JAHN-TELLER EFFECT AND SUPEREXCHANGE IN HALF-DOPED MANGANITES

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9.7 cm

While the A-type antiferromagnetic (AF) phase in the undoped $LaMnO_3$ is well understood and follows from the superexchange interactions due to e_g and t_{2g} electron excitations [1], the stability of the charge exchange (CE) phase in half doped manganites remains one of the outstanding problems. We investigate the stability of this phase within a microscopic model which describes a single plane as in $La_{0.5}Sr_{1.5}MnO_4$ compound. It includes: the kinetic energy $\propto t$ of e_g electrons moving in nearly degenerate orbitals and interacting by local Coulomb interaction U, the Jahn-Teller (JT) term $\propto E_{\rm JT}$ which induces orbital polarization, and the superexchange interactions $\propto J$, as derived for the pairs of Mn^{3+}–Mn^{4+}, Mn^{3+}–Mn^{3+}, and Mn^{4+}–Mn^{4+} ions [2]. Treating the electron-electron interactions within the Hartree approximation, and the superexchange within the mean-field approximation, we determine the magnetic, orbital and charge order parameters in various magnetic phases: G-type AF, A-type AF, C-type AF, and CE phase as functions of $E_{\rm JT}$ and J. By investigating the phase diagram at $T = 0$ we conclude that the cooperative JT effect plays a prominent role in stabilizing the CE phase, while its magnetic order could be explained only by somewhat stronger superexchange than that which follows from the spectroscopic parameters.

[1] L.F. Feiner and A.M. Oleś, Phys. Rev. B **59**, 3295 (1999).
[2] A.M. Oleś and L.F. Feiner, Phys. Rev. B **65**, 052414 (2002).

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