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Spin-Orbital Entangled States in Transition Metal Oxides [1]

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Superexchange models provide a theoretical framework for describing magnetic and optical properties of Mott insulators. Spin-orbital entanglement (SOE) determines finite temperature properties of systems with active orbital degrees of freedom, for instance the phase diagram of the RVO$_3$ perovskites (R=La,$\cdots$,Lu) [1]. To describe SOE one needs to use exact diagonalization of finite clusters, or combine it with the self-consistent Bethe-Peierls-Weiss (BPW) cluster method. The latter is employed to investigate the ground state of a bilayer in the (d^9) Kugel-Khomskii model [2], depending on Hund's exchange $\eta \equiv J_H/U$ (U is the intraorbital Coulomb element) and the e_g orbital splitting E_z/J ($J \equiv 4t^2/U$ is the superexchange constant). When spin and orbital degrees of freeedom are disentangled in mean-field theory (MFT), the G-type antiferromagnetic (G-AF), A-type antiferromagnetic (A-AF) and ferromagnetic (FM) order compete, see Fig. 1(a). The BPW approach gives a quite different phase diagram, see Fig. 1(b), including: (i) interlayer valence-bond phase with holes in $3z^2-r^2$ orbitals (VBz), (ii) alternating plaquette valence-bond (PVB), and (iii) two phases with SOE in the regime of strongly frustrated interactions, ESO and EPVB. In the d^1 spin-orbital model on a triangular lattice the Lanczos diagonalization suggests that the Goodenough-Kanamori rules are violated [3] — here the geometrical frustration prevents long-range order and leads to the spin-orbital liquid state that involves SOE on the bonds. However, ordered states may be stabilized on frustrated lattices by strong orbital-lattice coupling in presence of interorbital hopping, as for instance in KO_2 or RbO_2 [4].

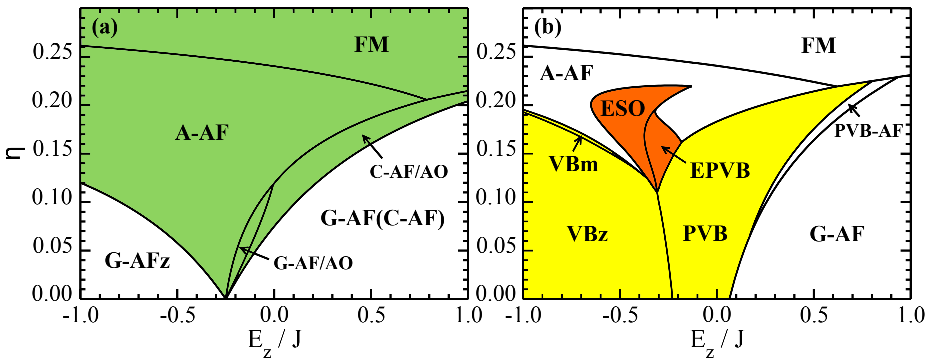

Figure 1: Phase diagrams of the d^9 bilayer model [2]: (a) MFT, and (b) BPW approach with a cubic cluster of 8 sites. Green area in (a) indicates phases with alternating orbitals; yellow area in (b) marks singlet phases while orange area indicates phases with SOE.

[1] P. Horsch, A. M. Oleś, L. F. Feiner, and G. Khaliullin, Phys. Rev. Lett. **100**, 167205 (2008).
[2] W. Brzezicki and A. M. Oleś, Phys. Rev. B **83**, 214408 (2011).
[3] J. Chaloupka and A. M. Oleś, Phys. Rev. B **83**, 094406 (2011).
[4] K. Wohlfeld, M. Daghofer, and A. M. Oleś, Europhys. Lett. **96**, in press (2011).

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