Quantum Monte Carlo simulations of the t-J_z model with stripes on the square lattice

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Finite temperature quantum Monte Carlo simulations are performed on the anisotropic t-J model and in particular on its Ising limit. Straight site-centered stripes are imposed by an on-site potential representing external mechanisms of stripe formation. In this model, we show that, even though charge inhomogeneity exists at a high temperature, the antiphase ordering of the spin domains between stripes occurs at a much lower temperature. The magnetic correlations at this spin ordering crossover are analyzed. The stripes show metallicity, with absence of hole attraction. Comparison between this model and others that have been proposed to explain or describe stripes, as well as possible relations with experimental features on underdoped cuprates are discussed.

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The nature of the underdoped region and of the pairing mechanism in high-T_c cuprates is still a matter of strong controversies. From the experimental point of view, the relationship between the pseudogap (PG) and the superconducting gap (SG) is still under intense discussion. Older data suggested a pseudogap smoothly connecting with the superconducting gap[1] while some more recent studies[2,3] emphasize a different origin and behavior of the PG and the SG, the PG ending inside the superconducting phase at a ''quantum critical point.''[4] From the theoretical point of view, the stripe scenario, which is an almost unavoidable consequence of neutron experiments results on $La_{2-x}Sr_xCuO_4$ (Refs. 5,6) and perhaps on $YBa_2Cu_3O_{6+\delta}$,[7] offers a natural explanation for PG. Consistently with the experimental controversy about the nature of PG, there are widely diverging views about the origin of stripes and its relationship with superconductivity. In the theory by Emery, Kivelson and co-workers,[8] the pseudogap is identified with the SG and stripes are a key ingredient to explain superconductivity in the cuprates. In another view,[9] stripes are regarded as competing with a uniform gas of hole pairs and hence with superconductivity. In yet another approach, the stripes exclude hole pairing.[10] There are even more important differences regarding the origin of stripes. In Ref. 8, charge inhomogeneity appears as a combined effect of phase separation and long-range Coulomb repulsion and the stripe phase can be thought as a Wigner crystal. According to White and Scalapino,[9] stripes are already present in the simple t-J model at physical values of the parameters. In Ref. 10, the driving mechanism is the formation of strong singlets across a hole. In this sense, the stripes may be regarded as domain walls.[11] On the other hand, in some other views, the stripes are not inherent to two-dimensional (2D) extended t-J models but are due to, for example, electron-phonon coupling.[12,13] Following these alternative views, in this paper we formulate a model assuming that the origin of stripes in the cuprates is nonintrinsic to the 2D electronic correlations and our main goal is to examine the physically relevant properties of such model.

It is also well known the difficulty of studying microscopic models of correlated electrons either by analytical or numerical techniques. The already mentioned work on variants of the t-J model by using the DMRG method[9,10] is affected by limitations of this method, particularly the open boundary conditions adopted. The widely used Lanczos diagonalization could not deal with clusters large enough to reproduce the charge inhomogeneities. In the present study, we use the conventional finite temperature quantum Monte Carlo (QMC) method (world-line algorithm)[14] which allows the study of reasonable large clusters with fully periodic boundary conditions. As it is well-known, QMC simulations of fermionic models are affected by strong ''minus sign problem''[15] that virtually makes impossible these kinds of studies at very low temperatures. However, as we discuss below, in the model we consider the ''minus sign problem'' is not as much severe as in the plain 2D t-J model, and hence we are able to look at physical features which appear at not too low temperatures.

Let us first introduce the model here studied. In the first place, as in many other studies on this subject,[16–20] we impose the presence of straight site-centered stripes by an on-site potential. This on-site potential represents the effects of Coulomb potential due to out-of-plane ions, electron-phonon coupling, a-b plane anisotropy or other structural details, etc. Since in-plane long-range Coulomb repulsion can not be included in QMC simulations, its effects can eventually also be represented by the on-site potential. The confinement of holes to the stripes strongly reduces the ''minus sign problem.'' As we show below, this problem strongly constrains the values of the on-site potential accessible in the simulations. A further alleviation of this problem comes from reducing quantum spin fluctuations. We are thus lead to an anisotropic t-J model, and in the Ising limit to the so-called t-J_z model.[21,22] Again, the ''minus sign problem'' strongly constrains the off-diagonal exchange term we can deal with. On the other hand, this Ising limit is not only convenient from the numerical point of view but has an additional value, specially if one is interested in finite temperature effects. In fact, a three-dimensional (3D) AF (short- or long-range) order would imply, at a mean-field level, a staggered field acting on the 2D t-J model and in turn would induce an enhancement of the zz-component of the Heisenberg term as a second order process.

The Hamiltonian of the anisotropic t-J model is

$$H_{tJ} = -t \sum_{\langle ij \rangle, \sigma} (\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} \left(\frac{\gamma}{2} (S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z - \frac{1}{4} n_i n_j \right) \quad (1)$$

where the notation is standard. The stripes are induced by an effective on-site potential[23]

$$H_{\text{str}} = \sum_i e_{si} n_i , \quad (2)$$

$e_{si} = -2e_s < 0$ ($2e_s$) for sites on (outside) the stripe. Then, the total Hamiltonian of our model is $H = H_{tJ} + H_{\text{str}}$. Most of our calculations were performed on an 8×8 cluster with fully periodic boundary conditions and with eight holes which corresponds to a filling of $x = 1/8$. The imposed stripes involves columns separated by three-leg ladders, as in the original picture in Ref. 5.

Our simulations were done at $J/t = 0.35$, a value generally accepted to describe the cuprates, and also at $J/t = 0.7$. In this second case, we have seen essentially the same physical behavior but at a higher temperature scale and with a milder minus sign problem. As usual, t is chosen as the unit scale of energy and temperature. e_s was varied between 0.3 and 2.0, and $\gamma = 0.0$ (the Ising limit), 0.25 and 0.5 were examined. In the limit $e_s \to \infty$ each stripe would be at quarter filling. Simulations were also performed for the 12×12 cluster with twelve holes and also two equidistant stripes. This corresponds to a smaller density $x = 1/12$ and the spin domains in between the stripes are five-leg ladders.

The QMC algorithm employed is a straightforward extension of the world-line one successfully used to study the 2D Heisenberg model.[14] In addition to the cube and plaquette local moves, we have kept the global moves that change the total S_z of the system. Most of the calculations were performed with $\tau = \beta/M = 0.083$, where $\beta = 1/T$ and M is the Trotter number. The average of the sign of $\exp -\beta H$, is shown in Fig. 1(a). It can be seen that $\langle \text{sgn} \rangle$ is smaller for larger γ and for smaller e_s. In few words, the more isotropic is the spin space and the more homogeneous is the hole movement in real space, the worse becomes the minus sign problem. In Fig. 1(b), the hole occupancy of sites on the stripes are shown as a function of temperature for various sets of parameters (J, e_s, and γ). As expected, the stripe filling increases monotonically as T decreases. At large temperature there is already a filling of the stripes larger than the nominal one ($x = 1/8$) and it is driven solely by the on-site potential. As the temperature goes to zero, the stripe density saturates at a value smaller than 1/2 and it is apparent a small dependence on J, i.e., there is a correction due to the magnetic correlations of the t-J model. In Fig. 1(c), the hole density profile is shown for $J = 0.35$ and several values of e_s at the lowest temperatures reached. The sharpness of these profiles could be measured by neutron scattering.[24]

We start now to show the main features observed.[25] Results of the computation of magnetic and charge static structure factors $S(\mathbf{k})$ and $C(\mathbf{k})$ (Fourier transformed spin-spin and hole-hole correlations functions, respectively) are partially summarized in Fig. 2(a). In the 8×8 cluster ($x = 1/8$), at a rather large T there is a crossover in the peak of the structure factor from $(k_x, k_y) = (\pi, 0)$ (with the x axis perpendicular to the stripes direction) to $(2\delta, 0)$ with $\delta = \pi/4$. This crossover, together with the behavior shown in Fig. 1(b) indicates a nontrivial behavior of the charge ordering. One is tempted to term this crossover as the ''charge ordering'' temperature,[26] although this concept is somewhat arbitrary in our model. The most important feature is that at a temperature much lower than this crossover there is a second crossover in the spin sector signaled by a change in the peak of the magnetic structure factor from (π, π) to $(\pi \pm \delta, \pi)$. This

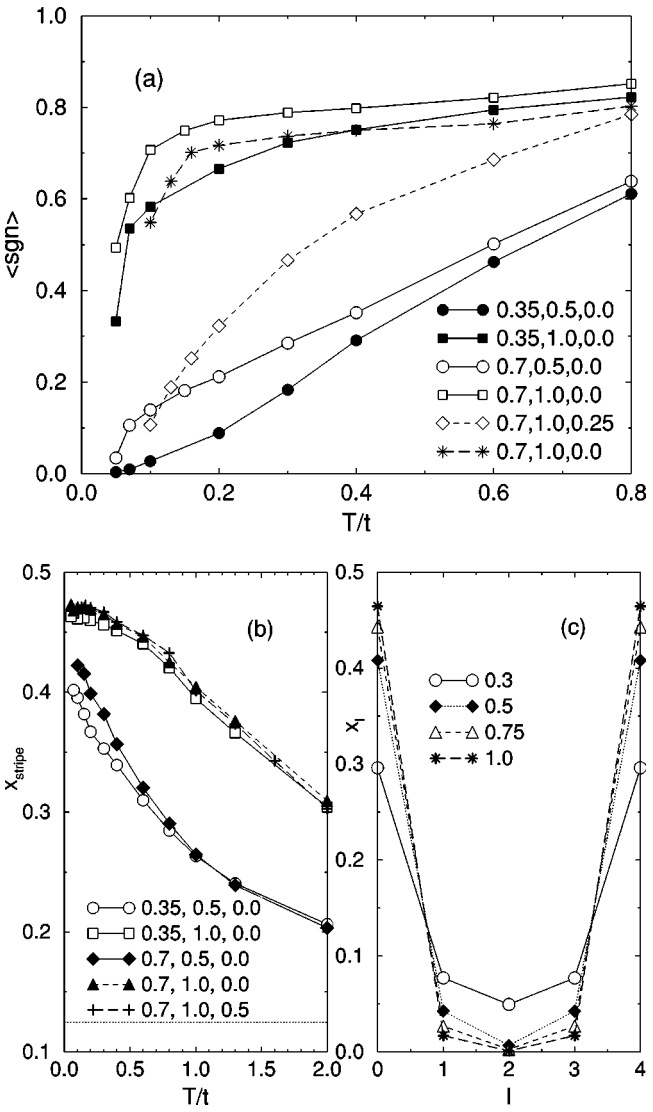

FIG. 1. (a) Averaged sign in QMC simulations on the 8×8 cluster with eight holes. The sets (J, e_s, γ) are indicated on the plot. Stars correspond to 12×12, twelve holes ($x = 0.083$). (b) Hole density on the stripes vs temperature, 8×8 cluster. The dotted line corresponds to the uniform hole distribution ($x = 1/8$). (c) Hole density profile ($l = 0$ and 4 correspond to the stripes) for the t-J_z model with $J = 0.35, T < 0.1$ and for several values of e_s as indicated on the plot ($T = 0.15$ for $e_s = 0.3$).

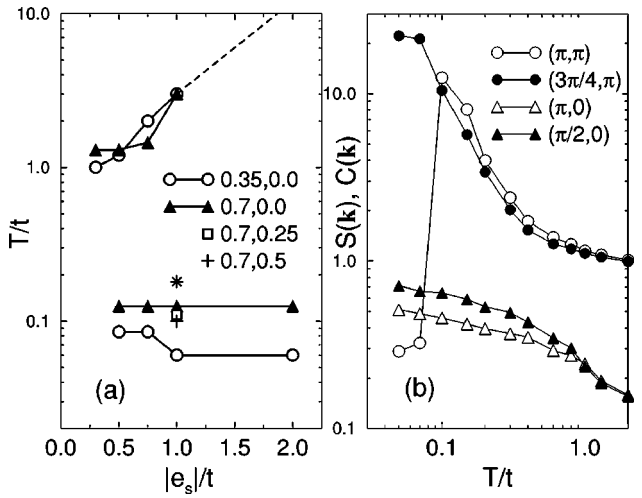

FIG. 2. (a) Phase diagram in the temperature-on-site potential plane. The curves at high (low) T correspond to a crossover in the charge (magnetic) structure factor. The sets $(J,\ \gamma)$ are indicated on the plot. The star corresponds to 12×12, $x=0.083, J=0.7, \gamma=0.0$. (b) Magnetic and charge static structure factors vs. temperature for $J/t=0.35, |e_s|=0.5, \gamma=0$.

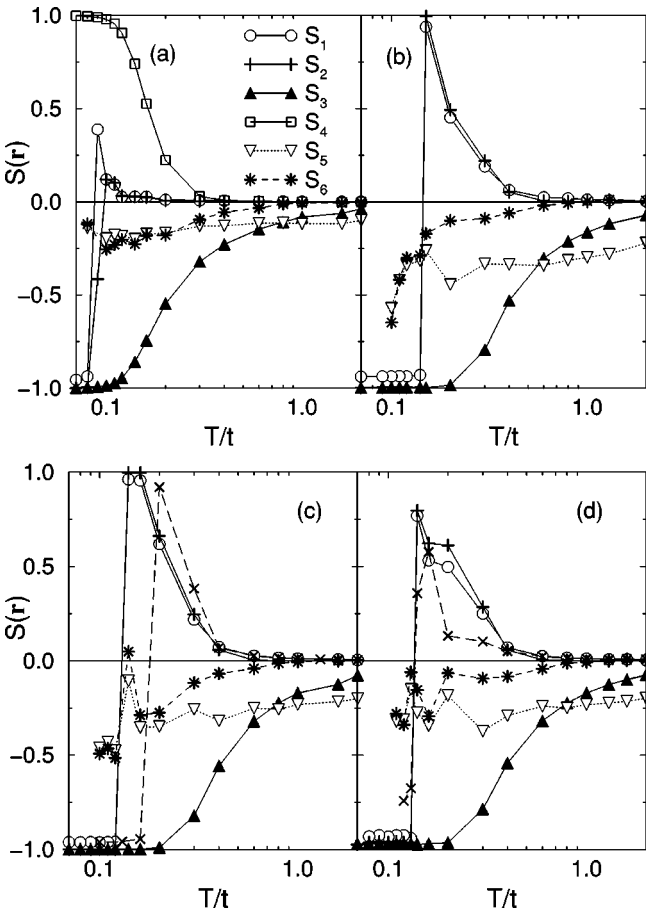

FIG. 3. Spin-spin correlations (defined in the text) vs temperature on the 8×8 cluster, for (a) $J/t=0.35, e_s=1.0, \gamma=0$, (b) $J/t=0.7, e_s=0.75, \gamma=0$, (c) $J/t=0.7, e_s=1.0, \gamma=0.0$ (crosses: S_1, 12×12 cluster), and (d) $J/t=0.7$, $e_s=1.0$, $\gamma=0.25$. (crosses: S_1, $\gamma=0.5$). Correlations S_5 and S_6 have been multiplied by 5.

peak very much resembles the one observed in neutron scattering experiments[5,7] signaling the presence of the ''incommensurate phase'' in underdoped cuprates. Following Ref. 8, we call T_2^* this lower crossover at which a ''spin ordering'' occurs. A similar behavior is observed in the 12×12 lattice with 12 holes ($x=0.083$). Following the behavior observed in underdoped cuprates, T_2^* occurs at a temperature higher than the one observed for similar parameters but for $x=0.125$. The peaks of $S(\mathbf{k})$ and $C(\mathbf{k})$ are the same as above except that for this smaller hole doping, $\delta=\pi/6$. A more detailed evolution of the peaks with temperature is shown in Fig. 2(b). In particular, the crossover in the charge sector is rather smooth. In the spin sector, the weight of the (π,π) peak is strongly reduced below the crossover, but $S(\pi\pm\delta,\pi)$ is definitely nonzero above it.

We have detected important hysteresis effects in the crossover region. The results shown in Fig. 2(b) were obtained by starting the simulation from a configuration with π-shifted spin domains. If the starting configuration consists of in-phase spin domains the crossover temperature is pushed to smaller values. In this case, for many values of the parameters J, e_s, and γ (specially for large J and e_s) we could not detect that crossover to the lowest temperature attainable. In most cases, starting from a randomized spin configuration, behaviors similar to those of Fig. 2 are recovered but we cannot rule out the possibility of in-phase domains being more stable than or degenerate with antiphase domains[7,27] at low temperatures and for very large J and e_s.

We can analyze the crossover in the spin sector at a more microscopic level by looking at the real-space spin-spin correlations that experience the most important changes at this crossover. These correlations are between sites two lattice spacings apart in the same row across a stripe (labeled S_1), and between sites belonging to the center leg of two consecutive three-leg ladders in the same row (S_2). For completeness we have also computed the correlations between nearest neighbor (NN) sites in the center leg of a three-leg ladder (S_3), and between sites at the maximum distance along this leg (S_4). S_5 and S_6 are the correlations between NN and next NN (NNN) sites along the stripes. The spin-spin correlations have been normalized in such a way that their maximum (minimum) value is $+1$ (-1) for the z components of the two spins fully aligned or ferromagnetic (FM) (respectively, antialigned or AF). In Fig. 3(a), corresponding to $J/t=0.35, e_s=1.0$ it can be seen that the correlations S_1 and S_2 across the stripe are positive at high temperature and they increase as T is lowered. Around $T\approx0.12$ these correlations reach their maximum value and as the temperature is further lowered they suddenly become fully AF and remain negative down to the lowest temperature reached. These changes from FM to AF indicate that the intervening mostly hole-free ladders are in-phase (antiphase) above (below) $T\approx0.11$. S_3 and S_4 [only shown in Fig. 3(a)] show a monotonic behavior as the temperature is decreased. They indicate a full polarization of the spin domains at low temperatures. A similar behavior can be observed for smaller e_s and larger J [Fig. 3(b)]. For the $e_s=1.0$ but $J=0.7$ [Fig. 3(c)], T_2^* increases and it increases further for smaller density (x

$=0.083$ on the 12×12 cluster). The same features survive when a XY term in the exchange interaction is included, as it can be seen in Fig. 3(d) for $\gamma=0.25$ and 0.5. As the Heisenberg interaction is made more isotropic, T_2^* slightly decreases. Results for $\gamma=0.5$ suggest that the spin ladders are not going to be fully polarized in the isotropic limit $\gamma=1.0$.[17] As discussed below, the correlations along the stripe S_5 and S_6 are much smaller than the previous ones and hence they show a more erratic behavior, specially below the crossover temperature. Above this temperature, these correlations are AF, and the NN correlation is in general larger (in absolute value) than the NNN one, although for $J=0.35$ and just above T_2^* the opposite behavior is true in agreement with the analysis made in Ref. 10 which is valid for small J/t. A note of caution should be made. Since translational invariance in the direction perpendicular to the stripes is broken, the spin-spin correlations depends on the hole density on each site (e.g., $\langle S_i^z S_i^z\rangle=\langle n_i\rangle$) which in turn has a smooth variation with temperature as shown in Fig. 1(b). However, the changes in the spin-spin correlations, specially at low temperatures, are much stronger than the variation of the hole density, so one could safely ignore that dependency.

Our final study concerns the other important issue that is the relationship between stripes and hole pairing. A sign of hole attraction is the presence of largest hole-hole correlations at smallest distances. Taking into account the remark made earlier about the broken translational invariance the hole-hole correlations $C(\mathbf{r}_i,\mathbf{r}_j)=\langle n_i n_j\rangle$ result proportional to the hole density at each site. It is then expected that $C(\mathbf{r}_i,\mathbf{r}_j)$ along the stripe $C_s(\mathbf{r})$ as shown in Fig. 4(a), present a smooth increase as the temperature is reduced, while the correlations along the first column next to the stripe C_1 are smoothly decreasing. However, near and below T_2^* these correlations behave roughly independently of T. The same behavior can be observed for $C(\mathbf{r}_i,\mathbf{r}_j)$, with $\mathbf{r}_i$ on the center leg of a three-leg ladder and $\mathbf{r}_j$ on the column next to it C_{c1} [Fig. 4(b)]. The normalization adopted is such that

$$\sum_y C[(x,y_0),(x,y)]=\langle N_{h,x}\rangle,$$

where y_0 is the y coordinate of a reference site on column x, and $\langle N_{h,x}\rangle$ is the number of holes on that column. Then, $C(\mathbf{r},\mathbf{r})=1$.

In Figs. 4(c) and 4(d) we show $C(\mathbf{r}_i,\mathbf{r}_j)$ at several points $(\mathbf{r}_i,\mathbf{r}_j)$ after being averaged in a region $\Delta T\approx0.2$ above and below the crossover temperature. It may be noticed that there is no abrupt changes as T_2^* is crossed since the averaged correlations immediately above and below it fall within each other error bars. The first place to look for hole pairs are on the stripes, where the largest hole density is located. The results for the hole-hole correlations along the stripes [Fig. 4(c)], for all the parameter sets studied, show that $C_s(r)$ are *smallest* at nearest neighbor (NN) sites and largest at the maximum possible distance, although they are approximately constant beyond NN sites. This behavior is consistent with a *metallic* behavior of the stripes, as expected in the cuprates.[6] Results for $J=0.7$ are virtually indistinguishable from the ones for $J=0.35$, for the same $e_s=1$. In the metastable in-phase state, degenerate with the antiphase state within error bars at the same low temperatures, the largest correlations also occur at the largest distance but with a more pronounced π modulation, indicating a stronger coupling with the spin surrounding. The same short distance repulsion is obtained for $C_1(r)$ and also when $\mathbf{r}_i$ belongs to the stripe and $\mathbf{r}_j$ to the first column next to it (C_{s1}) [Fig. 4(c)]. In Fig. 4(d), similar results are shown for the 12×12 cluster, $x=0.083$. An alternative scenario[12] assumes that hole pairs with $d_{x^2-y^2}$ symmetry are formed due to short-range AF correlations inside the spin domains located in between the stripes as well-known results on small cluster calculations show.[28] Again, due to the dependence of the hole-hole correlations with the local hole density, the correlations between sites along the central leg of the spin domains are extremely small and hence they are almost completely masked by errors. However, the correlations between a site on the central leg of the three-leg ladder and a site on the first column next to it,

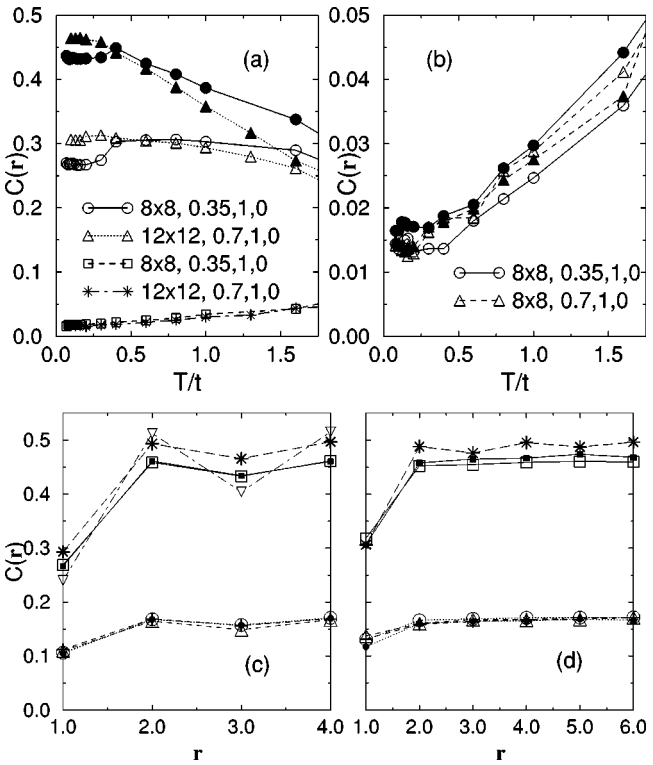

FIG. 4. (a) Hole-hole correlations along the stripe C_s vs temperature. Lattice size J, e_s, and γ are indicated on the plot. Open (full) circles and triangles correspond to NN (maximum distance) sites. Squares and stars indicate C_{s1} (see text) at the maximum distance. (b) Hole-hole correlations on the "spin" ladder C_{c1}. Open (full) symbols correspond to NNN (maximum distance) sites. (c) Hole-hole correlations for the 8×8 cluster, $J=0.35, e_s=1.0, \gamma=0$ above (open circles, squares, and triangles) and below (full circles and squares, plus) T_2^*. C_s (squares), C_{s1} (circles), and C_1 (triangles, plus) are shown. The last two correlations have been multiplied by 10. The down triangles correspond to C_s but for the metastable in-phase state. The stars indicate exact results for an eight site t-J_z ring at quarter filling at $T=T_2^*$. (d) same as (c) but for the 12×12 cluster, $J=0.7$, $e_s=1.0$, and $\gamma=0$.

which are almost identically zero on the 12×12 cluster, acquire on the 8×8 cluster and $x=0.125$, very similar values to those of C_{s1}. These correlations could then become important as the hole density is further increased. Figures 4(c) and 4(d) also show exact diagonalization results for hole-hole correlations on $L=8$ and $L=12$ t-J_z rings at quarter filling ($T=T_2^*=0.08,0.18$, respectively). They are very similar to the correlations C_s along the stripes except for a small shift due to the fact that the hole density on stripes is slightly smaller than $x=0.5$. In addition, as shown earlier, S_1 shows that contiguous spin ladders are almost completely AF coupled in a 2D square lattice. This combined behavior suggests, at least for the t-J_z limit, a generalized spin-charge separation, or more properly, a separation between the spin background and the stripes.[29,10]

In summary, we have studied an anisotropic t-J model, close to the Ising limit, where straight site-centered stripes are imposed by an on-site potential reflecting a mechanism which is not intrinsic to the 2D short-range electronic correlations of that model. The results of the present study suggest that we are able to study with QMC simulations the temperature region between the formation of the stripes at a charge ordering temperature (more or less arbitrarily defined in our model) and the spin ordering process which takes place at a much lower temperature. This lower crossover, at which the spin domains become antiphase domains and an incommensurate magnetic order appears, should correspond in the cuprates to the opening of the pseudogap. In this sense, this result that stems from a model where the stripes are caused by long-range Coulomb interaction, electron-phonon couplings, or other mechanisms that are described by an on-site potential, is at variance with recent results in which the stripes are originated in the pure t-J model.[9,10] In that and other approaches,[11] the stripes are the *consequence* of antiphase domain formation and both features should occur simultaneously. The results of the present study, including the behavior of spin-spin correlations along the stripes, open the possibility of experimentally discriminate the mechanism leading to stripe formation and hence to determine to what extent the stripes are universal to the cuprates or depend on particular details of the various compounds. The hole-hole correlations along and near the stripes show a metallic behavior with no indications of hole attraction. The question arises if a hole attraction on the stripes could appear by taking the isotropic Heisenberg term in the model. One should take into account that, as previous exact results show,[21] hole attraction is actually enhanced in the t-J_z model with respect to the fully isotropic t-J model. In addition, to give more support to our result, it has been suggested that stripes could be introduced in a uniform t-J model by taking an Ising spin interaction at the stripes links.[20] An improvement on statistical errors in order to deal with larger hole densities and lower temperatures would be necessary to detect signs of hole attraction inside the intervening regions between stripes.[30]

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