The Novel Spin-Charge Patterns in Correlated Electron Systems Described by Extended Hubbard Hamiltonian

K. Rościszewski and A.M. Oleś*

M. Smoluchowski Institute of Physics, Jagiellonian University
Reymonta 4, 30-059 Kraków, Poland

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Inhomogeneous spin and charge orderings in doped two-dimensional correlated electron systems described by the extended Hubbard Hamiltonian were investigated. At the crossover from stripe phases to charge order phases, the novel types of ordering connected with highly symmetric superlattice-type spin and charge patterns were identified. In particular, the emergence of local hexagonal-like symmetry is of interest as such patterns are generic in complex, nonlinear dynamic systems.

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1. Introduction

Inhomogeneous charge and spin orderings in doped cuprates, so-called stripe phases, attracted much attention due to their possible role in the high temperature superconductivity [1]. They were discovered both in cuprates [2] and nickelates [3]. In general, they are present in systems with relatively small doping $\delta = 1-n$ (typically 1/8, where n is the band filling) and for medium to strong on-site Coulomb repulsion U and not too large intersite repulsion V [4]. For systems with larger hole concentrations the stripes are replaced by charge order (CO) [5, 6]. The theoretical investigations of the stripes and CO in two- and three-dimensional systems with Coulomb inter- and intra-site repulsion are numerous and involve various theoretical approaches [7, 1]. They allowed to understand the leading mechanisms of magnetic and/or charge instabilities leading to the symmetry broken ordered

*corresponding author; e-mail: roscis@if.uj.edu.pl (K. Rościszewski and A.M. Oleś)

states, but as a rule strong simplifying assumptions about the ground state symmetry were made in most papers. Therefore the hypothetical presence of many phases, in particular those showing complex spin and charge symmetry patterns, was not fully investigated.

In the present paper we would like to provide some interesting examples of such phases. They can be considered to be intermediate between stripes and CO phases and as such deserve a proper attention. The stripes and the usual two-sublattice CO phases were discussed in many separate investigations and therefore here we will not comment much on them.

2. Theory

We studied the ground state of the standard single-band extended Hubbard Hamiltonian,

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j . \tag{1}$$

Here $c^{\dagger}_{i\sigma}$ are creation operators for an electron with spin $\sigma = \uparrow, \downarrow$ at site i, and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ are electron number operators. The hopping elements are finite, $t_{ij} = -t$, on the bonds $\langle i,j \rangle$ which connect nearest neighbors and zero otherwise. The sum $\langle i,j \rangle$ runs over all nearest neighbor pairs. Coulomb interactions U and V are expressed in the units of the hopping element $t = 1$.

We considered two-dimensional (2D) square clusters containing $N = 64$ sites with periodic boundary conditions, with hole doping $\delta = 1-n = \frac{1}{8}, \frac{1}{4}, \frac{1}{2}$ away from half-filling ($n = 1$), where n is an electron density. First, the calculations within the Hartree–Fock (HF) approximation were performed to determine the ground state wave function $|\Psi_{\rm HF}\rangle$ and in the next step the HF wave function was modified to include the electron correlation effects. We used local ansatz [8] for the correlated ground state, $|\Psi\rangle = \exp(-\sum_{\mu} \alpha_{\mu} O_{\mu})\ |\Psi_{\rm HF}\rangle$, where O_{μ} are properly chosen local operators and α_{μ} are the corresponding variational parameters. In this way, the ground state wave function can be optimized and energetically unfavorable configurations, such as double occupancies at one site, and too large charge and spin fluctuations on the neighboring sites are suppressed. The variational parameters $\{\alpha_{\mu}\}$ were fixed by minimizing the total energy E in the correlated ground state. To avoid the burden of working with all α_{μ} simultaneously (the number of different α_{μ} amounts to several hundreds) we used the local increments (LI) expansion [9], the method which made correlation treatment of solids reasonably "non-expensive".

HF computations were run starting from different initial charge and spin configurations. The minimized energy $E_{\rm HF}$ has a multitude of local minima. In this respect too few HF starting configurations may result in a failure to find the true ground state minimum. For the sake of present study, for each set of U and $V < \frac{1}{2}U$ we picked 50 different, carefully chosen starting configurations. In this way

we wanted to make an account for any (possible a priori) ground state known from the literature, such as antiferromagnetic order, various stripe phases, polaronic-like configurations and various CO phases with nonhomogeneous charge density and magnetization distribution. As a result we obtained numerous HF-stable phases with different energy and/or different spin and charge patterns. For each such phase we performed the LI correlation computations obtaining the final (total) energy, $E = E_{\mathrm{HF}} + E_{\mathrm{corr}}$. The minimal value of E was used to identify the true ground state. More technical details can be found in Ref. [4].

3. The novel superlattice-type phases

3.1. $U = 6$, *low doping* $\delta = \frac{1}{8}$

In the intermediate coupling regime and for the lightly doped systems ($\delta = \frac{1}{8}$) variety of stripe-like structures for small values of V up to $V = 1.0$ was found. At larger V one finds instead nine-site antiferromagnetic islands separated by non-magnetic domain walls in both horizontal and vertical directions. Such pattern can clearly be termed a superlattice (see Fig. 1) and are intermediate between stripes and CO phases sharing common features with both of them. Indeed, for $V = 1.3$ vertical stripe phases are stable again but simultaneously strong charge density modulation on domain walls develops. For still larger V imperfect (space inhomogeneous) CO phase sets in [4].

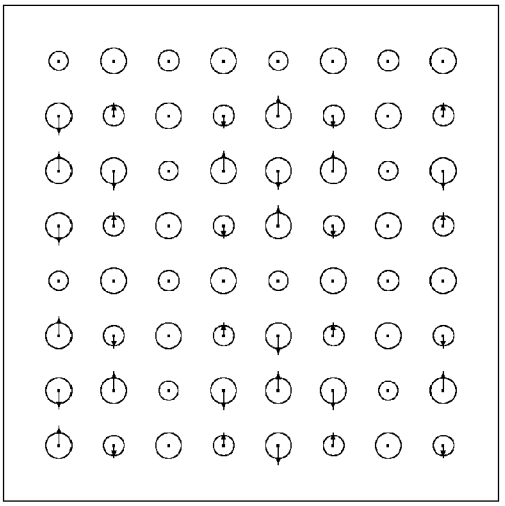

Fig. 1. Magnetic and charge order as obtained for an 8×8 cluster with $U = 6$, $V = 1.2$ at doping $\delta = \frac{1}{8}$. The circle diameters correspond to the on-site charges, and the arrow lengths to the spin values expressed in nearest neighbor atom–atom distance which is taken to be unity.

3.2. $U = 6$, large doping: $\delta = \frac{1}{2}$

For large doping and $V < 1.5$ spin and charges show superlattice-type ordering while CO sets in for larger V. Typical pattern is shown in Fig. 2 (for $V = 0$), i.e., regularly placed antiferromagnetic polaronic islands with small magnetic moments. The shape of the islands (for different V) can change a little bit but as a rule the islands form small magnetically ordered squares.

The polarons are well separated from each other and resemble Zhang–Rice singlets at low doping [10]. Here these states occur in otherwise non-magnetic (unpolarized) background and demonstrate generic tendency towards antiferromagnetism which survives locally even in large doping regime.

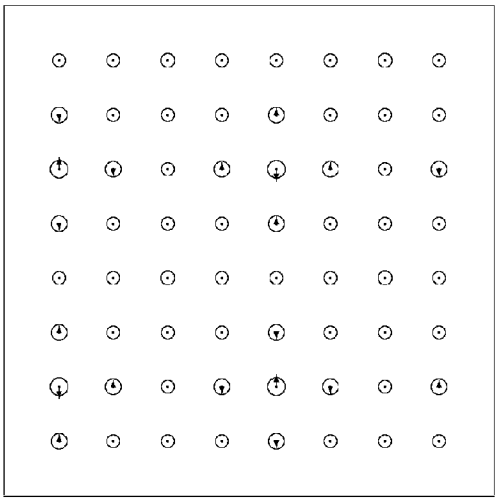

Fig. 2. Magnetic and charge order as obtained for an 8×8 cluster with $U = 6$, $V = 0$ at large doping $\delta = \frac{1}{2}$.

Let us note that for lower doping $\delta = \frac{1}{4}$ for all studied values of V (i.e., $0 < V < 3$) such intermediate superlattice-type patterns are absent. In this case one finds first vertical and diagonal stripes for lower values of V, and usual CO phases for $V > 1.65$.

3.3. The medium to strong coupling regime $U = 8$ and large doping: $\delta = \frac{1}{2}$

For medium to strong coupling regime and low dopings $\delta = \frac{1}{8}$, $\frac{1}{4}$ only stripe phases and imperfect CO for $V > 1.8$ are the most stable. No intermediate superlattice-type structures were found which suggests that such structures are suppressed by a higher value of V. However, for the large doping $\delta = \frac{1}{2}$ the situation is again much the same like that found for intermediate coupling $U = 6$. Highly symmetric superlattice-type spin and charge patterns are the most stable

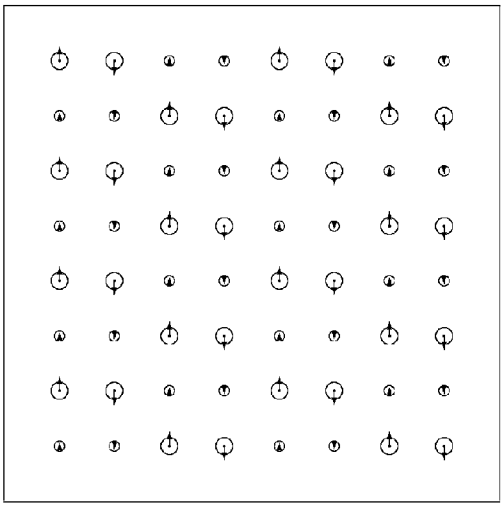

Fig. 3. Local hexagonal, magnetic, and charge order as obtained for an 8×8 cluster with $U = 8$, $V = 0.4$ at large doping $\delta = \frac{1}{2}$.

ones for $V < 1.2$. In our opinion, the most interesting finding is sporadic appearance of local hexagonal-like order shown in Fig. 3.

We attribute the mechanism which governs formation of such hexagonal phase to belong to the realm of nonlinear, nonequilibrium phenomena. We believe that for large doping in the regime of strong on-site interactions any starting charge configuration necessarily must show strong charge gradients which together with large Coulomb interaction suffice to drive local transitions belonging to the same category as nonlinear Benard–Marangoni convection with hexagonal convection cells [11].

The mechanisms leading to novel structures such as the ones shown in Fig. 3 are not yet completely understood. Several factors contribute: strong local Coulomb interaction U polarizes the sites with enhanced electron density, while the intersite Coulomb interaction V induces a complicated pattern of the charge density wave. Even at the sites with lower electron densities small magnetic moments are formed which helps again to lower the interaction energy due to the on-site term $\propto U$.

One can conclude that a multitude of inhomogeneous spin and charge ordered ground states is possible in the doped, strongly correlated electron systems in two dimensions. While for weak (strong) intersite Coulomb interaction the stripe phases (charge order phases) are generic, the phase situations is not simple for the intermediate coupling. The local symmetry of the most stable patterns does not need to mirror the underlying lattice symmetry but is rather governed by a complicated balance of several competitive factors. In particular, the novel superlattice patterns and the charge order with a local hexagonal symmetry are manifestations of such competition in strongly correlated electron systems.

Therefore the spontaneous symmetry breaking found in geometrically unfrustrated lattice gives complex structures (with coexisting charge and magnetic order) characterised by large unit cells.

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