Mean-field approximation for a model HTSC cuprate

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***Abstract*—In the framework of the charge triplet model and $S = 1$ pseudospin formalism, we used the mean field approximation typical of spin-magnetic systems to construct a phase diagram for HTSC cuprates**

***Keywords*—HTSC cuprates, "unparticle" approach, charge triplet model, pseudo-spin formalism, mean-field approximation, Caron-Pratt approach, phase diagrams**

I. Introduction

Today there is no consensus on a theoretical model that allows, within the framework of a single scenario, to describe the phase diagram of cuprates, including the pseudogap phase, strange metal phase, and the HTSC mechanism. Numerous experimental data show the inapplicability of the BCS theory and question the very existence of pairing "bosonic glue" in cuprates. The BCS paradigm involves using a single-particle "k-momentum" representation. However, a more appropriate description of strong local and nonlocal correlations, short coherence length of "Cooper pairs", is achieved within the framework of the "coordinate", or local, representation. At the present time, realization of the "beyond quasiparticle", or "unparticle" description of cuprates is becoming more and more popular. The pseudo-spin formalism is one of the most promising "unparticle" approaches. This allows one to use many results that are well known for spin-magnetic systems, including a description of phase transitions, topological structures, domains, and domain walls. Hereafter we consider a simplified minimal microscopic ("toy") model of the CuO_4 centers in cuprates which allows us to derive all the local order parameters within an unified approach and show that all the main features of superconductivity, spin and charge orders can be explained on equal footing.

II. Results and discussion

The "on-site", or the Hilbert space of the CuO_4 plaquettes, to be a main element of crystal and electron structure of the high-T_c cuprates, is reduced to states formed by only three effective valence centers $[CuO_4]^{7-,6-,5-}$ (nominally $Cu^{1+,2+,3+}$, respectively), forming a charge triplet. Such an approach for cuprates immediately implies introduction of unconventional on-site quantum superpositions with different charge, spin and orbital momenta. or with an uncertainty of the charge, spin, and orbital density. To describe the diagonal and off-diagonal, or quantum local charge order we start with a simplified *charge triplet model* that implies a full neglect of spin and orbital degrees of freedom [1]. Three charge states, the bare Cu^{2+}-center, the hole Cu^{3+}-center, and the electron Cu^{1+}-center are assigned to three components of the $S = 1$ pseudo-spin triplet with the pseudo-spin projections $M_S = 0, +1, -1$, respectively. The $S = 1$ spin algebra includes the eight independent nontrivial pseudo-spin operators, the three dipole and five quadrupole ones:

$$\hat{S}_z; \hat{S}_\pm = \mp\frac{1}{\sqrt{2}}(\hat{S}_x \pm i\hat{S}_y); \hat{S}_z^2; \hat{T}_\pm = \{\hat{S}_z, \hat{S}_\pm\}; \hat{S}_\pm^2 . \quad (1)$$

Both $\hat{S}_+(\hat{S}_-)$ and $\hat{T}_+(\hat{T}_-)$ can be anyhow related with conventional single particle creation (annihilation) operators, however, these are not standard fermionic ones.

The pseudo-spin raising/lowering operators $\hat{S}_+^2/\hat{S}_-^2$ do change the pseudo-spin projection by ± 2 and create an on-site hole/electron pair, or composite boson, with a kinematic constraint $(\hat{S}_\pm^2)^2 = 0$, that underlines its "hard-core" nature. In lieu of $\hat{S}_\pm$ and $\hat{T}_\pm$ operators one may use two novel operators:

$$\hat{P}_\pm = \frac{1}{2}(\hat{S}_\pm + \hat{T}_\pm);\ \hat{N}_\pm = \frac{1}{2}(\hat{S}_\pm - \hat{T}_\pm)\,, \quad (2)$$

which do realize transformations $Cu^{2+} \leftrightarrow Cu^{3+}$ and $Cu^{1+} \leftrightarrow Cu^{2+}$, respectively. Taking into account the $s = 1/2$ spin state of the Cu^{2+}-center we should introduce the spin-charge operators $\hat{P}_\pm^\nu$ and $\hat{N}_\pm^\nu$ which do transform both the charge and spin state. The on-site, or local $S = 1$ pseudo-spin state can be written as follows

$$|\Psi\rangle = \cos\theta\cos\phi e^{-i\alpha}|-1\rangle + \sin\theta e^{i\beta}|0\rangle + \cos\theta\sin\phi e^{i\alpha}|+1\rangle. \quad (3)$$

The on-site off-diagonal order parameter with a d-wave symmetry

$$\langle\hat{S}_\pm^2\rangle = \frac{1}{2}(\langle\hat{S}_x^2 - \hat{S}_y^2\rangle \pm i\langle\{\hat{S}_x, \hat{S}_y\}\rangle) = \frac{1}{2}\cos^2\theta\sin 2\phi\, e^{\pm 2i\alpha}\,, \quad (4)$$

which is nonzero only for the on-site spinless Cu^{1+}-Cu^{3+} superpositions can be addressed to be a local complex su-

perconducting order parameter. Unconventional nonzero local mean values of the Fermi-like operators $\hat{P}^{\nu}_{\pm}$ and $\hat{N}^{\nu}_{\pm}$

$$\langle \hat{P}^{\nu}_{\pm} \rangle \propto \mp \frac{1}{2} \sin 2\theta \sin\phi \, e^{\mp i(\alpha-\beta)}; \tag{5}$$

$$\langle \hat{N}^{\nu}_{\pm} \rangle \propto \mp \frac{1}{2} \sin 2\theta \cos\phi \, e^{\mp i(\alpha+\beta)} \tag{6}$$

imply the local charge and spin density uncertainty.

Effective $S=1$ pseudo-spin Hamiltonian which does commute with the z-component of the total pseudo-spin $\sum_i S_{iz}$ thus conserving the total charge of the system can be written to be a sum of potential and kinetic energies: $\hat{H} = \hat{H}_{pot} + \hat{H}_{kin}$, where

$$\hat{H}_{pot} = \sum_i (\Delta_i \hat{S}^2_{iz} - \mu \hat{S}_{iz}) + \sum_{i<j} V_{ij} \hat{S}_{iz} \hat{S}_{jz} \,, \tag{7}$$

with a charge density constraint:$\sum_i \langle \hat{S}_{iz} \rangle = 2N\,\Delta n$, where Δn is the deviation from a half-filling. The first single-site term in $\hat{H}_{pot}$ describes the on-site density-density interactions, or local correlations, $\Delta = U/2$, U being the local correlation parameter. The second term may be related to a pseudo-magnetic field $\parallel Z$ with μ being the hole chemical potential. The third term in $\hat{H}_{pot}$ describes the nonlocal correlations. Kinetic energy $\hat{H}_{kin} = \hat{H}^{(1)}_{kin} + \hat{H}^{(2)}_{kin}$

$$\hat{H}^{(1)}_{kin} = -\sum_{i<j} \sum_{\nu} [t^{p}_{ij} \hat{P}^{\nu}_{i+} \hat{P}^{\nu}_{j-} + t^{n}_{ij} \hat{N}^{\nu}_{i+} \hat{N}^{\nu}_{j-} + \frac{1}{2} t^{pn}_{ij} (\hat{P}^{\nu}_{i+} \hat{N}^{\nu}_{j-} + \hat{P}^{\nu}_{i-} \hat{N}^{\nu}_{j+}) + h.c.] \,. \tag{8}$$

$$\hat{H}^{(2)}_{kin} = -\sum_{i<j} t^{b}_{ij} (\hat{S}^2_{i+} \hat{S}^2_{j-} + \hat{S}^2_{i-} \hat{S}^2_{j+}) \,, \tag{9}$$

is a sum of one- and two-particle transfer contributions. It is worth noting, the single-particle transport is determined by the three terms with different transfer integrals. The complete Hamiltonian must include the antiferromagnetic Heisenberg exchange coupling for the $s=1/2$ Cu^{2+}-centers

$$\mathcal{H}_{exc} = \frac{1}{4} \sum_{i<j} J_{ij} \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j \,, \tag{10}$$

where $\boldsymbol{\sigma} = 2\hat{P}_0 \mathbf{s}$, $\hat{P}_0 = 1 - \hat{S}^2_z$ are the on-site spin density operators. Using the mean-field approximation (MFA) which is the typical one for spin-magnetic systems we get several MFA phases according to the number of independent local order parameters. Within the two-sublattice (AB) approximation with nn (nearest neighbors) inter-site coupling we arrive at a checkerboard charge order (CO, or CDW with $\mathbf{q}=(\pi,\pi)$) with "pseudo-antiferromagnetic" order parameter $L_z = \langle S_{zA} \rangle - \langle S_{zB} \rangle$, spin-antiferromagnetic insulating phase (AFMI) with local spin order parameter $\langle \boldsymbol{\sigma} \rangle$, Bose superfluid/superconducting phase (BS) with local order parameter $\langle S^2_{\pm} \rangle$, and the two Fermi-type metallic phases, the hole- and electron-like ones, characterized by a superposition of nonzero local order parameters $\langle P^{\nu}_{\pm} \rangle$ and $\langle N^{\nu}_{\pm} \rangle$, respectively. Interestingly, this approximation does provide analytical expressions for the phase transition lines [2]. It should be noted that the

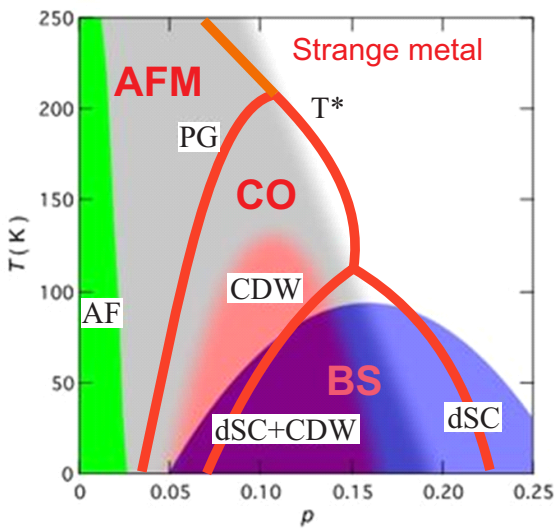

Fig. 1. (Color online) The MFA T-p (p the hole doping) phase diagram for the model cuprate calculated with parameters quite arbitrarily chosen as $\Delta = 0.25$, $V = 0.375$, $t^{p} = 0.67$, $t^{n} = 0$, $t^{pn} = 0$, $t^{b} = 0.67$ (all in units of the exchange integral J) to obtain a visual agreement with experimental phase diagram typical for cuprates.

local mean values of fermionic operators similar $\langle \hat{P}^{\nu}_{\pm} \rangle$ and $\langle \hat{N}^{\nu}_{\pm} \rangle$ have been introduced by Caron and Pratt [3] to describe the Hubbard model in the real coordinate space. The P-and N-modes interact/mix due to the PN (NP) contribution in $H^{(1)}_{kin}$, which leads to "strange" properties of the Fermi-type metal phases with a specific coexistence of hole and electron carriers, characteristic of both hole and electron doped systems.

Fig. 1 shows the MFA, even under extremely simplifying assumptions, can reproduce quite well all the principal features of the real phase diagram.

All the MFA phases are characterized by nonzero local order parameters, i.e. they have a "Néel" character, However, the MFA "hides" the existence of a true quantum ground state, a "quantum background", such as the Anderson's RVB (resonating valence bond) phase, formed by a system of electron-hole dimers [1]. It is with the formation of this phase that puzzling "pseudogap" behavior can be associated. Obviously, the existence of this "MFA-hidden" quantum state leads to a significant suppression of the magnitude of the local order parameters for CDW and superconducting (BS) phases observed experimentally.

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