Two dimensional model for correlated e_g electrons in doped nickelates

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9.7 cm

The magnetic and orbital instabilities in e_g band are relevant for the appearence of novel phases with orbital and magnetic order, discovered in doped nickelates such as $La_{2-x}Sr_xNiO_4$ [1]. We investigate this problem using two-dimensional Hubbard type model with two e_g orbitals, with anisotropic hopping (dependent on orbital-phases) and with intraorbital Coulomb and Hund's exchange interactions. The insulating undoped phase corresponds to two electrons per site.

The calculations were carried on 8×8 cluster: first, using Hartree-Fock approximation; next, including the correlations implemented within (space-nonhomogeneous) Local-ansatz-like method. Comaprison with mean-field (Hartree) results [2] is made. For parameters of the model Hamiltonian which, presumably, are applicable to nickelates we found that for the dopings ranging from 1/8 to 1/2 the most stable phases consist of ferromagnetically ordered lines of spins with antiferromagnetic coupling between them (C-AF phase). It was found that the correlations renormalised the HF ground state energies but in no case was the renormalised HF ground state switched with higher laying metastable states. It was also found that the orbital ordering in space is weak but couples to the spin order.

[1] J. M. Tranquada, et al., Phys. Rev. B **67**, 012404 (2003).

[2] R. Frésard, M. Raczkowski,, and A. M. Oleś, Phys. Stat. Sol. (b) **242**, 370 (2005).

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