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Magnetic and optical properties of Mott insulators with orbital degrees of freedom

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The temperature dependence and anisotropy of optical spectral weights associated with different multiplet transitions is determined by the spin and orbital correlations. To provide a systematic basis to exploit this close relationship between magnetism and optical spectra, we present and analyze the spin-orbital superexchange models for a series of representative orbital-degenerate transition metal oxides with different multiplet structure. The magnetic and optical properties depend on two parameters, the superexchange energy J and the ratio η of Hund's exchange to the intraorbital Coulomb interaction, and on the actual orbital state. In e_g systems important corrections follow from charge transfer excitations, and we show that $KCuF_3$ can be classified as a charge transfer insulator, while $LaMnO_3$ is a Mott insulator with moderate charge transfer contributions. On the example of $LaVO_3$ we describe a case where the full quantum spin-orbital physics must be considered [1]. Thus information on optical excitations, their energies, temperature dependence and anisotropy, combined with the results of magnetic neutron scattering experiments, provides an important consistency test of the spin-orbital models, and indicates whether orbital and/or spin fluctuations are important in a given compound.

[1] G. Khaliullin, P. Horsch, and A. M. Oleś, Phys. Rev. B **70**, 195103 (2004).

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