MICROSCOPIC THEORY OF MAGNETIC INTERACTIONS IN $KCuF_3$ AND $LaMnO_3$ — THE ROLE OF CHARGE TRANSFER

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9.7 cm

Magnetic interactions in correlated insulators with orbital degrees of freedom are described by superexchange spin-orbital models, which are characterized by nontrivial quantum effects [1]. We analyze the spin interactions in A-type antiferromagnetic phase of $KCuF_3$ with one hole in e_g orbital ($S = 1/2$) and of $LaMnO_3$ with $t_{2g}^3 e_g$ high-spin ($S = 2$) electronic configuration. The spin exchange constants along cubic axes J_{ab} and J_c sensitively depend on three parameters: (i) overall energy scale $J = 4t^2/U$, where t is $(dd\sigma)$ hopping and U is on-site Coulomb repulsion, (ii) the Hund's exchange $\eta = J_H/U$, and (iii) the parameter $R = 2U/(2\Delta + U_p)$, where Δ and U_p are charge transfer (CT) energy and Coulomb repulsion on oxygen, and (iv) on the e_g orbital order. One finds that quasi one-dimensional spin interactions $J_c \gg |J_{ab}|$ in $KCuF_3$ are intrinsically related to its CT type insulating state. On the contrary, the effects of CT superexchange terms are moderate in a Mott insulator $LaMnO_3$. Finally, using partial optical sum rules [2], we discuss experimental constraints on the microscopic parameters of $LaMnO_3$.

[1] L. F. Feiner, A. M. Oleś, and J. Zaanen, Phys. Rev. Lett. **78**, 2799 (1997).
[2] G. Khaliullin, P. Horsch, and A. M. Oleś, Phys. Rev. B **70**, 195103 (2004).

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