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STRIPE PHASES IN THE HUBBARD MODEL

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We investigate the magnetic and charge ordering in the stripe phases obtained while using correlated wave functions for finite 8×8 clusters described by the Hubbard model with extended hopping. Nonmagnetic vertical (01) site-centered domain walls and (11) bond-centered stripes are found for the parameters of $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$, respectively, at doping $\delta = 1/8$. The obtained half-filled domain nonmagnetic walls reproduce the maxima observed in neutron scattering for $La_{2-x}Sr_xCuO_4$.

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Nonhomegeneous charge and spin orderings in real space, the so-called *stripe phases*, were first predicted in Hartree–Fock (HF) calculations for the Hubbard model [1], and observed in neutron scattering for $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ only a few years later [2]. Neutron scattering experiments performed on single crystals of $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ reveal static antiferromagnetic (AF) spin domains, separated by charged domain walls (DWs), seen as two kinds of superlattice peaks [2], displaced along the (10) and (01) directions from $\boldsymbol{k} = (\pi, \pi)$ to $\boldsymbol{k} = [\pi(1 \pm 2\eta), \pi]$ and $\boldsymbol{k} = [\pi, \pi(1 \pm 2\eta)]$ ($\eta \simeq \delta$), and the charge-order X-ray peaks displaced by 4η with respect to $\boldsymbol{k} = (0, 0)$. These results imply that DWs with the density of one doped hole per two atoms (*half-filled domain walls* [3]) are located at every fourth vertical line. In contrast, the recent experimental results for $YBa_2Cu_3O_{6.6}$ [4] suggest diagonal (11) DWs ("diagonal stripes").

The experimentally observed vertical half-filled stripes [2] are unstable in the HF calculations against the filled DWs (with one doped hole per one DW atom) [3]. Other methods, such as the density matrix renormalization group [5] and the dynamical mean field theory [6], give stable stripe phases with half-filled DWs in a broad range of parameters. This indicates the importance of local electron correlations which may be explicitly included by modifying the HF states within the local ansatz (LA) method [7]. Indeed, it gives a stripe phase with vertical half-filled nonmagnetic DWs, stable at doping $\delta = 1/8$ in a broad range of Coulomb interaction U in the Hubbard model with the nearest-neighbor hopping t, with and without static phonons [8]. Here we study the stripe phases using realistic parameter sets for cuprate superconductors which include second- and third-neighbor hoppings [9, 10].

The cuprates are described by the Hubbard Hamiltonian [9, 10]

$$H_1 = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) are creation (anihilation) operators for an electron ($\sigma = \uparrow, \downarrow$) at the site i. The hopping elements t_{ij} are nonzero for the first ($t_{ij} = t$), second ($t_{ij} = t'$) and third ($t_{ij} = t''$) neighbors on a square lattice. We consider 8×8 clusters with periodic boundary conditions, with hole doping $\delta = 1/8$ which corresponds to the underdoped regime of the cuprates ($\delta = 1 - n$), where n is an electron density. The actual number of holes is $N_{\rm h} = N\delta$, where $N = 64$ is the number of sites. We choose $t = 1$ as an energy unit and vary the Coulomb interaction U in the range of $6t < U < 12t$ which includes the typical values for the cuprates [9, 10].

The stripe phases were obtained self-consistently within the nonhomogeneous HF approximation. As we do not consider (unstable) spin spirals, we used the simplest close-shell version of the HF method which leads to the HF wave function $|\Phi_0\rangle$, being the product of two Slater determinants for up and down spins. Such functions serve next to construct variational wave functions [7], $|\Psi_0\rangle = \exp\left(-\sum_i \eta_i O_i\right)|\Phi_0\rangle$, where $O_i = n_{i\uparrow} n_{i\downarrow} - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle$ are the local operators, and η_i are the corresponding variational parameters. The averages $\langle \cdots \rangle$ are determined by averaging over the wave function $|\Phi_0\rangle$ of the respective HF state. By construction the local operators describe the correlations which go *beyond* the HF state. This method captures the leading contribution to the correlation energy for the present *nonhomogeneous* states. The variational parameters η_i are fixed by minimizing the total energy in the correlated ground state, $E_0 = \langle\Psi_0|H|\Psi_0\rangle / \langle\Psi_0|\Psi_0\rangle$. As a measure of stability of various textures it is convenient to introduce the energy gain per one doped hole [3], $E_{\rm h} = [E_0(\delta) - E_0(\delta = 0)]/N_{\rm h}$, where $E_0(\delta = 0)$ is the reference energy of the undoped AF phase ($n = 1$). Note that for the HF energies (no correlations included) the energy gain per hole is defined in the same way.

For the characterization of charge and magnetization distribution in the correlated states $\{|\Psi_0\rangle\}$ it is convenient to introduce two functions which are directly measured in elastic coherent scattering experiments: (i) the X-ray elastic scattering function $C(\boldsymbol{k})$ which is a Fourier transform of the density distribution, and (ii) $S(\boldsymbol{k})$, related to the elastic unpolarised neutron scattering. In order to show the charge and spin structure in real space we also introduce after White and Scalapino [5] the averaged charge density $n_{\rm h}$ and spin density S_π

$$n_{\rm h}(l_x) = 1 - \frac{1}{L_y} \sum_{l_y=1}^{L_y} \langle n_{(l_x,l_y),\uparrow} + n_{(l_x,l_y),\downarrow} \rangle, \tag{2}$$

$$S_\pi(l_x) = \frac{1}{L_y} \sum_{l_y=1}^{L_y} (-1)^{l_x+l_y} \frac{1}{2} \langle n_{(l_x,l_y),\uparrow} - n_{(l_x,l_y),\downarrow} \rangle, \tag{3}$$

where $\boldsymbol{l} = (l_x, l_y)$ labels the lattice sites. The densities (2) and (3) are well designed to analyze vertical DWs; analogous formulae with the summations performed along one of the diagonal directions are used instead for diagonal DWs.

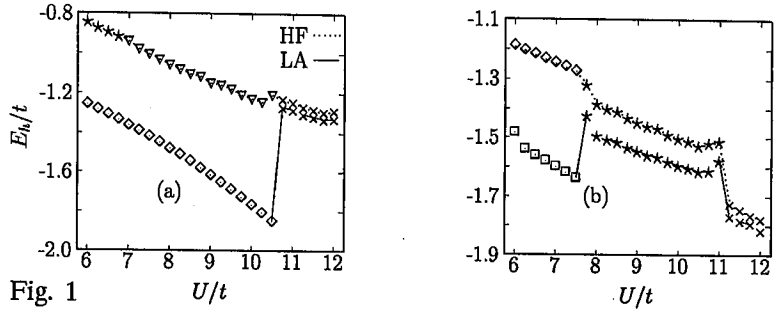

Fig. 1

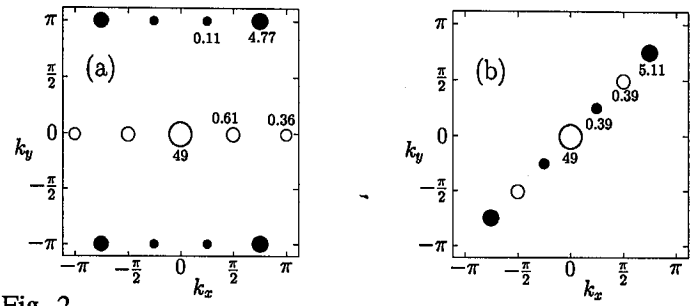

Fig. 2

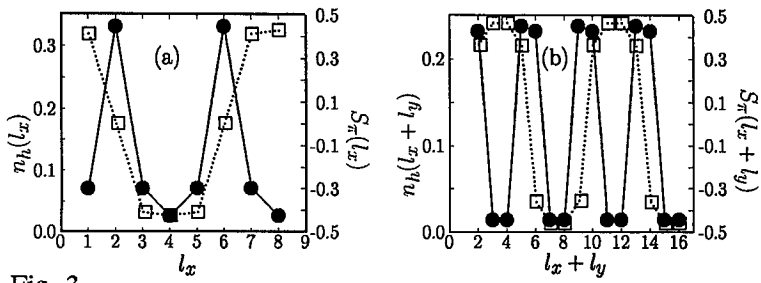

Fig. 3

Fig. 1. Energy per one doped hole E_h/t for various stripe phases in HF (top) and LA (bottom). (a) LSCO parameters: $\diamond$ — vertical nonmagnetic DWs; ∇ — diagonal AF DWs; $\star$ — vertical DWs with quadrupling of unit cell; $\times$ — polaron structures with FM intersecting diagonal DWs. (b) YBCO parameters: $\square$ — vertical FM DWs; $\diamond$ — vertical magnetic walls with quadrupling of unit cell; $\star$ — diagonal FM DWs; $\times$ — polaron structure as in (a). Except for polaron structures ($\times$) all DWs are half-filled.

Fig. 2. Structure factors $S(\boldsymbol{k})$ (full circles) and $C(\boldsymbol{k})$ (open circles) of the half-filled striped phases obtained for: (a) LSCO parameters, (b) YBCO parameters ($U = 10t$). The numbers accompanying the circles indicate the peaks intensity.

Fig. 3. Charge $n_h(l_x)$ (solid circles) and spin $S_\pi(l)$ (open squares) structure functions as obtained for the half-filled (10) and (11) stripes for the parameters of Fig. 2.

We consider here two sets of parameters: (i) for $La_{2-x}Sr_xCuO_4$, $t' = -0.11t$ and $t'' = 0.04t$ (LSCO), and (ii) for $YBa_2Cu_3O_{6+x}$, $t' = -0.30t$ and $t'' = 0.20t$ (YBCO) [10]. The instability towards stripe order is generic, and we have verified that the HF charge and magnetization distribution for particular stripe phases do

not change significantly in the presence of electron correlations. However, which of different HF wave functions corresponds to the correlated ground state depends on the correlation energy (Fig. 1). Here we concentrate ourselves on the characterization of the phases obtained for the realistic value of $U = 10t$. In agreement with intuition, more correlation energy is gained in the structure with nonmagnetic half-filled DWs, and this stripe phase is found in the correlated ground state in a broad range of U values for the LSCO hopping parameters (Fig. 1a). This stripe phase is robust, is found in the strong-coupling regime $U \simeq 10t$ which corresponds to doped La-based cuprates [9, 10], and was also found before for the Hubbard model with nearest-neighbor hopping ($t' = t'' = 0$) [8].

The scattering pattern $S(\boldsymbol{k})$ (Fig. 2a) agrees with the experimentally observed [2] maxima at $\boldsymbol{k} = [\pi(1 \pm 2\eta), \pi]$ and $\boldsymbol{k} = [\pi, \pi(1 \pm 2\eta)]$ with $\eta = \delta$. The charge and spin density distribution (Fig. 3a) shows the AF domains separated by nonmagnetic walls. As a result, one finds the difference by a factor of two between charge and magnetic unit cell.

The polaron-like structure found for the LSCO parameters at $U > 10.75t$, with intersecting ferromagnetic (FM) diagonal (11) and $(1\bar{1})$ walls and large magnetic (FM–AF) islands at the intersection points, can be seen as precursor phases indicating the instability towards diagonal (11) stripes at large U/t. The diagonal walls are promoted by increasing second-neighbor hopping, and indeed, similar diagonal FM half-filled diagonal DWs separating oblique AF domains consisting of two atoms in a row (column) (Figs. 2b and 3b) are found for the YBCO hopping parameters and for $7.75t < U < 11t$ (Fig. 1b). We believe that this stripe phase with the peaks in $S(\boldsymbol{k})$ at $\boldsymbol{k} = [\pi(1 \pm 2\eta), \pi(1 \pm 2\eta)]$ ($\eta = \delta$) describes the experimental situation in $YBa_2Cu_3O_{6.6}$ [4].

In summary, the vertical nonmagnetic and half-filled stripe scenario found in lanthanum based cuprates is confirmed by the present calculations. We note, however, that the bond-centered stripes of White and Scalapino [5], unstable in the present approach, would give the same peaks in neutron scattering.

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