Quantum Monte-Carlo phase diagram for a model cuprate

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We introduce a minimal model for CT (charge transfer) unstable 2D cuprates with the on-site Hilbert space reduced to only three effective valence centers, nominally $Cu^{1+,2+,3+}$ ions and make use of the S=1 pseudospin formalism. It is worth noting that the $\hat{S}^2_+$ ($\hat{S}^2_-$) operator creates an on-site hole (electron) pair, or composite boson, with a kinematic constraint $(\hat{S}^2_\pm)^2 = 0$, that underlines its "hard-core" nature. Obviously, the pseudospin nematic average $\langle S^2_\pm \rangle$ can be addressed to be a local complex superconducting order parameter; $(1 - \langle \hat{S}^2_{iz} \rangle)$ to be an on-site Cu^{2+} spin density. Focusing on the unconventional bosonic-like physics of the model cuprate we neglect the one-particle transport (on-site $\Delta S_\pm$ terms) we write out the effective S=1 pseudospin Hamiltonian for the CuO_2 plane of the model cuprate as follows:

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

with a charge density constraint: $\frac{1}{2N} \sum_i \langle S_{iz} \rangle = \Delta n$ where Δn is the deviation from a half-filling. The first single-site term describes the effects of a bare pseudo-spin splitting, or the local energy of $M^{0,\pm}$ centers and relates with the on-site density-density interactions. The second term may be related to a pseudo-magnetic field $\mathbf{h}_i \parallel Z$, in particular, a real electric field which acts as a chemical potential (μ is the hole chemical potential, and h_i is a (random) site energy). The third term in $\hat{H}_{ch}$ describes the effects of the short- and long-range inter-site density-density interactions including screened Coulomb and covalent couplings. The fourth term describes the two-particle bosonic transport. It is worth noting that in the limit of large negative Λ we arrive at the Hamiltonian of the hard-core bosons[1]. The effect of the nonisovalent substitution in the model cuprate $La_{2-x}Sr_xCuO_4$ was modeled via a Sr^{2+} induced impurity potential region within CuO_2 plane with varied parameters Δ and V.

Despite its seeming simplicity the model is believed to capture the salient features both of the hole- and electron-doped cuprates. Concept of the electron and hole centers, differing by a composite local boson, and electron-hole pairing are shown to explain central points of the cuprate puzzles, in particular, the HTSC itself and pseudogap phenomena.

Making use of two different QMC methods, the standard stochastic series expansion (SSE) with loop updates and a continuous time world-line QMC, we studied the ground-state and finite-temperature properties of the Hamiltonian (1) given different parameters values. Our QMC calculations for the model CT unstable cuprates shows a step-by-step evolution under doping of the parent insulating state into an uncoventional inhomogeneous supersolid (mixed charge order - Bose superfluid, or CO+BS) phase formed by electron and hole CuO_4 centers. The simulation does reproduce main features of the $T-x$ phase diagrams for doped cuprates, in particular, the suppression of antiferromagnetism, a pseudogap regime due to charge ordering, formation of a local superconductivity at $T > T_c$, and global 2D superconductivity.

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