

Abstract Submitted
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Charge, spin, orbital and lattice degrees of freedom in manganites: The CE phase PEDRO SCHLOTTMANN, Florida State University — The CE phase of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ (LCMO) is stable for $x \geq 0.5$ and displays long-range magnetic, charge and orbital order. The magnetic order of the Mn spins arises from the competition of the superexchange and double-exchange interactions and the checkerboard charge and the orbital order is the consequence of the Jahn-Teller coupling of the e_g orbitals to the lattice. Using a mean-field slave-boson approach for the e_g electrons in two orbitals per site with excluded multiple occupancy and Hund's rule coupling between the e_g and t_{2g} states, we obtain the tight-binding band structure of the CE phase. The unit cell of the CE phase consists of 16 sites. The 32 e_g bands in the Brillouin zone are grouped into two sets of 16 bands separated by a charge order gap. The charge order gap does not directly affect the ground state and low-energy properties of the CE phase. A strong coupling to the Q_2 and Q_3 Jahn-Teller modes leads to a gap at the Fermi level for the half-filled case, yielding an orbitally ordered insulating ground state. The phase diagram is obtained by comparing the ground state energies of the A, B, C, CE and G phases. As a function of x the experimental phase sequence of LCMO is reproduced. Work supported by the Department of Energy under grant DE-FG02-98ER45707. P. Schlottmann, Phys. Rev. B **62**, 439 (2000); **73**, 214428 (2006); **77**, 104446 (2008); **80**, 104428 (2009).

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