Competition of the magnetic and charge ordering in orthonickelates

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Rare-earth orthonickelates $RNiO_3$ have attracted continuous interest of researchers in the last decades [**?**]. We consider these systems as Jahn-Teller (JT) magnets [**?**], in which the low-energy state is formed by a charge multiplet $[NiO_6]^{10-,9-,8-}$ (nominally $Ni^{2+,3+,4+}$) with different spin and orbital ground states. The Ni^{3+} ion in the low-spin configuration of the NiO_6 octahedron $t_{2g}^6 e_g^1$ forms a JT center with a ground orbital doublet ^2E. However, the orbital degeneracy in $RNiO_3$ is lifted due to the charge disproportionation with the formation of Ni^{4+} and Ni^{2+} centers [**?**, **?**]. In this case, the electronic structure of the orthonikelate can be represented as a system of local composite spin-triplet bosons with the configuration e_g^2;$^3A_{2g}$ moving in a lattice of non-magnetic centers with the configuration t_{2g}^6. The phase diagram for such a triplet boson system in the mean-field approximation [**?**] shows the phases of charge ordering, antiferromagnetic insulator, and spin-triplet superconductor, as well as the phase-separated states. With all the variety of possible phase states, the type of phase transition to the charge-ordered state, as well as the accompanying effects of structure change in nickelates remain beyond the scope of the model [**?**]. The aim of the present work is to describe these key properties, which leads to the need to include a full octet of low-energy states in the model and to account for the interaction of the electron subsystem with the lattice.

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