Introduction

The rich phase diagram of La$_{1-x}$Ca$_x$MnO$_3$ is the consequence of the interplay of charge, spin, orbital and lattice degrees of freedom. The end-compounds LaMnO$_3$ and CaMnO$_3$ are antiferromagnetic (AF) insulators, while for intermediate $x$ the system is either a ferromagnetic (F) metal or a charge-ordered AF and may display phase separation. The Jahn-Teller coupling to the lattice manifests itself in changes of the Mn-O-Mn bond lengths and angles, as well as orbital order.

Model

A simple cubic lattice of mixed-valent Mn ions with the $t_{2g}$-spins ($S=3/2$, treated classically, interacting via AF superexchange $J$) are oriented in the spin arrangements of the A, B, C and G phases. The multiple occupancy of the $e_g$ levels at each site is prevented by a large Coulomb interaction within an auxiliary boson mean-field approximation. The $e_g$-electrons (coupled via Hund's rule to the $t_{2g}$-electrons) hop between neighboring sites with amplitude $t$, giving rise to the F double-exchange. The Jahn-Teller coupling to the $E_g$ phonon modes lifts the degeneracy of the $e_g$-levels and reduces the ground-state energy for the A and C phases.

Results

The phase diagram is obtained by comparing the energies of the A, B, C and G phases for each $x$ and $J/t$. The hopping for the ferromagnetic B and antiferromagnetic G phases is isotropic and no Jahn-Teller distortions are obtained for these phases. The $t_{2g}$ spin-configurations in the A and C phases gives rise to anisotropic hopping of the $e_g$-electrons. It is unfavorable for an $e_g$-electron with spin $\sigma$ to hop between sites which have the $t_{2g}$-spins pointing in the opposite direction. This is a consequence of the Hund's rule coupling, which strongly reduces the hopping amplitude. The Jahn-Teller distortion then reduces the ground state energy of the A and C phases and enhances the range of stability of these phases at the expense of the B and G phases.

Distortions of the octahedra can also introduced by noncubic crystalline field splittings and interactions between $e_g$-electrons at neighboring sites. An extensive discussion of the A-phase is presented in Ref. 3.

Conclusions

The correct sequence of phases as a function of $x$ is obtained for $J/t$ of the order of a few percent. Staggered orbital long-range order is obtained for the A-phase.

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References