Monte Carlo simulations of a model cuprate

Yury Panov, Alexander Moskvin, Vasilii Ulitko

Ural Federal University, Institute of Natural Sciences and Mathematics

Ekaterinburg, Russia

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Abstract

One of the topical problems of the high-T_c cuprate physics is the coexistence and competition of antiferromagnetic, superconducting, and charge orderings, 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.

The use of the pseudospin formalism and Monte Carlo method is very fruitful for constructing phase diagrams and studying the features of the thermodynamic properties for such systems.

Model

A minimal model for the CuO_4 centers in CuO_2 plane in cuprates [1,2]:

CuO_4 center state	effective Cu ion state	pseudospin $S=1$ state	conventional spin state
CuO_4^{7-}	Cu^{1+}, $3d^{10}$	-1	0
CuO_4^{6-}	Cu^{2+}, $3d^9$	0	$\pm\frac{1}{2}$
CuO_4^{5-}	Cu^{3+}, $3d^8$	$+1$	0

1. A.S. Moskvin, True Charge-Transfer Gap in Parent Insulating Cuprates, *PRB* **84**, 075116 (2011)

2. A.S. Moskvin, Perspectives of Disproportionation Driven Superconductivity in Strongly Correlated 3d Compounds, *J.Phys.:Cond.Mat.* **25**, 085601 (2013)

Further development

- A.S. Moskvin, Y.D. Panov, Electron-Hole Dimers in the Parent Phase of Quasi-2D Cuprates, *Phys. Solid State* **61**, 1553 (2019)

- A. S. Moskvin, Y. D. Panov, Nature of the Pseudogap Phase of HTSC Cuprates, *Phys. Solid State* **62**, 1554 (2020)

Effective pseudospin Hamiltonian (1 of 2)

Effective pseudospin Hamiltonian $S = 1$ of the model cuprate

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

Here,

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

 – the on-site and inter-site nearest-neighbour density-density correlations.

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

 – the antiferromagnetic Heisenberg exchange coupling for the CuO_4^{6-} centers, $\boldsymbol{\sigma} = P_0 \mathbf{s}/s$, the on-site spin density $P_0 = 1 - S_z^2$, $\mathbf{s}$ is the spin $s = 1/2$ operator.

Effective pseudospin Hamiltonian (2 of 2)

Effective pseudospin Hamiltonian $S = 1$ of the model cuprate

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

* $\mathcal{H}_{tr}^{(1)} = -t_p \sum_{\langle ij \rangle} \left(P_i^+ P_j + P_j^+ P_i \right) - t_n \sum_{\langle ij \rangle} \left(N_i^+ N_j + N_j^+ N_i \right)$
$$- \frac{t_{pn}}{2} \sum_{\langle ij \rangle} \left(P_i^+ N_j + P_j^+ N_i + N_i^+ P_j + N_j^+ P_i \right)$$

  – the correlated one-particle transport, P and N operators are the combinations of the pseudospin $S = 1$ operators:
  $P^+ \propto (S_+ + T_+), \quad N^+ \propto (S_+ - T_+), \quad T_+ = S_z S_+ + S_+ S_z.$

* $\mathcal{H}_{tr}^{(2)} = -t_b \sum_{\langle ij \rangle} \left(S_{+i}^2 S_{-j}^2 + S_{+j}^2 S_{-i}^2 \right)$ is the two-particle transport.

* $-\mu \sum_i S_{zi}$ accounts for the charge constraint, $\langle \sum_i S_{zi} \rangle = const.$

The sums run over the sites of a 2D square lattice, $\langle ij \rangle$ means the nearest neighbors.

The uniform distribution of random unit vectors

It is well known, that the uniform distribution of randomly generated vectors over the unit sphere is given by the following state selection algorithm:

1. $\phi = 2\pi\gamma_1$;
2. $\theta = \arccos\gamma_2$,

where $\gamma_{1,2}$ are random numbers in the $[0, 1]$ range.

The (ϕ, θ)-histogram is shown on the left panel, and this produces the flat (ϕ, z)-histogram (right panel).
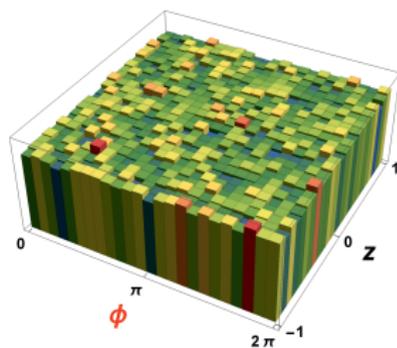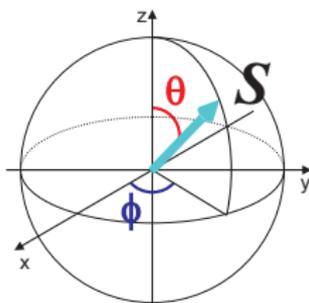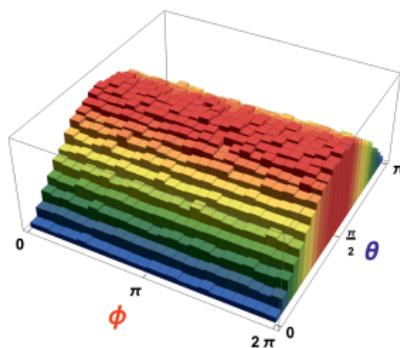
The spin $S = 1$ problem

The wave function of the $S = 1$ triplet is a point in the octant of the unit sphere:

$$|\Psi\rangle = c_{+1} |{+1}\rangle + c_0 |0\rangle + c_{-1} |{-1}\rangle, \quad c_{\pm 1} = \sin\frac{\theta}{2}\cos\frac{\phi}{2} e^{\mp i\frac{\alpha}{2}}, \quad c_0 = \cos\frac{\theta}{2} e^{i\frac{\beta}{2}},$$

where $0 \leq \theta \leq \pi$, $0 \leq \phi \leq \pi$, $0 \leq \alpha \leq 2\pi$, $0 \leq \beta \leq 2\pi$.

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

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

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.

State selection algorithm (1 of 2)

- caclulation of n_1, $-1 + n + |n| \leq n_1 \leq 1 + n - |n|$, from equation $G_1(n_1; n) = \gamma$, where γ is a random uniformly distributed quantity, $0 \leq \gamma \leq 1$,

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

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

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

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

- calculation of $\cos\frac{\theta_i}{2}$ from equation
$\cos\dfrac{\theta_i}{2} = \sqrt{1 - |n_i|}\,\operatorname{sn}\left(\gamma_i K\left(m(n_i)\right), m(n_i)\right)$, 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 $\cos\frac{\theta_i}{2} = \gamma_i$.

State selection algorithm (2 of 2)

- calculation of $\cos\phi_i$ from equation $\cos\phi_i = \dfrac{n_i}{1 - \cos^2\frac{\theta_i}{2}}$. If $n_i = 0$ and $\cos\frac{\theta_i}{2} = 1$, ϕ_i is a random uniformly distributed quantity, $0 \le \phi_i \le \pi$.

The (ϕ, θ)-histogram is shown on the left panel, and this produces the flat (ϕ, z)-histogram (right panel).
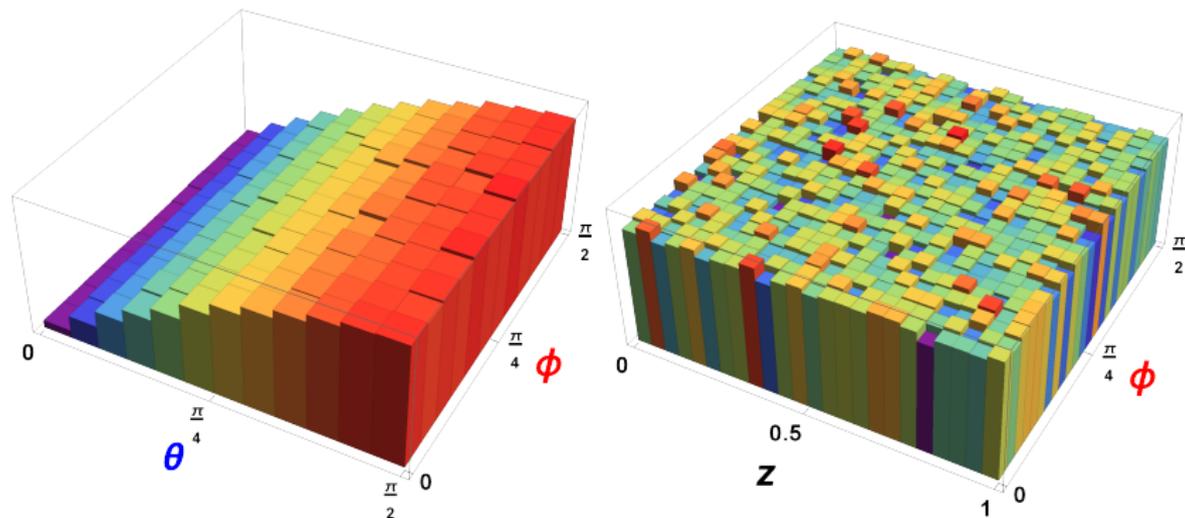
Monte Carlo simulation

In Monte Carlo simulation, we calculated the structure factors

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

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).

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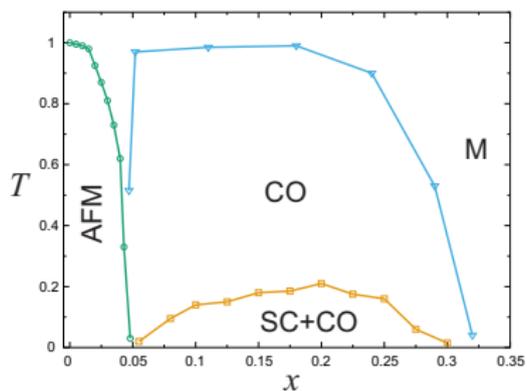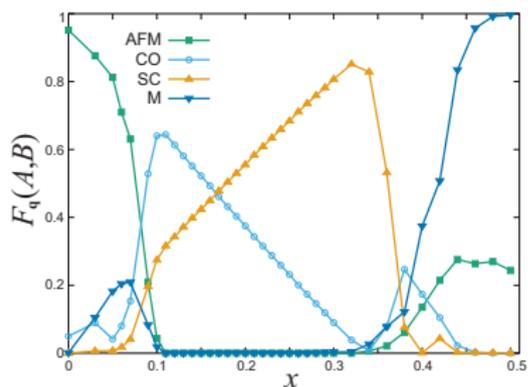
Left panel: The dependencies on the charge doping of the structure factors in the ground state calculated with parameters $\Delta = 0.8$, $V = 0.625$, $J = 1$, $t_p = 0.35$, $t_n = 0$, $t_{pn} = -0.24$, (all in units of the t_b).

Right panel: The Monte Carlo $T\,\text{-}\,x$ (x the charge doping) phase diagram for the model cuprate calculated with $\Delta = 0.8$, $V = 0.625$, $J = 1$, $t_p = 0.35$, $t_n = 0$, $t_{pn} = -0.24$, (all in units of the t_b). 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.

References

1. A.S. Moskvin, True Charge-Transfer Gap in Parent Insulating Cuprates, *PRB* **84**, 075116 (2011)

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