energy state at several momenta are shown in Fig. 1(a) using a PBC 4×6 cluster, at a representative coupling set. At $\lambda=1.0$ all the correlations are negative, compatible with the results in Refs. 11 and 13. As λ is reduced, the magnitude of C_{AH} decreases but it remains negative for the momenta of most relevance, namely, $(\pi/3,\pi/2)$ [the closest on the 4×6 cluster to $(\pi/2,\pi/2)$] and $(0,\pi)$-$(\pi,0)$. In Fig. 1(b) the AF spin correlations are shown at $(0,\pi)$ and $\lambda=0.0$. There is a good agreement with the results observed in the $\lambda=1.0$ limit.[11] Similar conclusions are reached in the (π,π) case [Fig. 1(c)] at moderate anisotropy and for $(\pi/3,\pi/2)$ (not shown), although in this case the correlation along the short direction is approximately zero. The across-the-hole correlations remain even with Ising anisotropy.

On the other hand, for momenta $(0,0)$ and (π,π) with PBC (and also at $k_y=0$ and π, with CBC) a transition to a *ferromagnetic* (FM) correlation occurs at small λ. This tendency is dangerous for the stripe formation, which will not occur in a spin-polarized background. Calculating the NN spin correlations *without* hole projection, i.e., involving all the links of the cluster for several couplings and $0.0 \leqslant \lambda \leqslant 1.0$, similar trends were observed, including the change of sign for $\lambda \to 0.0$. This suggests that the C_{AH} λ dependence at $(0,0)$ and (π,π) for the one-hole results can be ascribed to an overall decrease of the AF tendency on the clusters studied, which is replaced by a tendency toward ferromagnetism. A comparison of data at several couplings and lattice sizes supports this interpretation. Fortunately, the results are also in agreement with an early analysis by Barnes *et al.*[22] that reported a reduction in the FM tendency upon an increase of the cluster size for the Ising limit of the t-J model. Thus, it is believed that the FM state found in some sectors of the one-
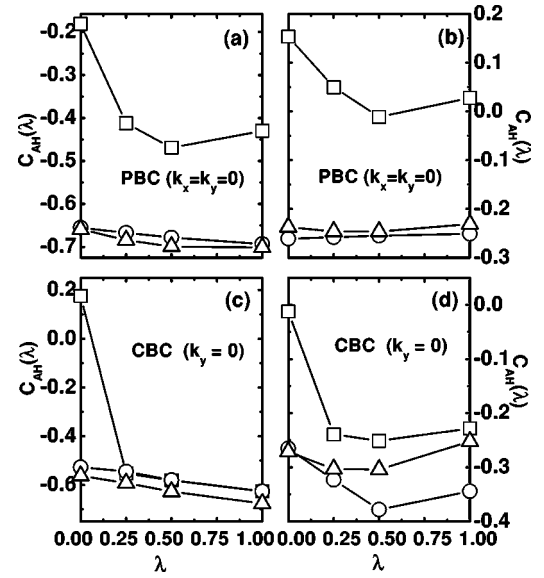

FIG. 2. Spin-spin correlations vs λ for the most probable ground-state hole configuration (stripe) using 4×4 clusters with two holes, PBC and CBC. (a) Spin-spin correlations across the hole calculated along the stripe; PBC were used in both directions. Squares are for $J=0.2$ and $t'=t''=0.0$; circles for $J=0.2$, $t'=-0.35$, and $t''=0.25$; and triangles for $J=0.4$, $t'=-0.35$, and $t''=0.25$. In all three cases $k_x=k_y=0$. (b) Same as (a) but now the spin-spin correlations across the hole are calculated across the stripe. (c) Same as (a) but now using CBC $k_y=0$ (the stripe runs along the PBC direction). (d) Same as (b) but now using CBC $k_y=0$.

hole problem at finite J will disappear as the clusters grow.[23] In fact, if a compromise between couplings and cluster size is followed to avoid the FM region, the qualitative "shape" of the $\lambda=1.0$ one-hole wave function can be preserved as $\lambda \to 0.0$. In conclusion, the FM tendency in some subspaces of the one-hole sector is expected not to be detrimental to stripe formation, and studies with more holes shown below support this view. Nevertheless, care must be taken with the stripe-FM competition in these systems.

Consider now two holes on four-leg ladders. Similarly as in Ref. 13, stripes are formed with the two holes mainly located at two lattice spacings along the rung. Then, correlations along and across the stripe must be considered separately. As in Fig. 2, the introduction of a second hole on a 4×4 cluster using the *extended* t-J model stabilizes robust C_{AH} both along and across the stripe, in PBC and CBC, even for values of λ 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.[24]

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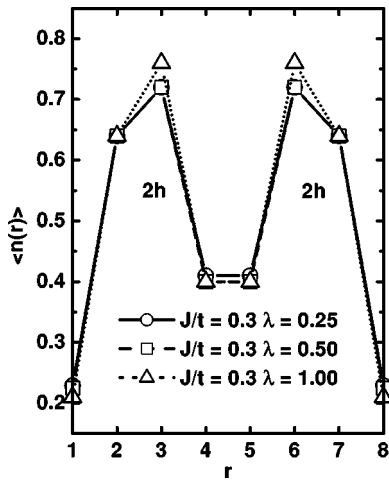
FIG. 3. Rung hole density $\langle n(r) \rangle$ vs rung index r using the DMRG technique (243 states) on a 4×8 cluster with four holes, CBC (OBC along the direction shown, with invariance under reflections assumed).

with four holes ($J = 0.3$, $t' = t'' = 0.0$; 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 π shift across the stripe is shown for a CBC 4×6 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]
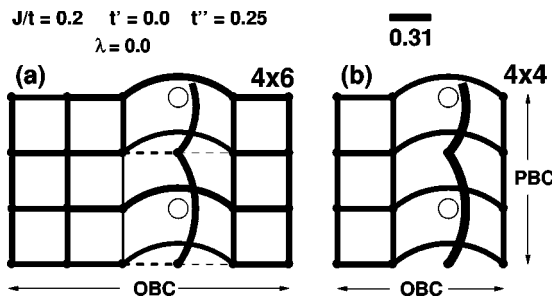

FIG. 4. (a) Spin-spin correlations for two mobile holes projected at their most probable configuration (circles) in the two-hole ORBA ground state of a 4×6 cluster using CBC ($k_y = 0$), $J = 0.2$, $t' = 0.0$, $t'' = 0.25$, and $\lambda = 0.0$. Solid lines indicate AF correlations (thickness proportional to absolute value); dashed lines indicate ferromagnetic correlations. (b) AF spin-spin correlations of the CBC 4×4 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). 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.
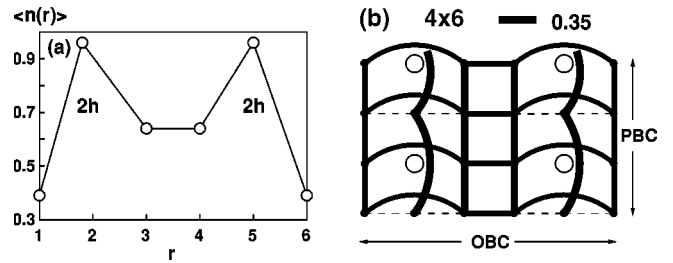

FIG. 5. (a) Rung hole density $\langle n(r) \rangle$ vs rung index r calculated using the ORBA on a 4×6 cluster with four holes, $J = 0.2$, $t' = 0.0$, $t'' = 0.25$, and $\lambda = 0.0$, using CBC with $k_y = 0$. (b) Spin-spin correlations for four mobile holes at their most probable configuration in the four holes ORBA ground state of (a).

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 Sz 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 4×4 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 π 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).

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.[26] 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.

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[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_{AH} is more AF in the OBC direction and its dependence with λ is less monotonic than in the PBC direction.

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[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 λ. The maximum AF correlation at zero doping for $\lambda=0.0$ is -0.25 and for $\lambda=1.0$ is ≈ -0.35.

[26] In the intermediate J/t region it is still unclear whether stripes or a hole-paired state is stable.