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Unconventional spin-charge phase separation in a model 2D cuprate

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In cuprates, the competition of static magnetic order, bulk superconductivity and charge-density waves has attracted a lot of attention over the years, but its nature remains a challenge [1]. Recently [2] it was argued that cuprates should be addressed to be the *d*-*d* charge transfer (CT) unstable systems whose description implies accounting of the three many-electron valence states $CuO_4^{7-,6-,5-}$ (nominally $Cu^{1+,2+,3+}$) on an equal footing as a well-defined charge triplet. This allows us to introduce a minimal model for cuprates with the on-site Hilbert space reduced to only these three charge states, three effective $Cu^{1+,2+,3+}$ valence centers where the electronic and lattice degrees of freedom get strongly locked together, and make use of the $S = 1$ pseudospin formalism [2–8]. Such a formalism constitutes a powerful method to study complex phenomena in interacting quantum systems characterized by the coexistence and competition of various ordered states [9].

At variance with spinless ground states of the "electron" Cu^{1+} and "hole" Cu^{3+} centers the $s = 1/2$ Cu^{2+} centers are coupled by a rather strong Heisenberg exchange interaction that can compete with the on-site and inter-site charge density interactions. To describe a competition of the spin and charge degrees of freedom in cuprates we proposed recently a simplified 2D spin-pseudospin model [10, 11]. Within atomic limit the charge degree of freedom is assumed to be described by an effective $S = 1$ pseudospin Hamiltonian:

$$\hat{H}_{\rm ch} = \sum_i (\Delta_i S_{iz}^2 - \mu S_{iz}) + \sum_{i<j} V_{ij} S_{iz} S_{jz}, \qquad (1)$$

with a charge density constraint: $nN = \sum_i \langle S_{iz} \rangle = \text{const}$. The first term, or on-site pseudospin anisotropy, describes the effects of the on-site density-density interactions: $\Delta = U/2$, where U is a conventional correlation parameter. In the second "pseudo-Zeeman" term μ is a hole chemical potential. The third "pseudo-Ising" term describes the effects of the inter-site density-density interactions. Formally Hamiltonian $\hat{H}_{\rm ch}$ corresponds to a classical spin-1 Ising model with a single-ion anisotropy in the presence of a longitudinal magnetic field. Conventional spin $s = 1/2$ degree of freedom can be build in our effective pseudospin Hamiltonian (1), if we transform conventional Heisenberg spin exchange Cu^{2+}-Cu^{2+} coupling as follows

$$\hat{H}_{\rm ex} = \sum_{i<j} (1 - \hat{S}_{iz}^2) J_{ij} (1 - \hat{S}_{jz}^2)(\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_j), \qquad (2)$$

where $(1 - \hat{S}_{iz}^2)$ is a projection operator which picks out the $s = 1/2$ Cu^{2+} center, J_{ij} is the conventional Cu^{2+}-Cu^{2+} exchange integral. Hereafter we restrict ourselves by nearest-neighbor couplings with repulsive inter-site correlation $V_{\rm nn} = V > 0$ and antiferromagnetic exchange integral $J_{\rm nn} = J > 0$. The atomic limit, that is a full neglect of any transfer terms seems to be the most important limitation of the model, however, we believe it catches principal features of the spin-charge competition in cuprates.

Within a two-sublattice approximation, the generalized mean-field approximation (MFA) technique points to the five homogeneous ground state (GS) solutions or phases of the spin-pseudospin system, termed here as COI, COII, COIII, AFM, and FIM [11]. The COI is a charge-ordered phase without spin centers, in the COII and COIII phases the charge order is diluted by the non-interacting spins, the AFM phase corresponds to a checkerboard antiferromagnetic spin ordering, while in "ferrimagnetic" FIM phase the charge and spin orders coexist. In a "weak" exchange limit, at $J < 4V$, all the GS phases (COI, COII, COIII, FIM) anyhow correspond to various types of the charge order. In a "weak" inter-site coupling limit, at $V < J/4$, there are only COI and AFM phases. However, the MFA cannot reproduce some important features of the spin-charge competition related with formation of inhomogeneities and phase separation. Here we present the results of classical Monte-Carlo (MC) calculations.

The model spin-charge Hamiltonian $\hat{H} = \hat{H}_{\rm ch} + \hat{H}_{\rm ex}$ has been analyzed by means of MC simulations on a large two-dimensional square lattice 256×256 under periodical boundary conditions with the heat-bath algorithm in a "weak" inter-site correlation limit ($V < J/4$). The MC algorithm used in this analysis implies "mobile"

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charges [12, 13]. As an initial state, we choose a random distribution of charges (pseudospins) and spins with a fixed total z-component of pseudospins for a given value of n. In numerical calculations, we used the Ising type spin-spin interaction with the same account of the on-site occupation dependence as in expression (2).

The behavior of the system strongly depends on the sign and value of the on-site correlation stabilizing CO ($\Delta < 0$) or AFM ($\Delta > 0$) phase, respectively. We show that homogeneous ground-state AFM solutions found in the MFA [10, 11] are unstable with respect to a phase separation with the charge and spin subsystems behaving like immiscible quantum liquids. Temperature dependence of the specific heat and spin susceptibility for the AFM phase at $n = 0.1$ are shown in Fig. 1. The

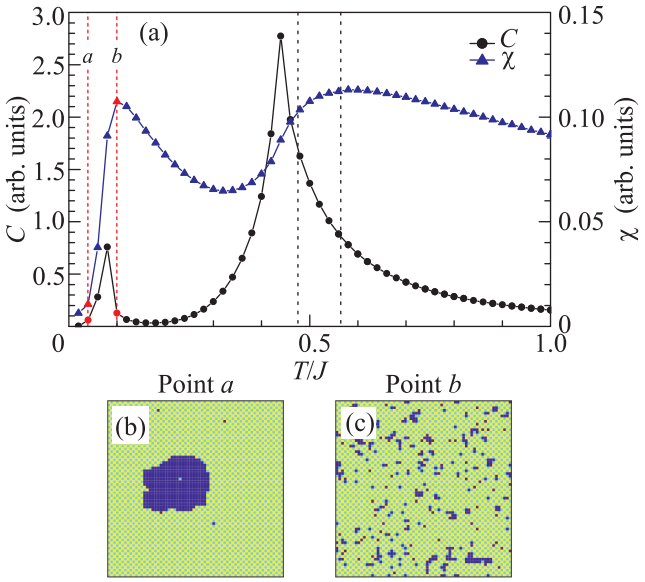

Fig. 1. (Colour online) (a) – The temperature dependence of the specific heat and the magnetic susceptibility for the AFM phase at $n = 0.1$, $\Delta = 0.5$, $V = 0.1$, $J = 1$. The Ising type high-temperature peak corresponds to the AFM ordering in spin subsystem at $T^{\star} \approx 0.45\,J$. Two lines above $T_{\rm AFM}$ at $T \approx 0.465\,J$ and $T \approx 0.562\,J$ point to critical temperatures for 2D diluted ($n = 0.1$) and concentrated ($n = 0.0$) Ising model (see, e.g., Ref. [14]), respectively. (b), (c) – The low-temperature peak corresponds to the charge droplet condensation shown in representative MC snapshots at temperatures below (b) and above (c) $T_{\rm PS}$. The snapshots are made on square lattice 64×64 to better visualize the checkerboard structure. Blue color in the snapshots points to doped charge distribution, $\langle S_z \rangle = 1$, yellow and green colors correspond to the on-site spin values: $\langle s_z \rangle = \pm 1/2$, respectively

snapshots at $T < T_{\rm PS}$ (b) and $T > T_{\rm PS}$ (c) show that the puzzling peculiarity at $T_{\rm PS} \approx 0.08\,J$ is related with a condensation of doped charges in the charge droplets, or a "third-order" phase transition (see, e.g., Ref. [12]) to the phase separated state with coexistence of homogeneous phases with $n = 0$ and $n = 1$, respectively. The inhomogeneous droplet phase reduces the energy of the system and changes the diagram of the GS. Charge doping does suppress the long-range spin order, but the phase separation of doped charges and short-range spin order exists for a whole range of the charge doping.

In the COI phase, the doped charges remain distributed randomly over the CO matrix up to $T = 0$ as for the near-neighbor interaction the energies of all possible distributions of extra charges over the CO matrix are equal. For this reason the GS energy of the COI MFA solutions exactly matches the energy of the low-temperature MC state and the entropy of the low-temperature state in the doped CO phase is higher than in the doped AFM phase.

We calculated the concentration dependencies of specific heat and susceptibility. Also, we considered briefly the localization of the doped charges within antiphase 180° domain walls of AFM domain structure.

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