One-Dimensional Metallic Behavior of the Stripe Phase in $La_{2-x}Sr_xCuO_4$

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Using an exact diagonalization method within the dynamical mean-field theory we found stable stripe phases in the two-dimensional Hubbard model doped by $0.03 < \delta < 0.2$ holes, with a crossover from diagonal to vertical site-centered stripes at doping $\delta \simeq 0.05$. The doping dependence of the size of magnetic domains and chemical potential shift $\Delta\mu \propto -\delta^2$ are in quantitative agreement with the experimental results for $La_{2-x}Sr_xCuO_4$. The one-dimensional metallic behavior along the domain walls explains the observed suppression of spectral weight along the Brillouin zone diagonal.

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It is commonly believed that the understanding of normal state properties of high-temperature superconducting cuprates (HTSC) will provide important clues for the understanding of superconductivity itself. The undoped compounds, La_2CuO_4 and $YBa_2Cu_3O_6$, are insulators and exhibit long-range antiferromagnetic (AF) order, which is rapidly destroyed and replaced by short-range AF correlations as holes are doped into the CuO_2 planes [1,2]. Incommensurate charge and spin order, discovered first in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ [3], suggests that the strong competition between hole propagation and AF order in the CuO_2 planes leads to segregation of holes in regions without AF order. These regions form one-dimensional (1D) structures, so called *stripes*, which act as walls between AF domains [4]. The essentially identical momentum dependence of the magnetic scattering in $La_{2-x}Sr_xCuO_4$ [1,5] provides evidence for the *stripe phases* in this class of materials.

If indeed realized in a broad range of doping, the stripe phase should have measurable consequences. Studies of $La_{2-x-y}Nd_ySr_xCuO_4$ showed a chemical potential shift in underdoped and overdoped cuprates responsible for the breakdown of the Fermi liquid picture, with a decreased spectral weight at the Fermi level μ [6], and a real gap for charge excitations around momentum $(\pi/2, \pi/2)$ [7,8]. It is therefore interesting to investigate whether such puzzling features are fingerprints of a stripe phase and follow from strong Coulomb interactions at Cu ions.

Stripe phases were first found in the Hartree-Fock (HF) approximation [9], with empty (filled by holes) domain walls in an insulating ground state. In contrast, the calculations which include electron correlations indicate that the ground state of an AF system with strong short-range Coulomb repulsion is a stripe phase with populated domain walls at low doping [10–12]. Hence a partially filled band might be expected, responsible for charge transport along the walls. These results clearly emphasize the need for a reliable and controlled approximation scheme in order to study the physics of stripe phases.

In this Letter we present the results of a *nonperturbative* solution of the dynamical mean-field theory (DMFT) [13] equations for the stripe phase obtained for the two-dimensional (2D) Hubbard model. The DMFT approach allows us to treat the hole correlations using *local self-energy* [14]. Recently we have shown that within DMFT one obtains the correct dispersion and spectral weights of quasiparticle (QP) states in the Hubbard model at half filling ($n = 1$) [15].

Here we investigate long-range stripe order in the 2D Hubbard model at zero temperature,

$$H = -\sum_{mi,nj,\sigma} t_{mi,nj} a^{\dagger}_{mi\sigma} a_{nj\sigma} + U \sum_{mi} n_{mi\uparrow} n_{mi\downarrow} . \quad (1)$$

The square lattice is covered by N supercells containing L sites each. Positions $\mathbf{R}_{mi} \equiv \mathbf{T}_m + \mathbf{r}_i$ of nonequivalent sites $i = 1, \ldots, L$ within the unit cell m are labeled by a pair of indices $\{mi\}$. We restrict the hopping term to nearest neighbors $\{mi\}$ and $\{nj\}$ only, $t_{mi,nj} = t$. The one-particle Green's function in the stripe phase is given by an $(L \times L)$ matrix, $G_{ij\sigma}(\mathbf{k}, i\omega_\nu)$, on the imaginary energy axis $\omega_\nu = (2\nu + 1)\pi T$ with fictitious temperature T. It contains a site- and spin-dependent *local self-energy* [13,14],

$$G^{-1}_{ij\sigma}(\mathbf{k}, i\omega_\nu) = (i\omega_\nu + \mu)\delta_{ij} - h_{ij}(\mathbf{k}) - \Sigma_{i\sigma}(i\omega_\nu)\delta_{ij} , \quad (2)$$

where μ is the chemical potential, and $h_{ij}(\mathbf{k})$ is an $(L \times L)$ matrix which describes the kinetic energy, $h_{ij}(\mathbf{k}) = \sum_n \exp[-i\mathbf{k}(\mathbf{R}_{0i} - \mathbf{R}_{nj})] t_{0i,nj}$. The local Green's functions for each nonequivalent site i are calculated from the diagonal elements of the Green's function matrix (2), $G_{i\sigma}(i\omega_\nu) = N^{-1} \sum_{\mathbf{k}} G_{ii\sigma}(\mathbf{k}, i\omega_\nu)$. Self-consistency of site i with its effective medium requires

$$\mathcal{G}^0_{i\sigma}(i\omega_\nu)^{-1} = G^{-1}_{i\sigma}(i\omega_\nu) + \Sigma_{i\sigma}(i\omega_\nu) , \quad (3)$$

similar to the situation in thin films [16].

For the solution of the effective impurity model with hybridization parameters $V_{i\sigma}(k)$, and diagonal energies $\varepsilon_{i\sigma}(k)$ for each nonequivalent site i in the stripe supercell,

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we employed the exact diagonalization method of Caffarel and Krauth [17]. By fitting $\mathcal{G}^0_{i\sigma}(i\omega_\nu)$ on the imaginary energy axis, the parameters of an effective DMFT-impurity cluster, $V_{i\sigma}(k)$ and $\varepsilon_{i\sigma}(k)$, with $k = 1, \ldots, n_s$ sites [17], are obtained. After solution of the effective cluster problem using Lanczos algorithm, the local Green's function $G_{i\sigma}(i\omega_\nu)$ was determined. Self-consistency is implemented by extracting from Eq. (3) the new self-energy for $G_{ij\sigma}(\mathbf{k}, i\omega_\nu)$ for the next iteration. We have verified the convergence of the Green's function using, for the same type of domain wall order, different supercells with appropriate boundary conditions. Rapid convergence with respect to n_s has also been found when we used $n_s = 6$, 8, and 10. Finally, the Green functions (2) serve to determine the spectral function,

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi}\frac{1}{LN}\mathrm{Im}\sum_{mi,nj,\sigma} e^{-i\mathbf{k}(\mathbf{R}_{mi}-\mathbf{R}_{nj})} G_{mi,nj,\sigma}(\omega)\,.$$

Below we summarize the results obtained for $U = 12t$, a value representative for $La_{2-x}Sr_xCuO_4$ (neglecting small hopping elements to further neighbors), and for a broad range of hole doping ($\delta = 1 - n$), $0.03 < \delta < 0.2$, where we found that the ground state contains populated domain walls. Several different initial configurations have been used for searching for the minimum of the ground state energy at a given doping δ. We have verified that magnetic polarons are unstable in this whole doping regime, as also found using the slave-boson method by Seibold *et al.* [11].

First, for $0.03 < \delta \leq 0.05$, diagonal stripe supercells are stabilized by a (weak) charge-density wave superimposed with a spin-density wave (SDW) along the wall. Such states are precursors of the undoped AF Mott insulator [18], with the SDW domain wall unit cells consisting of four sites, $|0\rangle - |\uparrow\rangle - |0\rangle - |\downarrow\rangle$, and small moments at magnetic sites. Second, *site-centered vertical stripes with populated domain walls* were found to be stable structures in a range of doping $0.05 < \delta < 0.17$, in agreement with neutron scattering experiments [3] (Fig. 1). This phase is stabilized by electron correlations [10–12] and by the kinetic energy gains on the populated domain walls which are largest if the domain walls are nonmagnetic. Finally, at doping $\delta > 0.17$ the bond-centered stripe phase of White and Scalapino [12] is energetically favored, kinks and antikinks along the domain walls develop, and the stripe structure gradually melts.

The size of AF domains in the site-centered stripe phase shrinks with increasing doping for $\delta \leq 1/8$. For example, the charge unit cell contains eight (four) sites at doping $\delta = 1/16$ ($\delta = 1/8$), while the electron density is almost constant on the sites of the walls, being $n_i \simeq 0.850$ and $n_i \simeq 0.830$, respectively. In agreement with the results of the slave-boson calculations [11] and numerical density matrix renormalization group [12], the self-consistent DMFT densities in the stripe unit cell are characterized by much smoother variations than in the corresponding HF states

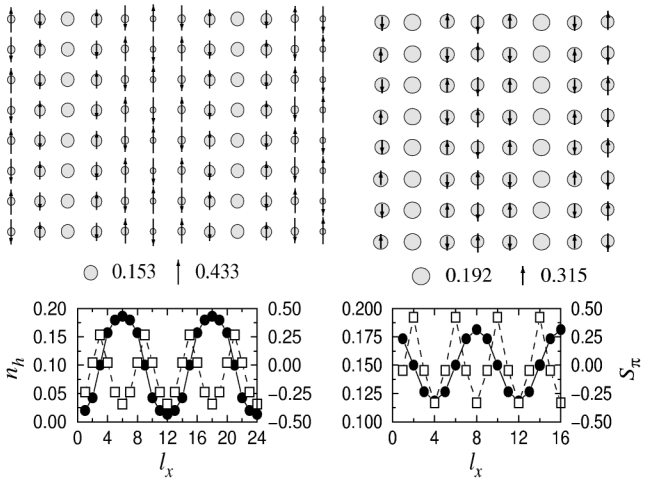

FIG. 1. Vertical site-centered stripe phases for $\delta = 1/12$ (left) and $\delta = 0.15$ (right) at $U = 12t$. Top part shows doped hole (circles) and magnetization density (arrows); their spatial variations are represented by $n_h(l_x)$ (empty squares) and $S_\pi(l_x)$ (filled circles) in the lower part.

[9]. Beyond $\delta = 1/8$ we find a lock-in effect of the same structure with a charge (magnetic) unit cell consisting of four (eight) sites, and the doped hole density, $n_h(l_x) = 1 - \langle n_{(l_x,0),\uparrow} + n_{(l_x,0),\downarrow}\rangle$, increasing faster within the AF domains than on the wall sites (Fig. 1). The magnetic domain structure is best described by the modulated magnetization density, $S_\pi(l_x) = L_y^{-1}\sum_{l_y}(-1)^{l_x+l_y}\frac{1}{2}\langle n_{(l_x,l_y),\uparrow} - n_{(l_x,l_y),\downarrow}\rangle$, projected on the direction perpendicular to the wall [12].

The stability of the above stripe phases is investigated by the energy change per one doped hole, $E_h = [E_0(\delta) - E(0)]/\delta$, where $E_0(\delta)$ is the ground state energy at doping δ, and $E(0)$ is the reference energy of an AF state at $\delta = 0$, both found within the DMFT. The energy E_h/t is a monotonically increasing function of doping [Fig. 2(a)], showing that the diagonal and vertical stripe phases are stable against macroscopic phase separation. As two most pronounced features one observes (i) two phase transitions between stripe phases discussed above and (ii) decreasing excitation energy with increasing δ which indicates that the stripe phases are gradually destabilized with increasing doping. The energy difference between the stripe phases with bond-centered and site-centered domain walls is typically small, e.g., $\Delta E_h \sim 0.05t$ for $\delta \simeq 1/8$. Therefore, one expects strong transverse stripe fluctuations which might enhance superconducting correlations in the ground state [18]. The errors in E_h estimated by increasing the impurity model from $n_s = 8$ to $n_s = 10$ sites do not exceed 0.7%. However, corrections from transverse stripe fluctuations are likely to be larger, but we believe that they do not change our qualitative conclusions.

We have found that the chemical potential shifts downwards with hole doping, $\Delta\mu \propto -\delta^2$ [Fig. 2(b)], in agreement with the experimental results of Ino *et al.* [6], and with the Monte Carlo simulation of the 2D Hubbard model [19]. Therefore, the charge susceptibility is enhanced

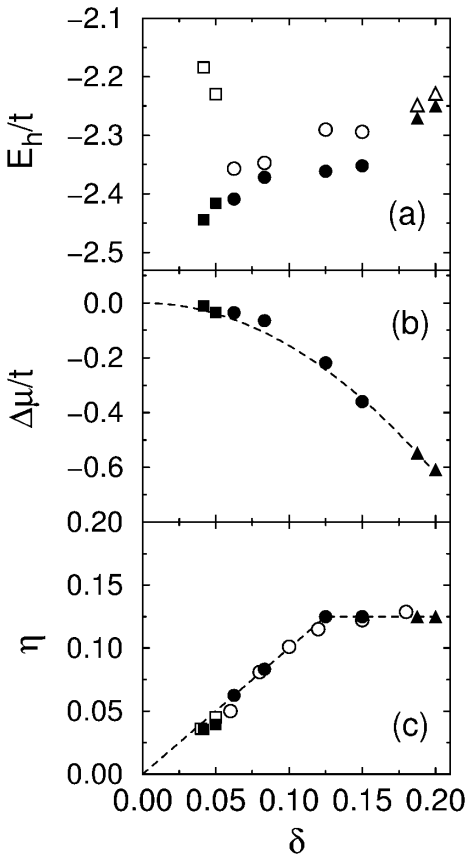

FIG. 2. Evolution of the stripe phases with doping δ ($U = 12t$): (a) energy per doped hole E_h/t; (b) shift of the chemical potential $\Delta\mu/t$ and the quadratic fit $\Delta\mu/t = a\delta^2$ with $a = -15.57$ (dashed line); (c) shift η of the maxima of the magnetic structure factor $S(\mathbf{Q})$. Filled symbols show the data obtained for diagonal SDW stripes with $\mathbf{Q} = [(1 \pm \sqrt{2}\,\eta)\pi, (1 \pm \sqrt{2}\,\eta)\pi]$ (squares), and vertical site-centered (circles) and bond-centered (triangles) with $\mathbf{Q} = [(1 \pm 2\eta)\pi, \pi]$. Empty symbols in (a) stand for the excited states, while in (c) they show the data points of Yamada *et al.* [5] (circles) and Wakimoto *et al.* [20] (squares).

towards $\delta \to 0$, reproducing a universal property of the Mott-Hubbard metal-insulator transition [19].

As both the bond-centered and site-centered stripe phases have the same size of the magnetic unit cell, they give the same pattern in neutron scattering and are thus indistinguishable experimentally. The neutron scattering structure factor $S(\mathbf{Q})$ in the stripe phase has the maxima shifted away from the $M = (\pi, \pi)$ point to $\mathbf{Q} = [(1 \pm 2\eta_{\text{vert}})\pi, \pi]$ points for the structures of Fig. 1 {and to $\mathbf{Q} = [\pi, (1 \pm 2\eta_{\text{vert}})\pi]$ for equivalent horizontal stripes}. The present calculations give a linear dependence $\eta_{\text{vert}} = \delta$ for $\delta \leq 1/8$ and $\eta_{\text{vert}} = 1/8$ for $\delta > 1/8$ [Fig. 2(c)]. Such a behavior was observed by Yamada *et al.* [5] and indicates a unique stability of populated domain walls in the stripe phase. The correlations included within the DMFT play thereby a crucial role, as other filling and periodicity of the stripe phase were found in HF calculations [9]. It is quite remarkable that the points found at low doping [Fig. 2(c)], obtained for the diagonal stripe structures with the maxima of $S(\mathbf{Q})$ at $\mathbf{Q} = [(1 \pm 2\eta_{\text{diag}})\pi, (1 \pm 2\eta_{\text{diag}})\pi]$ with $\eta_{\text{diag}} \simeq \delta/\sqrt{2}$, agree perfectly well with the recent neutron experiments of Wakimoto *et al.* [20].

Let us focus on the spectral function $A(\mathbf{k}, \omega)$ of the stripe phases. The photoemission spectra ($\omega \leq \mu$) consist of the lower Hubbard band at $\omega - \mu \sim -4.8t$ and low-energy states, separated well from the Hubbard band and extending over an energy range of $\sim 2t$. The QP states known from the dispersion of a single hole in the t-J model survive in the stripe phase up to $\delta = 0.15$ (Figs. 3 and 4), and are characterized by a considerable spectral weight and a bandwidth $\sim 2J$ (here $J/t = 4t/U = 1/3$) [15]. Because of the stripe structure we find that the directions $\Gamma - X$ and $\Gamma - Y$ are nonequivalent.

At $\delta = 1/12$ we found a reduced spectral weight around the Fermi energy μ at the X point (Fig. 3); it originates from the quasi-1D electronic structure of the site-centered stripe phase [21] and explains the *flat band* around the X point and the Fermi level crossing at $(\pi, \pi/4)$, both observed in recent angle-resolved photoemission (ARPES) experiments [7,8]. On the contrary, such QP states are not seen in ARPES around the Y point, as the structure factor vanishes [22], and one only resolves the spin-polaron QP band with dispersion $\sim 2J$.

As the most spectacular result, a *gap* for charge excitations opens at the Fermi energy in the underdoped regime around the S point (Fig. 3). Little or no spectral weight is found at μ for $\mathbf{k} = (\pi/4, \pi/4)$ and $\mathbf{k} = (0, \pi/4)$ where, notably, the 1D quarter-filled stripe band should show Fermi level crossings [21]. This behavior agrees quantitatively with the ARPES measurements on $La_{2-x}Sr_xCuO_4$ [7] and $La_{1.28}Nd_{0.6}Sr_{0.12}CuO_4$ [8].

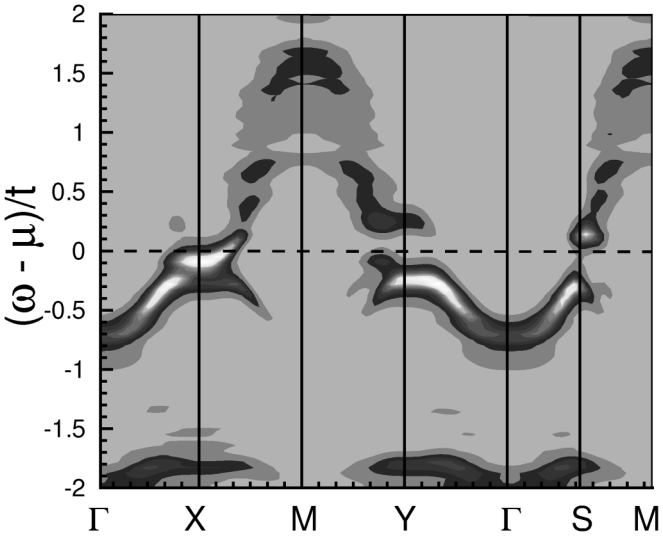

FIG. 3. Spectral function $A(\mathbf{k}, \omega)$ of the stripe phase at $\delta = 1/12$ with $U = 12t$, as obtained along the main directions of the 2D Brillouin zone, with $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, $M = (\pi, \pi)$, and $S = (\pi/2, \pi/2)$.

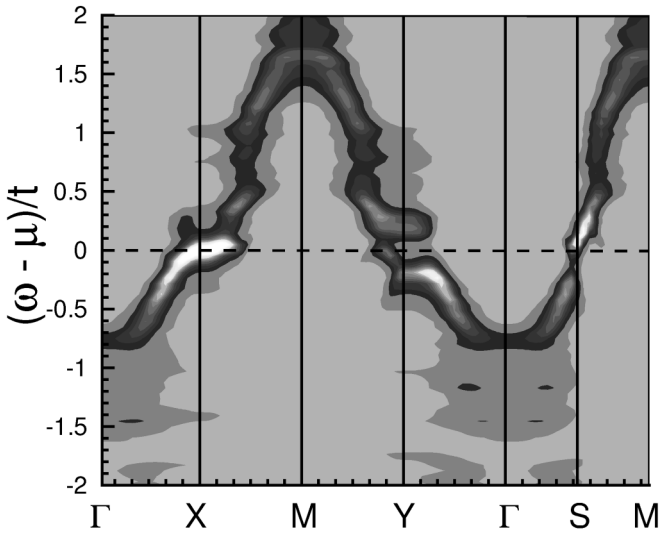

FIG. 4. $A(\mathbf{k}, \omega)$ as in Fig. 3 but at $\delta = 0.15$.

In order to understand these results we analyzed the electronic structure of $H = -t \sum_{\langle ij \rangle, \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_i U_i S^z_i$, where U_i is a spin potential at site $i = (i_x, i_y)$ in the stripe supercell. Local energy contributions $V_{i_x} \equiv U_{(i_x,i_y)} |\langle S^z_{(i_x,i_y)} \rangle|$, independent of i_y for vertical stripes, are treated as parameters, with $V_0 = 0$ on the nonmagnetic domain wall. By numerical analysis we found a condition $V_2 \geq 2V_1$ for vanishing photoemission weight at μ for $\mathbf{k} = (\pi/4, \pi/4)$, which is satisfied by the spin densities found in the DMFT at $\delta = 1/12$, with $V_2 \simeq 2.07t$ and $V_1 \simeq 0.99t$. The strong renormalization of spin densities next to the domain walls with respect to the HF values is due to charge fluctuations included in DMFT and demonstrates that local correlations play a crucial role in understanding the ARPES spectra of HTSC [7,8].

The ARPES spectral weight at $\delta = 1/12$ around $\omega - \mu \sim -2t$ originates entirely from the bands of stripe supercell (Fig. 3). As expected, spectral weight is transferred from that energy region to the inverse photoemission part $\omega > \mu$ with increasing doping (Fig. 4). Finally, we observed that the gaps found at the Y and S points are gradually filled by spectral weight as the stripe order melts.

Summarizing, we have shown that stripe phases with populated domain walls are well described by the DMFT in a broad range of δ. Their spectral properties show an interesting superposition of the QP's known from doped 2D antiferromagnets with a 1D metallic behavior. Experimental features, such as (i) the incommensurability of spin fluctuations [3,5], (ii) the chemical potential shift $\Delta\mu \propto -\delta^2$ [6], and (iii) the distribution of the photoemission spectral weight near the X and S points [7,8], find a natural explanation as signatures of stripe phases in $La_{2-x}Sr_xCuO_4$ at low and intermediate doping.

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[1] M. A. Kastner *et al.*, Rev. Mod. Phys. **70**, 897 (1998).
[2] C. Niedermayer *et al.*, Phys. Rev. Lett. **80**, 3843 (1998).
[3] J. M. Tranquada *et al.*, Phys. Rev. B **54**, 7489 (1996).
[4] V. J. Emery and S. A. Kivelson, Physica (Amsterdam) **209C**, 597 (1993).
[5] K. Yamada *et al.*, Phys. Rev. B **57**, 6165 (1998).
[6] A. Ino *et al.*, Phys. Rev. Lett. **79**, 2101 (1997); **81**, 2124 (1998).
[7] A. Ino *et al.*, J. Phys. Soc. Jpn. **68**, 1496 (1999).
[8] X. J. Zhou *et al.*, Science **286**, 268 (1999).
[9] J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989); D. Poilblanc and T. M. Rice, *ibid.* **39**, 9749 (1989); M. Kato *et al.*, J. Phys. Soc. Jpn. **59**, 1047 (1990); J. Zaanen and A. M. Oleś, Ann. Phys. (Leipzig) **6**, 224 (1996).
[10] C. Nayak and F. Wilczek, Phys. Rev. Lett. **78**, 2465 (1997).
[11] G. Seibold *et al.*, Phys. Rev. B **57**, 6937 (1997); G. Seibold *et al.*, *ibid.* **58**, 13 506 (1998); D. Góra *et al.*, *ibid.* **60**, 7429 (1999).
[12] S. R. White and D. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998); **81**, 3227 (1998).
[13] A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
[14] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[15] M. Fleck *et al.*, Phys. Rev. Lett. **80**, 2393 (1998); Phys. Rev. B **60**, 5224 (1999).
[16] M. Potthoff and W. Nolting, Eur. Phys. J. B **8**, 555 (1999).
[17] M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994).
[18] S. A. Kivelson, E. Fradkin, and V. J. Emery, Nature (London) **393**, 550 (1998).
[19] N. Furukawa and M. Imada, J. Phys. Soc. Jpn. **62**, 2557 (1993).
[20] S. Wakimoto *et al.*, Phys. Rev. B **60**, 769 (1999); **61**, 3699 (2000).
[21] An anisotropic 2D model with hopping amplitude t along the y direction has dispersion $\varepsilon_{\mathbf{k}} = -2t \cos k_y$ [see also M. I. Salkola *et al.*, Phys. Rev. Lett. **77**, 155 (1996)].
[22] The structure factor measures the weight of Bloch waves $e^{i\mathbf{kr}}$ in the correlated wave function of the stripe phase. A similar observation has also been made contemporary by R. S. Markiewicz, cond-mat/9911108 (unpublished).