Interplay between the orbital and magnetic order in monolayer manganites

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We adopt the two-dimensional model for e_g electrons in a monolayer [1] to describe an undoped and half doped manganite $La_{1-x}Sr_{1+x}MnO_4$ and study it using correlated wave functions. The effective Hamiltonian takes into account the kinetic energy, the crystal field splitting and on-site Coulomb interactions for e_g electrons. They interact with $S = 3/2$ core spins due to t_{2g} electrons. Furthermore, the model includes other important interactions in the manganites [2]: antiferromagnetic superexchange interaction between core spins, and the coupling between e_g electrons and Jahn-Teller modes. The model reproduces the antiferromagnetic order in the undoped $LaSrMnO_4$ compound, with occupied $3z^2 - r^2$ orbitals and elongated MnO_6 octahedra along the direction perpendicular to the Mn–O plane. In half doped $La_{0.5}Sr_{1.5}MnO_4$ manganite one finds rubust checkerboard-like charge order, in agreement with experiment [3]. However, the experimentally observed CE phase is more difficult to stabilize, and we discuss the necessary conditions to obtain it. Altogether, we conclude that the Jahn-Teller effect plays the crucial role, as shown in Ref. [4].

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