Abstract Submitted
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A Monte Carlo simulation study of phase transitions in spin-orbital models for iron pnictides[1] RYAN APPLEGATE, RAJIV SINGH, Department of Physics, University of California, Davis, CHENG-CHIEN CHEN, THOMAS DEVEREAUX, Department of Physics, Stanford University, Stanford — The common phase diagrams of superconducting iron pnictides show interesting material specificities in the structural and magnetic phase transitions. In some cases the two transitions are separate and second order, while in others they appear to happen concomitantly as a single first order transition. We explore these differences using Monte Carlo simulations of a two-dimensional Hamiltonian with coupled Heisenberg-spin and Ising-orbital degrees of freedom. In this spin-orbital model, the finite-temperature orbital-ordering transition results in a tetragonal-to-orthorhombic symmetry reduction and is associated with the structural transition in the iron-pnictide materials. With a zero or very small spin space anisotropy, the magnetic transition separates from the orbital one in temperature, and the orbital transition is found to be in the Ising universality class. With increasing anisotropy, the two transitions rapidly merge together and tend to become weakly first order. We also study the case of a single-ion anisotropy and propose that the preferred spin-orientation along the antiferromagnetic direction in these materials is driven by orbital order.

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