Defects, Disorder, and Spin-Orbital Polarons in Orbital Degenerate, Doped Mott Insulators

Adolfo Avella[1,2]

[1] *Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy*
[2] *CNR-SPIN, UOS di Salerno, I-84084 Fisciano (SA), Italy*

We elucidate the role played by charged defects and doped holes in doped Mott insulators with active orbital degrees of freedom and, in particular, in doped vanadate perovskites [1-5]. We use a degenerate Hubbard model extended by terms that describe crystal-field splittings and orbital-lattice coupling, as well as by the long-range Coulomb potential terms of charged defects and doped holes [1]. We show that the multiplet structure of the excited states generated in such systems by strong electron interactions is well described within the unrestricted Hartree-Fock approximation [1]. A soft gap of kinetic origin develops in the defect band and survives defect disorder. This behavior naturally emerges in the statistical distribution of gaps among different defect realizations, which turns out to be of Weibull type [2]. Our results provide clear indications that doped holes are bound to charged defects and form small spin-orbital polarons whose internal kinetic energy is responsible for the opening of the soft gap [3]. Such a generic behavior leads to complex non-hydrogen-like defect states that tend to preserve the underlying C-type spin and G-type orbital order [2]. Another fundamental characteristic of these systems is the persistence of spin and orbital order up to high doping, in contrast to the loss of magnetic order in high-Tc cuprates at low defect concentration. We show that the rotation of the t_{2g} orbitals, induced by the electric field of defects, is a very efficient perturbation that largely controls the suppression of orbital order in these compounds [4]. From the change of kinetic and superexchange energy, we can conclude that the motion of doped holes, which is the dominant effect for the reduction of magnetic order in high-T_c compounds, is of secondary importance here as well as the quadrupolar components of the Coulomb fields of doped holes. These rotations modify the spin-orbital polaron clouds and compete with orbital rotations induced by defects [5], but we find that the gradual decline of orbital order with doping has its origin in the off-diagonal couplings of orbital rotations induced by the charges of the doped ions.

References:

[1] A. Avella, P. Horsch, A.M. Oleś; Phys. Rev. B **87**, 045132 (2013)
[2] A. Avella, A.M. Oleś, P. Horsch; Phys. Rev. Lett. **115**, 206403 (2015)
[3] A. Avella, A.M. Oleś, P. Horsch; Phys. Rev. B **97**, 155104 (2018)
[4] A. Avella, A.M. Oleś, P. Horsch; Phys. Rev. Lett. **122**, 127206 (2019)
[5] P. Horsch, A.M. Oleś, A. Avella; Phys. Rev. B **103**, 035129 (2021)