Can FeCrAs be understood in terms of frustrated classical spins?\(^1\)

JOHN HOPKINSON, TRAVIS REDPATH, ALTON LEIBEL, Brandon University, HAE-YOUNG KEE, University of Toronto — Recently W. Wu et al. (EPL 85 17009 (2009)) have observed unusual non-Fermi liquid physics in a magnetically frustrated iron pnictide, FeCrAs. In this material, magnetic Cr atoms form distorted kagome planes which are coupled through planes of decoupled Fe trimers. We study a \(J_1\) (Cr-Cr) - \(J_2\) (Cr-Fe) classical extended Heisenberg model on this lattice by numerical minimization and classical Monte Carlo simulation. In our simplified model the Fe trimers are treated as single spins. In agreement with experiment, we find magnetic order for a wide range of parameters with wavevector \(k=(1/3,1/3,0)\). We derive exact expressions for the spin structure of the ground state. We calculate the heat capacity and magnetic susceptibility within this model and map out the phase diagram, which shows an unusual double transition in the vicinity of \(|J_1/J_2|=0.4\).

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