

Charge and Orbital Order in Transition Metal Oxides

Andrzej M. Oleś^{1,2}

¹ *M.Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, 30059 Kraków*

² *Max-Planck-Institut FKF, Heisenbergstrasse 1, 70569 Stuttgart, Germany*

Several novel types of complex ordered phases which arise in transition metal oxides will be discussed. The first example are the superconducting cuprates with their puzzling properties, frequently attributed to competing instabilities. In the normal phase the competition between the magnetic and kinetic energy leads to stripe phases characterized by the coexisting modulation of charge and magnetization and density. The possible types of such phases and their dependence on doping will be shortly discussed using the slave-boson approach to the Hubbard model [1]. As shown recently using the variational Monte Carlo and the Gutzwiller approach to the t - J model, charge modulation may also coexist with the d -wave superconducting resonating valence bond phase [2].

In transition metal oxides with orbital degrees of freedom interesting novel types of order arise already in Mott (or charge transfer) insulators. The main features of the spin-orbital superexchange which describes the magnetic and optical properties of Mott insulators with orbital degrees of freedom [3] will be discussed. In contrast to the SU(2) symmetry of spin superexchange, the orbital part of the superexchange obeys the lower cubic symmetry of the lattice and is therefore intrinsically frustrated. This intrinsic frustration and spin-orbital entanglement [4] induce enhanced quantum fluctuations, and we point out a few situations where this leads to unexpected consequences such as deviations from classical expectations or disordered states (e.g. orbital liquid state in the ferromagnetic manganites [5]). Strong coupling between the spin and orbital degrees of freedom will be discussed on the example of the RVO_3 perovskites, with R standing for rare-earth ion, $R=La, \dots, Lu$. We introduce a model [6] describing $(xy)^1(yz/zx)^1$ configuration of V^{3+} ions in the RVO_3 perovskites, and demonstrate that $\{yz, zx\}$ orbital fluctuations along the c axis are responsible for the huge magnetic and optical anisotropies observed in the almost perfectly cubic compound $LaVO_3$. The model demonstrates that the $GdFeO_3$ distortion plays a central role to explain the observed variation of orbital and magnetic transition temperature, T_{OO} and T_N , in the RVO_3 series with decreasing ionic radius r_R . The orthorhombic distortion which increases from $LaVO_3$ to $LuVO_3$ plays a crucial role by controlling the orbital fluctuations, and via the modified orbital correlations influences the onset of both magnetic and orbital order. The coupling between the spin ($S=1$) and orbital degrees of freedom explains also the observed dimerization of the ferromagnetic interactions in the C-AF phase of YVO_3 at finite temperature. This is an example of a Peierls dimerization instability of a ferromagnetic spin chain at finite temperature [7].

Finally, a few examples of the coexisting magnetic, orbital and charge order in nickelates [8] and manganites [9] will be briefly discussed.

[1] M. Raczkowski, R. Fresard, and A. M. Oleś, *Phys. Rev. B* **73**, 174525 (2006).

[2] M. Raczkowski, M. Capello *et al.*, *Phys. Rev. B* **76**, 140505(R) (2007).

[3] A. M. Oleś, G. Khaliullin, P. Horsch, and L.F. Feiner, *Phys. Rev. B* **72**, 214431 (2005).

[4] A. M. Oleś, G. Khaliullin, P. Horsch, L. F. Feiner, *Phys. Rev. Lett.* **96**, 147205 (2006).

[5] L. F. Feiner and A. M. Oleś, *Phys. Rev. B* **71**, 144422 (2005).

[6] P. Horsch, A.M. Oleś, L.F. Feiner, G. Khaliullin, *Phys. Rev. Lett.* **100**, 167205 (2008).

[7] J. Sirker, A. Herzog, A. M. Oleś, and P. Horsch, *Phys. Rev. Lett.* **101**, 167205 (2008).

[8] M. Raczkowski, R. Fresard, and A. M. Oleś, *Phys. Rev. B* **73**, 094429 (2006).

[9] M. Daghofer, A. M. Oleś *et al.*, *Phys. Rev. B* **73**, 104451 (2006).