Monte Carlo simulations of a model cuprate

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***Abstract*—We used the classical Monte Carlo method to construct phase diagrams of a model cuprate within the framework of a *S* = 1 pseudo-spin formalism**

***Keywords*—HTSC cuprates, charge triplet model, pseudo-spin formalism, classical Monte Carlo simulations**

I. Introduction

One of the topical problems of the high-T_c cuprate physics is the coexistence and competition of antiferromagnetic, superconducting, and charge orderings [1], the study of which is complicated by the presence of heterogeneity due to dopants or non-isovalent substitution, as well as to the internal electronic tendency to heterogeneity [2]. The use of the pseudo-spin formalism and Monte Carlo (MC) method is very fruitful for constructing phase diagrams and studying the features of the thermodynamic properties for such systems.

II. Model

A minimal model to describe the charge degree of freedom in cuprates [3], [4] implies that for the CuO_4 centers in CuO_2 plane the on-site Hilbert space reduced to a charge triplet formed by the three many-electron valence states $[CuO]_4^{7-,6-,5-}$ (nominally $Cu^{1+,2+,3+}$). These states can be considered to be the components of the $S = 1$ pseudo-spin triplet with projections $M_S = -1,\ 0,\ +1$. Effective pseudo-spin Hamiltonian of the model cuprate with the addition of the Heisenberg spin-spin exchange coupling of the $s = 1/2$ $[CuO]_4^{6-}$ (Cu^{2+}) centers can be written as follows:

$$\mathcal{H} = \mathcal{H}_{ch} + \mathcal{H}_{exc} + \mathcal{H}_{tr}^{(1)} + \mathcal{H}_{tr}^{(2)} - \mu \sum_i S_{zi}\,. \qquad (1)$$

Here, the first term

$$\mathcal{H}_{ch} = \Delta \sum_i S_{zi}^2 + V \sum_{\langle ij \rangle} S_{zi} S_{zj} \qquad (2)$$

describes the on-site and inter-site nearest-neighbour density-density correlations, respectively, so that $\Delta = U/2$, U being the correlation parameter, and $V > 0$. The sums run over the sites of a 2D square lattice, $\langle ij \rangle$ means the nearest neighbors. The second term

$$\mathcal{H}_{ex} = Js^2 \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j \qquad (3)$$

is the antiferromagnetic ($J > 0$) Heisenberg exchange coupling for the CuO_4^{6-} centers, where $\boldsymbol{\sigma} = P_0 \mathbf{s}/s$ operators take into account the on-site spin density $P_0 = 1 - S_z^2$, and $\mathbf{s}$ is the spin $s = 1/2$ operator. The third term

$$\begin{aligned} \mathcal{H}_{tr}^{(1)} \;=\; & -t_p \sum_{\langle ij \rangle} \left(P_i^+ P_j + P_j^+ P_i \right) \\ & -\; t_n \sum_{\langle ij \rangle} \left(N_i^+ N_j + N_j^+ N_i \right) \\ & - \frac{t_{pn}}{2} \sum_{\langle ij \rangle} \left(P_i^+ N_j + P_j^+ N_i + N_i^+ P_j + N_j^+ P_i \right) \end{aligned} \qquad (4)$$

where the transfer integrals t_p, t_n, t_{pn} describe the three types of the correlated "one-particle" transport. P and N operators are the combinations of the pseudospin S=1 operators [3]: $P^+ \propto (S_+ + T_+)$, $N^+ \propto (S_+ - T_+)$, $T_+ = S_z S_+ + S_+ S_z$. The next term

$$\mathcal{H}_{tr}^{(2)} = -t_b \sum_{\langle ij \rangle} \left(S_{+i}^2 S_{-j}^2 + S_{+j}^2 S_{-i}^2 \right) \qquad (5)$$

where the transfer integral t_b describes the two-particle ("composite boson") transport [3]. The last term with chemical potential μ is needed to account for the charge density constraint, $nN = \langle \sum_i S_{zi} \rangle = const$.

III. State selection algorithm

We write the on-site wave function of the charge triplet in the form as follows

$$|\Psi\rangle = c_{+1} |{+1}\rangle + c_0 |0\rangle + c_{-1} |{-1}\rangle\,, \qquad (6)$$

$$c_{\pm 1} = \sin\frac{\theta}{2} \cos\frac{\phi}{2} e^{\mp i \frac{\alpha}{2}}, \quad c_0 = \cos\frac{\theta}{2} e^{i \frac{\beta}{2}}, \qquad (7)$$

where $0 \le \theta \le \pi$, $0 \le \phi \le \pi$, $0 \le \alpha \le 2\pi$, $0 \le \beta \le 2\pi$. This state corresponds to a point in the octant of the unit sphere. We use the Metropolis algorithm for a system with conservation of the total charge. The charge at the site, n_i, is related to the parameters of the wave function by the expression

$$2n_i = (1 - \cos\theta_i) \cos\phi_i. \qquad (8)$$

We require when the states of sites 1 and 2 change simultaneously, the total charge of the pair is preserved, $n_1 + n_2 = n_1' + n_2' = 2n$, and the points representing states uniformly fill the allowed area in the octant.

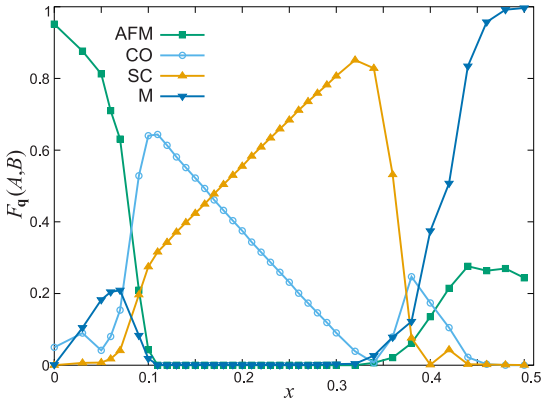

Fig. 1. (Color online) The dependencies on the charge doping of the structure factors in the ground state calculated with parameters $\Delta = 0.8$, $V = 0.625$, $J = 1$, $t_p = 0.35$, $t_n = 0$, $t_{pn} = -0.24$, (all in units of the t_b).

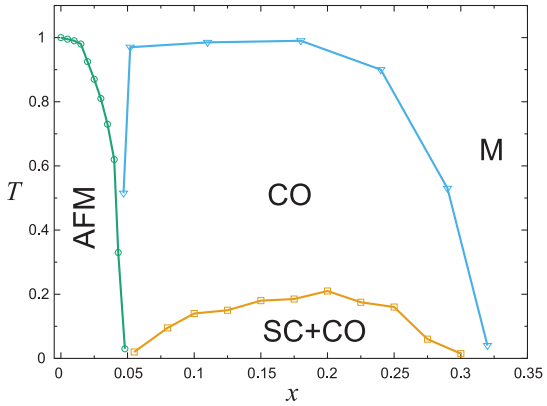

Fig. 2. (Color online) The MC T - x (x the charge doping) phase diagram for the model cuprate calculated with the same parameters as in Fig. 1.

The state selection algorithm consists of the following steps:

1) caclulation of n_1, $-1 + n + |n| \leq n_1 \leq 1 + n - |n|$, from equation

$$G_1(n_1; n) = \gamma, \tag{9}$$

where γ is a random uniformly distributed quantity, $0 \leq \gamma \leq 1$,

$$G_1(n_1; n) = \frac{\Phi(n_1) - \Theta(n)\,\Phi(-1 + 2|n|)}{\Phi(1 - 2|n|)}, \tag{10}$$

$$\Phi(x) = \operatorname{sgn} x \left[\frac{2\sqrt{1+|x|}}{\pi} \left(\frac{2\,\Pi\left(-1, \frac{\pi}{2} \,\middle|\, m(x)\right)}{1+|x|} - m(x)\,K\left(m(x)\right) \right) - \frac{1}{2} \right] + \frac{1}{2}, \tag{11}$$

$m(x) = \frac{1-|x|}{1+|x|}$, $\Theta(x)$ is the Heaviside step function, $\Pi\left(-1, \frac{\pi}{2} \,\middle|\, m\right) = \Pi_1(1, \sqrt{m})$ is the complete elliptic integral of the third kind, $K(m)$ is the complete elliptic integral of the first kind;

2) calculation of the value $n_2 = 2n - n_1$;

3) calculation of $\cos\frac{\theta_i}{2}$ from equation

$$\cos\frac{\theta_i}{2} = \sqrt{1 - |n_i|}\ \operatorname{sn}\left(\gamma_i K\left(m(n_i)\right), m(n_i)\right), \tag{12}$$

where γ_i, $i = 1, 2$, are the random uniformly distributed quantities, $0 \leq \gamma_i \leq 1$, $\operatorname{sn}(x, m)$ is the Jacobi function. If $n_i = 0$, we take $\cos\frac{\theta_i}{2} = \gamma_i$.

4) calculation of $\cos\phi_i$ from equation

$$\cos\phi_i = \frac{n_i}{1 - \cos^2\frac{\theta_i}{2}}. \tag{13}$$

If $n_i = 0$ and $\cos\frac{\theta_i}{2} = 1$, ϕ_i is a random uniformly distributed quantity, $0 \leq \phi_i \leq \pi$.

IV. Results

In MC simulation, we calculated the structure factors

$$F_{\mathbf{q}}(A, B) = \frac{1}{N^2} \sum_{lm} e^{i\mathbf{q}\,(\mathbf{r}_l - \mathbf{r}_m)} \left\langle A_l B_m \right\rangle, \tag{14}$$

where A_l and B_m are the on-site operators and the summation is performed over all sites of the square lattice. To determine the type of ordering, we monitored the following structure factors: $F_{(\pi,\pi)}(\boldsymbol{\sigma}, \boldsymbol{\sigma})$ for antiferromagnetic (AFM) order, $F_{(\pi,\pi)}(S_z, S_z)$ for the charge order (CO), $F_{(0,0)}(S^2_+, S^2_-)$ for the superconducting order (SC), $F_{(0,0)}(P^+, P)$ for the "metal" phase (M).

To illustrate the results of the MC simulation in Fig. 1 we presented the doping dependence of the main structure factors for the ground state of the model cuprate. Fig. 2 shows the MC simulation of the T - x phase diagram for model cuprate with the Hamiltonian (1) can reproduce some most important features of the real phase diagrams typical for the hole doped cuprates [1]. The critical temperatures for the AFM, CO, and SC phases were determined from the jump in the structure factor from zero to a certain finite value. Despite the preliminary nature of the results, the obtained phase diagrams show promising possibilities to describe the coexistence and competition of various phase orders in cuprates.

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