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Effective Hamiltonian for FeAs based superconductors[1] EFSTRATIOS MANOUSAKIS, Department of Physics and MARTECH, Florida State University, Tallahassee, Florida, 32306, USA and Department of Physics, University of Athens, Greece — The Fe-pnictide superconductors exhibit unusual properties attributed to electrons and holes occupying the Fe d-orbitals and the outermost occupied s and p pnictide orbitals. Starting from the atomic limit, we carry out a strong coupling expansion for the FeAs layer, where the on-site Coulomb repulsion parameters are assumed to be significantly larger than the hopping between Fe d orbitals and the hybridization parameters between the Fe d and As $4s$ or $4p$ orbitals; we derive an effective Hamiltonian that describes the low energy electron/hole behavior. If this condition for strong coupling expansion is not satisfied, still, we believe that our qualitative results capture important aspects of the physics in these materials. The hopping and the hybridization parameters are obtained by fitting the results of our calculations based on the local density approximation to a tight-binding model. The effective Hamiltonian, in the strong coupling limit, consists of three parts which operate on three sub-spaces coupled through Hund's rule and spanned by the following Fe orbitals: (a) the $d_{x^2-y^2}$; (b) the degenerate orbitals d_{xz} and d_{yz}; and (c) the d_{xy} and d_{z^2}. Each of these parts is an extended $t-t'-J-J'$ model and is characterized by different coupling constants and filling factors. For the undoped material the second subspace alone prefers a ground state characterized by a spin-density-wave order similar to that observed in recent experimental studies, while the other two subspaces prefer (π,π) antiferromagnetic order. The observed spin-density-wave order is imposed by the d_{xz}/d_{yz} subspace as the ground state of the total Hamiltonian of the undoped parent compounds. However, due to the above mentioned frustration the magnetic moment is small in agreement with observation. Our calculation illustrates in a simple manner the reason for the difference in the magnetic ordering between the Fe-pnictides and the cuprates. It also suggests a different evolution of the magnetic order upon electron versus hole doping.

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[1] installation from J. Ren, S. Meng and E. Kaxiras, Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA. Phys. Rev. B 78, 205112 (2008)