ENTANGLED SPIN-ORBITAL PHASES IN THE $\mathbf{d^9}$ MODEL

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9.7 cm

The phase diagram of the spin-orbital (SO) Kugel-Khomskii (d^9) model posed a challenging theoretical problem [1], yet it is still unknown. Here we investigate the phase diagrams of the d^9 model, depending on Hund's exchange J_H and the e_g orbital splitting E_z, for a bilayer and a monolayer square lattice using Bethe-Peierls-Weiss method with exact diagonalization of a cubic or square cluster coupled to its neighbors in ab planes by the mean-field (MF) terms. The cluster MF method confirms existence of singlet phases similar to those obtained by variational wave functions [2], and enables finite SO order parameter independent of spin and orbital ordering. For a bilayer we obtain phases with interlayer spin singlets stabilized by holes in $3z^2-r^2$ orbitals and with alternating plaquette valence-bond (PVB) as well as two new phases with SO entanglement, in addition to the antiferromagnetic (G-AF, A-AF) and ferromagnetic (FM) order. For a monolayer we obtained at temperature $T=0$: (i) the PVB phase, (ii) two AF phases with either $3z^2-r^2$ or x^2-y^2 orbitals occupied, and (iii) a FM phase. However, after including thermal fluctuations ($T>0$) we found the same entangled SO phases as for a bilayer at $T=0$. This shows that both quantum and thermal fluctuations can stabilize phases with exotic SO order while the classical spin order is destroyed.

[1] L. F. Feiner, A. M. Oleś, and J. Zaanen, Phys. Rev. Lett. **78**, 2799 (1997).
[2] A. M. Oleś, Acta Phys. Polon. A **115**, 36 (2009).

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