PHYSICAL REVIEW B VOLUME 59, NUMBER 18 1 MAY 1999-II

Stripe stability in the extended t-J model on planes and four-leg ladders

T. Tohyama
Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

C. Gazza
National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, Florida 32306

C. T. Shih
National Center for High-Performance Computing, Hsinchu, Taiwan

Y. C. Chen
Department of Physics, Tunghai University, Taichung, Taiwan

T. K. Lee
Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan

S. Maekawa
Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

E. Dagotto
National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, Florida 32306

(Received 30 September 1998)

The tendencies to phase-separation and stripe formation of the t-J model on planes and four-leg ladders have been here reexamined including hole hopping terms t',t'' beyond nearest-neighbor sites. The motivation for this study is the growing evidence that such terms are needed for a quantitative description of the cuprates. Using a variety of computational techniques it is concluded that the stripe tendencies considerably weaken when experimentally realistic $t'<0$, $t''>0$ for hole-doped cuprates are considered. However, a small $t'>0$ actually enhances the stripe formation. [S0163-1829(99)51218-6]

Growing experimental evidence suggests the existence of static stripe order in a variety of transition metal oxides, including hole-doped La_2NiO_4 and $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$.[1] In other cuprates, such as $La_{1.85}Sr_{0.15}CuO_4$ and $YBa_2Cu_3O_{6.6}$, the magnetic scattering is consistent with the presence of dynamic antiphase antiferromagnetic (AF) domains.[2] The origin of these charge inhomogeneities is controversial. Some authors believe they are caused by Jahn-Teller (JT) distortions.[3] Others favor a purely electronic explanation. For instance, hole domain walls were observed in Hubbard model Hartree-Fock calculations.[4] In addition, computational calculations for the two-dimensional (2D) t-J model have found striped tendencies consistent with neutron scattering experiments.[5,6] The existence of diagonal domain walls in four-leg t-J ladders has also been reported,[7] adding to the expected strong similarities between ladders and planes.[8] A third possibility is based on frustrated phase separation (PS) where the stripes arise from a combination of a short-range attraction and long-range Coulomb repulsion.[9]

In parallel to these developments recent angle-resolved photoemission (ARPES) experiments addressed the one-particle spectral function of the *undoped* insulator $Sr_2CuO_2Cl_2$.[10] The overall bandwidth and features along the $(0,0)$-(π,π) direction were found in agreement with theoretical t-J model predictions. However, the results along $(0,\pi)$-$(\pi,0)$ were puzzling since the ARPES quasiparticle-like peak has a clear energy maximum at $(\pi/2,\pi/2)$, while in the t-J model this line is almost flat. This difference is important and needs to be addressed.

The main explanation proposed for the t-J-ARPES discrepancy is based on the relevance of corrections in the form of electronic hopping amplitudes beyond the nearest-neighbor (NN) contribution. The importance of these terms was recognized from the analysis of the electronic structures of cuprates.[11] In all these calculations it was concluded that for a proper description of cuprates a next-NN (NNN) hopping of strength t' along the plaquette diagonal was necessary.[12] For hole-doped cuprates t' has been systematically found to be of *negative* sign in contrast to the NN-hopping amplitude t with positive sign, and of about 20% to 40% its magnitude. Electron-doped cuprates need $t'>0$.[13] Note that in regions where AF correlations are important, t is renormalized to smaller values while t' is not severely affected, thus enhancing the relevance of such NNN corrections. In addition, soon after the $Sr_2CuO_2Cl_2$ ARPES data[10] became available it was reported by Nazarenko *et al.*[14] that including a $t'<0$ NNN-hopping the agreement theory experiment was noticeably improved at all momenta. A similar result was also found by Lee and Shih.[15] Further work confirmed and improved this initial approach, showing that with the addition of an extra NNN t''–term connecting sites at distance $2a$ (a=lattice spacing) the results improved even

more.[16] Actually with these NNN corrections the hole-density dependence of the t-J spectra of small clusters was found in agreement with ARPES data.[17] In Ref. 14 it was remarked that there is no symmetry argument favoring the special case $t'=0$, as it occurs in gauge theories where local symmetries and renormalizability arguments fix the Hamiltonian. Since the existence of corrections to the t-J model are natural, the assumption $t'=0$ is mainly aesthetical.

The goal of the present paper is to address the much discussed tendency of the t-J model to phase-separate and/or form stripes performing the calculations in the presence of a realistic nonzero NNN-hopping amplitude. The t-J Hamiltonian employed here is defined as

$$H_{tJ}=-t\sum_{\langle \mathbf{ij}\rangle\sigma}(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}+\text{H.c.})+J\sum_{\langle \mathbf{ij}\rangle}(\mathbf{S_i}\cdot\mathbf{S_j}-n_{\mathbf{i}}n_{\mathbf{j}}/4),$$

where $\langle \mathbf{ij}\rangle$ are NN sites. No doubly occupancy is allowed, t is defined as positive, and the rest of the notation is standard. The contribution of the NNN terms is

$$H_{t't''}=-t'\sum_{\langle\langle \mathbf{km}\rangle\rangle\sigma}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{m}\sigma}-t''\sum_{\langle\langle\langle \mathbf{nr}\rangle\rangle\rangle\sigma}c^{\dagger}_{\mathbf{n}\sigma}c_{\mathbf{r}\sigma}+\text{H.c.},$$

where $\langle\langle \mathbf{km}\rangle\rangle$ denote a pair of sites along the diagonals of the elementary plaquettes, and $\langle\langle\langle \mathbf{nr}\rangle\rangle\rangle$ are pairs of sites located at distance $2a$ along the main axis.

To find information about the influence of t' and t'' on PS and stripe formation on the t-J model, here a variety of computational techniques have been employed. Let us start the analysis using the exact diagonalization (ED) method on planar systems. On 2D t-J clusters evidence in favor[18] and against[19] PS at small J/t has been recently presented. Our goal is not to add to this discussion, but rather to follow some of the approaches proposed in those papers and find the influence of NNN terms on the results. Let us start using ground state (GS) energies calculated by averaging with equal weight over a large number of twisted boundary conditions to reduce size effects.[20] Using this method the GS energies corresponding to the electronic density $\langle n\rangle=1$, the density under investigation (with N_e electrons), and the density corresponding to N_e+2 electrons were obtained for increasing values of J/t. When the three energies lie on a single line, PS occurs between half-filling and the average between the densities N_e/N and $(N_e+2)/N$.[21]

Figure 1(a) illustrates the influence of a NNN hopping on the PS tendencies of the t-J model using a 4×4 cluster. The largest density shown here corresponds to 13/16 and was obtained with information from 12, 14, and 16 electrons. For $t'=0$ the line separating the stable and unstable regions converge to a very small J/t as the density reaches 1.0.[21] However, even for an apparent ''small'' NNN hopping such as $t'=-0.2t$, the PS line now converges towards a larger J/t at half-filling. The effect is similar for $t'=-0.4t$. Although these small-cluster results should be considered only qualitative, the tendencies observed are clear and in agreement with a variety of calculations reported below. Then, it is apparent that a nonzero $t'<0$ amplitude reduces the tendencies towards PS in the t-J model near half-filling and small J/t.

Figure 1(b) contains the $\langle n\rangle=1$ binding energy defined as $\Delta_B=E(2)+E(0)-2E(1)$, where $E(n)$ is the GS energy

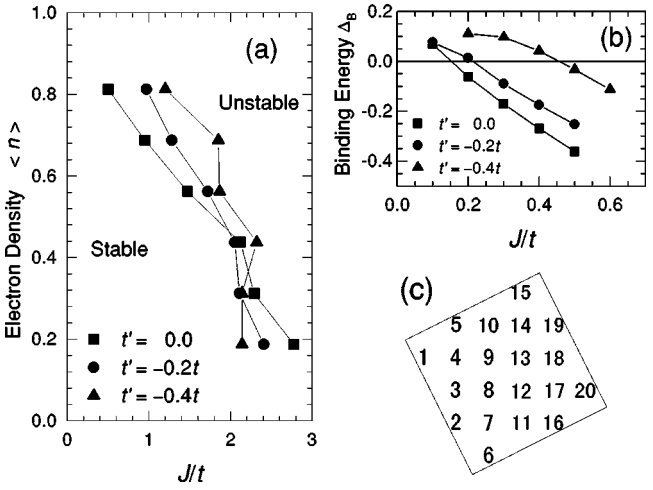

FIG. 1. (a) Stable and unstable regions of the extended t-J model on the $\langle n\rangle$-J/t plane. The results are obtained exactly on a 4×4 cluster with ''averaged'' boundary conditions (see text); (b) binding energy vs J/t of the extended t-J model on a 4×4 cluster, averaged boundary conditions, and using the NNN hoppings indicated; (c) site labeling used for the 20-site cluster.

(averaged over boundary conditions) for n holes. The results show that a $t'<0$ term reduces the attraction between holes. This is correlated with a reduction of the probability of stripe formation and PS [Fig. 1(a)] caused by the short-range AF-induced attraction. The pairing region is pushed up in couplings by a $t'<0$ since it follows PS.[22] Results qualitatively similar to those shown in Figs. 1(a) and 1(b) have been obtained using 18 and 20-sites clusters and other values of t'.[23]

To search for the dominant GS-hole configurations the matrix element $G_{ijkl}=\langle 0|n_h(i)n_h(j)n_h(k)n_h(l)|0\rangle$ was calculated.[5] Here (i,j,k,l) denote four sites of the 20-site cluster following the labeling convention shown in Fig. 1(c). The product of the four hole-number operators n_h is a projector that provides the GS weight of the configurations with the holes at (i,j,k,l). The configurations with the largest G_{ijkl} are $a=(4,7,14,17)$ (unbounded holes), $b=(3,7,13,17)$ (pairs of diagonally bounded holes), $c=(6,7,13,14)$ (NN-hole pairs), $d=(6,7,13,18)$ (another NN-hole pair configuration), $e=(2,8,13,19)$ [four-hole stripe along the (1,1) direction], $f=(1,2,3,6)$ (another type of four-hole domain hole), and $g=(3,8,12,17)$ [four-hole stripe along the (1,0) direction]. Figure 2(a) contains the results in the absence of NNN hoppings. In this case three regimes can be identified: (1) at small J/t the holes are unbounded; (2) for $J/t\sim0.5$ holes form pairs; and (3) at J/t above 0.7 ''diagonal'' stripes are preferred, as observed first in Ref. 5. Although these results are qualitative, the tendencies towards (1,1)-stripe formation are clear and also in agreement with four-leg ladder calculations.[6]

Figure 2(b) contains the results found for the same hole configurations but now using $t'=-0.2t$. Once again, in spite of the naively ''small'' value of t' its influence on GS properties is important. The (1,1) stripes are no longer competing with hole pairs and unbounded holes. Now the most relevant stripe configuration is the (1,0) stripe which dominates only for $J/t\sim1.9$ or larger. Results similar to those shown in Fig. 2(b) have been obtained using a variety of $t'<0$ and $t''>0$ amplitudes. Thus, it is clear that the stability of the stripes is

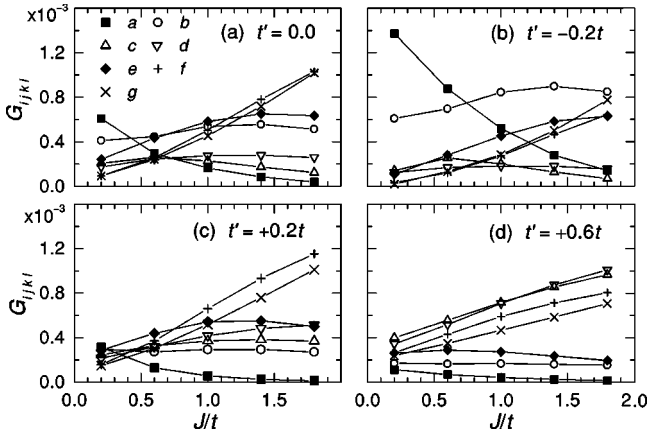

FIG. 2. G_{ijkl} for the seven configurations with the largest weight in the ground state (see text) vs J/t. (a) Results for $t'=0.0$; (b) same as (a) but for $t'=-0.2t$; (c) same as (a) but for $t'=+0.2t$; (d) same as (a) but for $t'=+0.6t$.

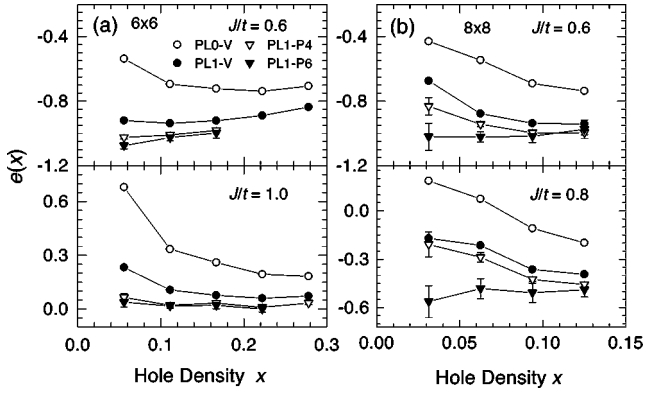

FIG. 3. (a) $e(x)$ (see text) vs x for several powers in the PL method, two values of J/t, and using a 6×6 cluster with $t'=-0.2t$; (b) same as (a) but using a 8×8 cluster.

sensitive to the presence of NNN-hopping amplitudes. Since such hoppings are expected to be realistic, the presence of stripes in electronic models for the cuprates with short-range interactions is called into question.

It is interesting to note that using $t'>0$, i.e., the ''wrong'' sign for hole-doped cuprates but relevant for electron-doped cuprates,[13] the tendencies to stripe formation are actually *enhanced* roughly in the small window $0<t'/t<0.2$ at all values of J/t. Now the crossing point between configurations a and f appears in Fig. 2(c) at $J/t\sim0.4$, while in Fig. 2(a) it occurred at $J/t\sim0.7$. Then, a small and positive t'/t can be used as a test ground of electronic models with tendencies towards stripe formation. As t'/t grows further stripes become unstable again, and actually for t'/t around 0.5 or larger the configurations with NN-hole pairs dominate for all the values of J/t explored here [Fig. 2(d)].

To understand the different influence of the sign of t' on the t-J model phase diagram, a discussion on the subtleties involving bare versus renormalized parameters is needed. It is known that at $t'=0$, the effective NN-hopping amplitude is dramatically reduced at half-filling since intersublattice hole hopping distorts the AF background. In this same regime effective nonzero t' and t'' amplitudes are generated, as deduced from the one-hole dispersion.[24] The sign of this effective t' which gives mobility to the dressed hole is *negative*, a well-known fact which manifests itself in the minimum of the hole-quasiparticle band at $(\pi/2,\pi/2)$. Adding a bare t' term of the same sign will enhance the hole mobility substantially, to the point where hole superstructures become unstable. This amplification of effects explains the results of Figs. 1(a) and 2(a) and 2(b). However, the addition of a bare t' in the Hamiltonian of *positive* sign can lead to a cancellation of effects, and a concomitant reduction of the hole mobility near half-filling. This will indirectly favor hole clustering since such structures arise from a competition of the potential energy gained by AF attraction and the kinetic energy. Spin correlations are enhanced with respect to $t'=0$,[13] since poorly mobile holes cannot scramble them. When t'/t is increased further eventually holes should become mobile again and the stripe tendencies will diminish. Figure 2(d) shows G_{ijkl} now for $t'/t=+0.6$. The dominant configurations have NN-hole pairs instead of stripes at all values of J/t shown.

The GS energy of the t-J model supplemented by a NNN term with $t'=-0.2t$ has also been calculated using the Power Lanczos (PL) method.[25] To search for indications of PS, the approach used in Refs. 19 and 26 is applied, namely the energy of the PS state is written as $E=N_s e_H+N_h e(x)$, where N_s is the number of sites, N_h the number of holes, e_H the energy per site of the Heisenberg model, x the hole density in a hole-rich phase, and $e(x)=[e_h(x)-e_H]/x$. If at a fixed coupling J/t, $e(x)$ is found to have a minimum at some density x_m and the overall density is smaller than x_m, then the system phase separates between a hole-free phase and a hole-rich one with density x_m. In Fig. 3 $e(x)$ is plotted vs x using 6×6 and 8×8 clusters with periodic boundary conditions (open-shell configurations). The energies denoted by PL0-V correspond to results using an optimized trial wave function taken from the set of Gutzwiller and resonant valence bond (RVB) wave functions.[19,25] PL1-V denote improved results now using the first Lanczos step applied to the previously optimized wave function.[27] PL1-Pn correspond to further improvements resulting from the application of n powers of the Hamiltonian over the PL1-V wave function. For additional details the reader is referred to Refs. 19 and 25.

At $J/t=1.0$ and after the application of six powers, the minimum of $e(x)$ in Fig. 3(a) is found to be at $x=0.22$. At $J/t=0.6$, the minimum shifts with increasing powers towards the smallest density studied here namely $x=0.056$. Similar results were obtained for the intermediate coupling $J/t=0.8$ (not shown). In addition, using an 8×8 cluster analogous trends are observed as shown in Fig. 3(b), although with larger error bars due to the sign problem. The minimal values of $e(x)$ are at the lowest doping density for $J/t=0.6$ and 0.8. Therefore it is concluded that the critical J_c/t for PS in the low hole density limit is at least ≈0.8, which is larger than in the $t'=0$ case where $J_c/t\approx0.6$.[19] The trends found here are qualitatively the same as observed using ED [Fig. 1(a)], namely a $t'<0$ moves the PS region towards larger J/t's.

Since the most robust computational evidence of stripe formation in one-band electronic models actually comes from the density-matrix numerical renormalization group

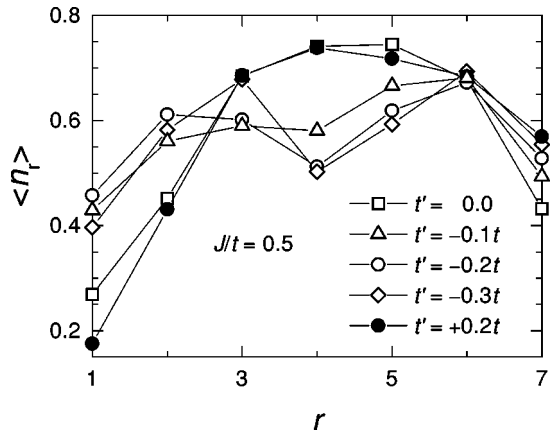

FIG. 4. Rung-density $\langle n_r \rangle$ vs r on a 4×14 cluster, $J/t=0.5$, 8 holes, studied with DMRG and open boundary conditions. Shown are only half the rungs, the rest is found by reflection. $r=1(r=7)$ is the end (middle) of the cluster. Results for several t''s are shown.

(DMRG) studies of four-leg t-J ladders, let us complete our analysis by studying the same clusters as in Ref. 7, following a similar methodology, but now adding NNN terms. The DMRG results reported here were obtained using $J/t=0.5$, $m=500$ states, and a truncation error $\sim 1\times10^{-4}$. In Fig. 4 the rung density $\langle n_r \rangle$ (i.e., the sum of the four-site densities forming a rung) is shown using a 4×14 cluster and 8 holes. Results for just half the lattice are provided for simplicity, since the rest are obtained by reflection. At $t'=0$, previous results[7] were reproduced as a test. They present a single broad peak indicative of GS clustering tendencies. Analyzing the hole-hole correlations the (1,1)-stripes were found to have a large weight in the GS.[7] However, when the NNN amplitude is turned on, the effect is weaken. Consider, for example, $t'=-0.2t$: now a two-peak structure is observed which is more suggestive of hole pairing than of stripe formation (note there are four holes in average on the portion of the cluster shown in Fig. 4). The effect is further enhanced for $t'=-0.3t$ where the two peaks are sharper. Here the holes were found to be unbounded residing in pairs at the extremes of the same rung. Then, as $|t'|$ grows a rapid transition from stripes to unbounded holes is observed. The melting of the stripes (assumed to be signaled by the melting of the single-peak in $\langle n_r \rangle$) roughly occurs at $t'\sim-0.1t$. More realistic values of the coupling are difficult to study as accurately as at $J/t=0.5$. However, it is expected that the short-range AF attraction will become weaker as J/t is reduced, and the tendencies to stripe formation will also be weaker in this regime. Note that once again a $t'>0$ maintains the stripe structure (single peak shown in Fig. 4 for $t'=+0.2t$), as in planar systems.

Summarizing, using a variety of computational techniques it has been shown that the tendencies to phase separation and stripe formation previously reported on planes and four-leg ladders are actually substantially weaken once realistic NNN-hopping amplitudes are added to the t-J model. The reason is that $t'<0$ terms enhance appreciably the mobility of holes, melting hole superstructures. Reciprocally, using a (small) $t'>0$ the stripes become more stable providing an interesting model for the analysis of their properties.

C.G. thanks the support of CONICET (Argentina). T.K.L. was supported by the NSC Grant No. 87-2112-M-001-016. E.D. was supported by the NSF Grant No. DMR-98-14350. S.M. was supported by the CREST and NEDO.

[1] J.M. Tranquada *et al.*, Nature (London) **375**, 561 (1995).
[2] J.M. Tranquada, Physica C **282-287**, 166 (1997).
[3] *Phase Separation in Cuprate Superconductors*, edited by E. Sigmund and K. A. Müller (Springer-Verlag, New York, 1994).
[4] J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989). See also D. Poilblanc and T.M. Rice, *ibid.* **39**, 9749 (1989).
[5] P. Prelovsek and X. Zotos, Phys. Rev. B **47**, 5984 (1993).
[6] S. White and D. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998).
[7] S. White and D. Scalapino, Phys. Rev. B **55**, 14 701 (1997).
[8] E. Dagotto and T.M. Rice, Science **271**, 618 (1996).
[9] U. Löw *et al.*, Phys. Rev. Lett. **72**, 1918 (1994); C. Castellani *et al.*, *ibid.* **75**, 4650 (1995).
[10] B.O. Wells *et al.*, Phys. Rev. Lett. **74**, 964 (1995).
[11] M.S. Hybertsen *et al.*, Phys. Rev. B **41**, 11 068 (1990); T. Tohyama and S. Maekawa, J. Phys. Soc. Jpn. **59**, 1760 (1990).
[12] For an alternative explanation see R.B. Laughlin, Phys. Rev. Lett. **79**, 1726 (1997); X.-G. Wen and P.A. Lee, *ibid.* **76**, 503 (1996).
[13] T. Tohyama and S. Maekawa, Phys. Rev. B **49**, 3596 (1994); R. Gooding *et al.*, *ibid.* **50**, 12 866 (1994).
[14] A. Nazarenko *et al.*, Phys. Rev. B **51**, 8676 (1995).
[15] T.K. Lee and C.T. Shih, Phys. Rev. B **55**, 5983 (1997).
[16] See, for example, references in Ref. 17.
[17] C. Kim *et al.*, Phys. Rev. Lett. **80**, 4245 (1998).
[18] C.S. Hellberg and E. Manousakis, Phys. Rev. Lett. **78**, 4609 (1997).
[19] C.T. Shih, Y.C. Chen, and T.K. Lee, Phys. Rev. B **57**, 627 (1998).
[20] D. Poilblanc, Phys. Rev. B **44**, 9562 (1991).
[21] C. Hellberg and E. Manousakis, J. Phys. Chem. Solids **59**, 1818 (1998).
[22] E. Dagotto *et al.*, Phys. Rev. B **49**, 3548 (1994); C.T. Shih *et al.*, Phys. Rev. Lett. **81**, 1294 (1998).
[23] On the 4×4 cluster calculations with $t''\neq0$ have strong size effects, and they were not pursued here.
[24] E. Dagotto *et al.*, Phys. Rev. Lett. **73**, 728 (1994).
[25] Y.C. Chen and T.K. Lee, Phys. Rev. B **51**, 6723 (1995).
[26] V.J. Emery *et al.*, Phys. Rev. Lett. **64**, 475 (1990).
[27] E. Dagotto and A. Moreo, Phys. Rev. D **31**, 865 (1985).