Charge transfer instability and phase diagram of a model doped cuprate

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Large body of experimental data points towards an unique charge transfer (CT) instability of parent insulating cuprates. True CT gap in these compounds is believed to be as small as 0.4-0.5 eV as derived from the midinfrared absorption measurements rather than 1.5-2.0 eV as usually derived from the fundamental absorption measurements. In fact we deal with a competition of the conventional ($3d^9$) ground state and a CT state with formation of electron-hole (EH) dimers which evolves under doping to an unconventional EH bosonic system, or EH Bose liquid formed by electron and hole CuO_4 centers having been glued in lattice due to strong electron-lattice polarization effects.[1] Making use of a quantum Monte-Carlo technique we study the evolution of the phase state of CuO_2 planes in a model CT unstable cuprate kind of $La_{2-x}Sr_xCuO_4$. Nonisovalent doping indeed gives rise to a nucleation of the inhomogeneous EH Bose liquid in supersolid CO+BS phase characterized by a charge (CO) and off-diagonal Bose superfluid (BS) order parameters which competition results in a generic T-x phase diagram. The simulation does reproduce main features of the doped cuprates, in particular, fast suppression of antiferromagnetism, a pseudogap regime due to charge ordering and formation of a local superconductivity. We have attempted to incorporate a broad enough collection of experimental (optical, Raman, photoabsorption, photoemission,...) results to demonstrate validity of the main message.

[1] A.S. Moskvin, Low Temp. Phys. **33**, 234 (2007).