VERTICAL VERSUS DIAGONAL STRIPE PHASES IN CUPRATES*

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Magnetic and charge ordering in the stripe phases in the Hubbard model are investigated in the regime of large on-site Coulomb repulsion, using correlated wave functions. We have found that the appearance of stripes is a robust feature, while vertical and diagonal stripe phases compete with each other. The Hartree–Fock approximation yields qualitative information on the hole and magnetization density in the stripes, but their stability can be decided only by including the electron correlations.

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1. Introduction

Nonhomogeneous charge and spin ordering in real space, so-called stripe phases, were first predicted in the Hartree–Fock (HF) [1] calculations and later observed in neutron scattering experiments for $La_{2-x}Sr_xCuO_4$ [2] and $YBa_2Cu_3O_{6+x}$ [3]. So far, the stripe phases were found using the Hubbard or $t-J$ model in the HF calculations [4,5], by using the density matrix renormalization group [6], in slave-boson approach [7], in the dynamical mean field theory [8], and also by using local ansatz [9]. In all these calculations the stripe phases oriented either along the (10) or along the (11) direction were found, independently of the applied method, when the Coulomb interaction U was sufficiently large as compared with the hopping element t.

The previous studies concentrated on the weakly interacting ($U < 4t$) and intermediate ($U \simeq 6t$) regime. In the present contribution we investigate the question which type of stripes, with vertical or diagonal domain walls, are more stable for the systems with very strong Coulomb interactions ($U > 8t$), as encountered in the cuprates.

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2. The model and variational method

We study the standard nondegenerate Hubbard Hamiltonian H with on-site repulsion U, and consider $U/t = 8$, 12 and 16, where t is the hopping element. The calculations were performed on two-dimensional 8×8 clusters with periodic boundary conditions, with hole doping $\delta = 1 - n = \frac{1}{8}$, where n is the electron density. We use exponential ansatz for the correlated ground state $|\Psi\rangle = \exp\left(-\sum_\mu \alpha_\mu O_\mu\right)|\Psi_{\rm HF}\rangle$, where O_μ are the local operators, α_μ are the corresponding variational parameters, and $|\Psi_{\rm HF}\rangle$ stands for HF ground state wave function. The operators O_μ are: $O_i^{(2)} = n_{i\uparrow}n_{i\downarrow} - \langle n_{i\uparrow}n_{i\downarrow}\rangle$, $O_{i\uparrow}^{(1)} = n_{i\uparrow} - \langle n_{i\uparrow}\rangle$, $O_{i\downarrow}^{(1)} = n_{i\downarrow} - \langle n_{i\downarrow}\rangle$, where $\langle ...\rangle$ denotes the average over HF ground state, and $n_{i\sigma}$ are the electron number operators. Thus, in total the subscript μ runs from 1 up to 3×64.

To include the effect of nearest-neighbor antiferromagnetic correlations we used in addition the composite operator $\sum_{ij}(n_{i\uparrow}n_{j\downarrow} - \langle n_{i\uparrow}n_{j\downarrow}\rangle)$, where the sum runs over all possible pairs $\{ij\}$ of nearest-neighbor sites. The latter operator takes into account all antiferromagnetic correlations on average.

The variational parameters α_μ are fixed by minimizing the energy E in the correlated ground state: $E = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$. To compute E and one-particle densities one needs numerous averages of the type: $\langle O_\mu H\rangle$, $\langle O_\mu O_\nu\rangle$, $\langle O_\mu H O_\nu\rangle$, and $\langle O_\mu n_{i\uparrow} O_\nu\rangle$. For the characterization of charge and magnetization distribution it is convenient to introduce two functions which are directly related to the elastic coherent scattering experiments: $C(\boldsymbol{k})$ and $S(\boldsymbol{k})$. First of them, the X-ray elastic scattering function $C(\boldsymbol{k})$ is: $C(\boldsymbol{k}) = \frac{1}{N}\sum_{ij}\langle n_i\rangle\langle n_j\rangle e^{i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)}$, where $\boldsymbol{R}_i$ are the real space lattice vectors. The second function $S(\boldsymbol{k})$ is related to the elastic neutron unpolarized spin scattering: $S(\boldsymbol{k}) = \frac{1}{N}\sum_{ij}\langle S_i^z\rangle\langle S_j^z\rangle e^{i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)}$.

3. Numerical results and conclusions

We have performed HF computations starting from different initial charge and spin configurations. As self-consistent solutions we obtained several stable and metastable (with higher energy) stripe phases. Most of them showed distinct symmetry. After including the correlation effects we verified that charge and magnetization distribution for particular stripe phases did not change significantly in the presence of electron correlations. However, the energies of stripe phases were strongly modified by the correlations.

For very large U a simple picture emerged. The most typical phases obtained were: (*i*) phase A: weakly ferromagnetic half-filled (on average one hole per two sites, forming a charge density wave) vertical (01) walls (two per used supercell); (*ii*) phase B: similar diagonal (11) half-filled weakly antiferromagnetic diagonal walls.

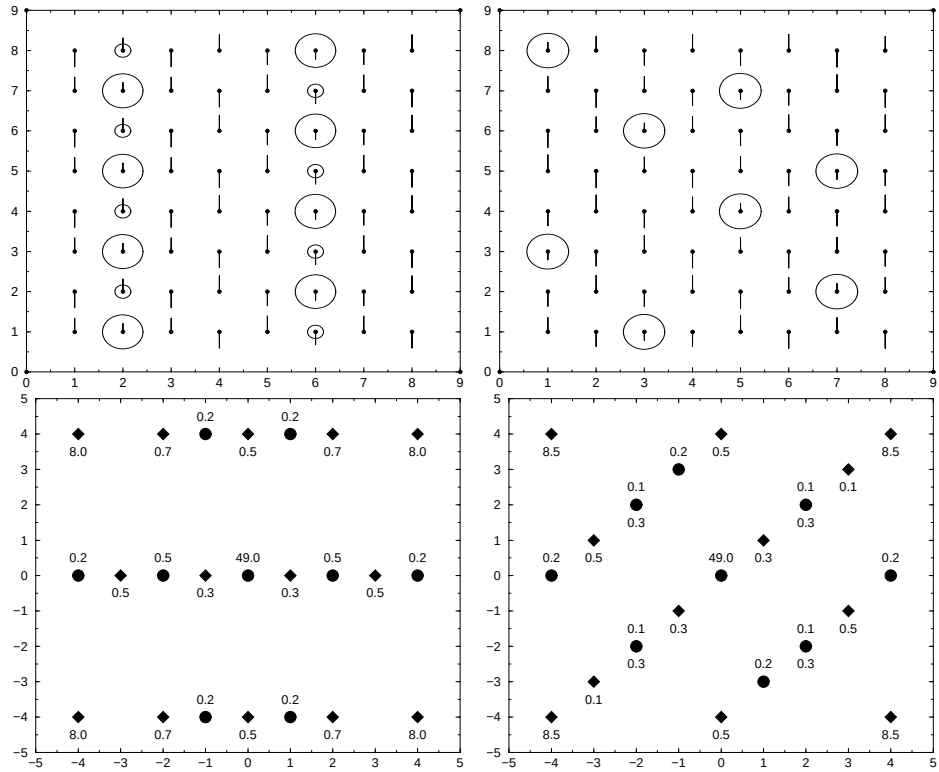

Fig. 1. *Left upper panel*: phase A: weakly half-filled ferromagnetic vertical stripes in 8×8 cluster, as obtained for $\delta = 1/8$ and $U = 12t$. Dots denote cluster sites, the diameters of empty circles correspond to the hole densities, while the lengths of thin bars to the magnetization density (the spin arrows tips were omitted). *Right upper panel:* phase B: weakly antiferromagnetic half-filled diagonal stripes. *Lower panels:* The scattering patterns in the reciprocal space: $C(\boldsymbol{k})$ for X-rays (dots) and $S(\boldsymbol{k})$ for neutrons (diamonds), corresponding to the phases shown in upper panels. The numbers denote the amplitudes.

TABLE I

The actual HF energies ($E_{\rm HF}$) obtained for these two phases as well as total correlated energies E_i (in units of t). The energies E_1, E_2 and E_3 correspond to correlation calculations using only Gutzwiller type local operators (E_1), a set extended by one particle operators (E_2), and including all (intrasite and intersite) operators (E_3).

	Phase A (vertical)				Phase B (diagonal)			
U	$E_{\rm HF}$	E_1	E_2	E_3	$E_{\rm HF}$	E_1	E_2	E_3
8	−38.37	−40.80	−41.13	−41.14	−38.22	−40.59	−40.90	−40.91
12	−31.14	−33.13	−33.56	−33.58	−31.11	−33.10	−33.48	−33.50
16	−27.38	−29.14	−29.67	−29.69	−27.42	−29.23	−29.68	−29.71

The stability of stripe phases changes with increasing U. For $U = 12$ ($U = 16$) the phase A (B) of Fig. 1 is the most stable (we take $t = 1$ as the energy unit). However, at $U = 8$ by far most stable phase is formed by intersecting (01) and (10) walls (this phase is not shown). Several other stripe phases were also found to be locally stable. In particular we remark on vertical nonmagnetic half-filled stripes, such as found earlier in Refs. [1,9] which were stable for intermediate values of U and when using only Gutzwiller type operators (E_1) (on top of it the important averages $\langle O_\mu H O_\nu \rangle$ were computed approximately by replacing H by its HF one-particle part [9]). We have found that these vertical nonmagnetic half-filled stripes are unstable (for $U = 12$, 16) or metastable (for $U = 8$) for very large U, and also when using more accurate and elaborate treatment of correlations.

It might seem that the diagonal (11) stripes form the ground state in the regime of large U ($U > 12t$). *This is however not the case.* In reality the energy distances between different metastable phases are tiny. If one included (as we did) more local operators, the resulting total energy increments would be just as big as the above mentioned energy distances. A similar situation occurs when taking into account: *(i)* relatively small second-nearest-neighbor hopping t' in H; *(ii)* three- and four-particle excitations in local operators (note that U is very large; at present no quantum-chemistry method does exist which would allow to obtain results for such a case); *(iii)* small lattice anisotropy which could be induced by static phonons [10]. Therefore, conclusive results about the stripe stability can be obtained only by including all these effects and treating the correlation effects in an accurate way.

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