

Interplay between crystal-field splitting and superexchange interaction in the t_{2g} orbital Mott insulator

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Abstract

With a model of the $d_{1(t_{2g})}$ -electron antiferromagnetic Mott insulator a competition of two typical interactions for orbital states of the t_{2g} -triplet levels has been investigated: The on-site electronic coupling with a local crystal field (LCF) tends orbitals to order, while the intersite superexchange (SE) induces their fluctuations. Both interactions coexist in perovskites: The LCF is induced by GdFeO 3-type structural deformations. In turn, the SE originates from virtual electronic hoppings, allowed by the Pauli principle, between nonorthogonal orbital states of adjacent sites. The dependence of the state of the orbitals (namely, a dispersion of their excitations and the quadrupole polarization) on a relation between the energy Δ of the triplet level splitting, caused by the D 3d-symmetry LCF, and the exchange energy J SE is analyzed. Two qualitatively different regimes of the collective orbital behavior have been established: the induced order and fast fluctuations. It has been found that a crossover between them occurs when Δ comes close to J SE, and in the parameter region about $\Delta \approx J$ SE the order and fluctuations affect the wave function in a comparable extent. Previous approaches based on either of the interactions fail in this window. The present study identifies validity ranges of the former theories, embracing the physics of the orbitals by the unified description. © 2012 American Physical Society.

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