

Relationships between electron band filling and type of charge and magnetic order

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Charge and spin orderings are studied on the infinite square lattice (ground state) and on the 4×4 cluster (finite temperatures) within the generalized Falicov-Kimball model with Hund coupling between localized and itinerant electrons. Using the restricted phase diagram method (RPDM), a number of simple rules of formation of various sorts of ground state phases are detected. In particular, relationships between density of current carriers (electrons or holes) and type of charge and magnetic arrangement are determined. In the mixed valence regime only axial (vertical or horizontal) stripes are found for intermediate values of the coupling constants. They are composed of ferromagnetic or antiferromagnetic chains interchanged with nonmagnetic ones. For band fillings close to the half filling, stripe phases oriented along one of the main diagonal direction are formed. The results suggest a possibility of tuning modulations of charge and magnetic superstructures with a change in doping.

Finite temperature properties of the model are examined by direct diagonalization of the Hamiltonian for the finite 4×4 cluster at the half filling. Magnetization, specific heat and susceptibility versus temperature and magnetic field are presented and compared to the characteristics calculated by other authors, as well as to some experimental data.