MICROSCOPIC APPROACH TO DILUTED MAGNETS BASED ON THE FALICOV-KIMBALL MODEL WITH HUND COUPLING

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The Falicov-Kimball model supplemented with the Hund coupling term is proposed as a relevant microscopic model for studies of diluted magnets. The model describes charge and magnetic order induced by on-site, charge-, and spin-dependent interactions between itinerant electrons and localized ions. Motivated by a discovery of the rich structure of ground-state phase diagrams, containing various charge and magnetic superstructures, we analyze the energy spectrum and determine finite temperature properties of the model at half filling. The analysis is based on calculations performed on the Bethe lattice using the Dynamical Mean Field Theory (DMFT) and on finite square clusters using exact diagonalization method. For the density of magnetic ions equal to 1 or 1/2 and not too small coupling constants we show that many-electron collective excitations derived from changes in positions of the ions or inversions their spins have much lower energy than single-electron excitations. From an analysis of the excitation spectrum structure we derive effective interactions between the ions. When the coupling constants are large enough the interactions reduce to two-body forces between ions occupying the nearest-neighboring sites.

9.7 cm

13.4 cm

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