HTS 2020 Modelling

7th International Workshop on Numerical Modelling of High Temperature Superconductors
22nd – 23rd June 2021, Virtual (Nancy, France)

Monte Carlo simulations of a model cuprate

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Objectives

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.

We use the pseudospin formalism and Monte Carlo method 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

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.

* $\mathcal{H}_{tr}^{(1)} = -t_p \sum_{\langle ij \rangle} \left(P_i^+ P_j + P_j^+ P_i \right) - t_n \sum_{\langle ij \rangle} \left(N_i^+ N_j + N_j^+ N_i \right) - \frac{t_{pn}}{2} \sum_{\langle ij \rangle} \left(P_i^+ N_j + P_j^+ N_i + N_i^+ P_j + N_j^+ P_i \right)$
  – the correlated one-particle transport, P and N operators are the combinations of the pseudospin $S=1$ operators:
  $P^+ \propto (S_+ + T_+)$, $N^+ \propto (S_+ - T_+)$, $T_+ = S_z S_+ + S_+ S_z$.

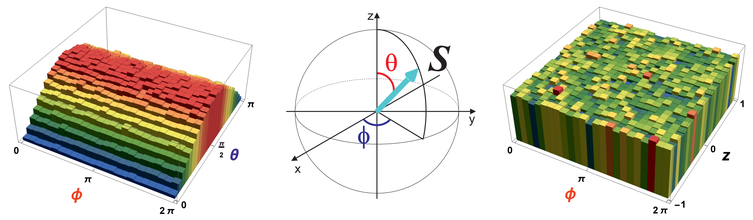
* $\mathcal{H}_{tr}^{(2)} = -t_b \sum_{\langle ij \rangle} \left(S_{+i}^2 S_{-j}^2 + S_{+j}^2 S_{-i}^2 \right)$
  – the two-particle transport.

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

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:

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

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

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

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

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

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

$m(x) = \frac{1-|x|}{1+|x|}$, $\Theta(x)$ is the Heaviside step function, $\Pi\left(-1, \frac{\pi}{2} \,\middle|\, m\right) = \Pi_1(1, \sqrt{m})$ 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 $\cos\frac{\theta_i}{2} = \sqrt{1 - |n_i|}\ \operatorname{sn}\left(\gamma_i K\left(m(n_i)\right), m(n_i)\right)$, where γ_i, $i = 1, 2$, are the random uniformly distributed quantities, $0 \le \gamma_i \le 1$, $\operatorname{sn}(x, m)$ 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 $\cos\phi_i = \frac{n_i}{1 - \cos^2\frac{\theta_i}{2}}$. If $n_i = 0$ and $\cos\frac{\theta_i}{2} = 1$, ϕ_i is a random uniformly distributed quantity, $0 \le \phi_i \le \pi$.

Monte Carlo simulation

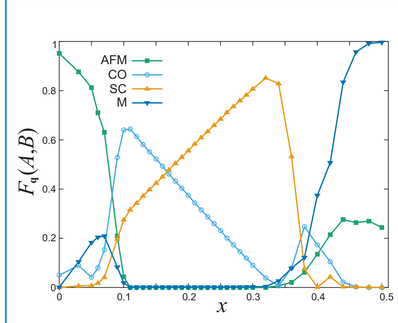
In Monte Carlo simulation, we calculated the structure factors

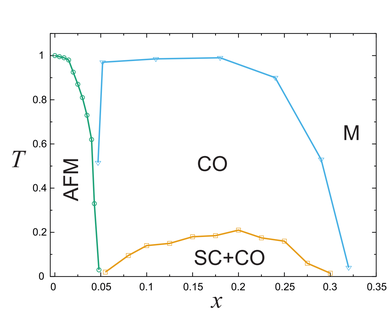
$$F_{\mathbf{q}}(A, B) = \frac{1}{N^2} \sum_{lm} e^{i\mathbf{q}\,(\mathbf{r}_l - \mathbf{r}_m)} \langle A_l B_m \rangle, \qquad (2)$$

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 - 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.

Acknowledgements

The research was supported by the Ministry of Education and Science of the Russian Federation, project FEUZ-2020-0054.

References

[1] A.S. Moskvin, True Charge-Transfer Gap in Parent Insulating Cuprates, *Phys. Rev. B* **84**, 075116 (2011)
[2] A.S. Moskvin, Perspectives of Disproportionation Driven Superconductivity in Strongly Correlated 3d Compounds, *J.Phys.:Cond.Mat.* **25**, 085601 (2013);
[3] A.S. Moskvin, Y.D. Panov, Electron-Hole Dimers in the Parent Phase of Quasi-2D Cuprates, *Phys. Solid State* **61**, 1553 (2019)
[4] A. S. Moskvin, Y. D. Panov, Nature of the Pseudogap Phase of HTSC Cuprates, *Phys. Solid State* **62**, 1554 (2020)