Charge, spin, orbital and lattice degrees of freedom in manganites

Pedro Schlottmann
Department of Physics, Florida State University, Tallahassee

The rich phase diagram of $La_{1-x}Ca_xMnO_3$ (LCMO) exhibiting several magnetic phases, orbital order, spin canting, charge order, Jahn-Teller distortions and phase separation is the consequence of the interplay of charge, spin, orbital and lattice degrees of freedom. The manganese ions are in a mixed valent state of two magnetic configurations, Mn^{4+} and Mn^{3+}. Each Mn ion has three localized *3d* electrons in t_{2g} orbitals with their spins ferromagnetically coupled to form a spin $S = 3/2$. The Mn^{3+} ions have an additional *3d*-e_g electron to form a total spin $(S + 1/2)$ via Hund's rule coupling. The e_g electrons hop between Mn sites with amplitude t with a multiple occupancy of the e_g levels being excluded at each site by a large Coulomb energy. The hopping of the e_g electrons gives rise to the ferromagnetic *double-exchange*, which competes with the antiferromagnetic *superexchange J* between the t_{2g} spins of the ions. The two e_g-orbitals also couple to the lattice degrees of freedom via the *Jahn-Teller* effect. Using a mean-field slave-boson formulation we calculate the ground state energy of the system for classical spins *S* oriented in the magnetic configurations of the A, B, C and G phases as a function of *x* and one model parameter, *J/t*. The experimental sequence of crossovers between ground states for LCMO was reproduced as a function of *x* for $J/t \approx 0.02$ [1]. Only the A, C and CE phases exhibit a Jahn-Teller distortion [2], leading to a contraction (expansion) of the c-axis for the A phase (C phase) and to long range orbital order. The effects of canting of the spins on the stability of the A and B phases and on phase separation is discussed. The model has been extended to electron-doping [3]. Preliminary results for the checkerboard charge and the orbital order of the CE-phase will be presented. There are 32 e_g bands (16 Mn ions in the unit cell) in the Brillouin zone of the CE phase which are grouped into two sets of 16 bands separated by a charge order gap. The charge gap does not directly affect the properties of the compound. If long-range orbital order is included an additional gap opens at the Fermi level.

The support by the Department of Energy under grant DE-FG02-98ER45707 is acknowledged.

[1] P. Schlottmann, Phys. Rev. B **62**, 439 (2000).
[2] P. Schlottmann, Phys. Rev. B **73**, 214428 (2006).
[3] P. Schlottmann, Phys. Rev. B **77**, 104446 (2008).