Abstract Submitted
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Fermion mediated state selection in the Kagome lattice and antiferromagnetism in FeCrAs[1] PATRICK J. O'BRIEN, Binghamton University, SHIVAM GHOSH, Cornell University, MICHAEL J. LAWLER, Binghamton University, Cornell University, CHRISTOPHER L. HENLEY, Cornell University — We study classical spins on a kagome lattice with weak Hund's coupling J_H to hopping electrons. For each filling, the effective RKKY interactions at all distances are extracted both by fits of the total electronic energy to a database of random spin configurations, as well as second order perturbation theory in J_H. We apply this to model the Cr antiferromagnetic order found below 125K in FeCrAs [2], in which one Cr d band split by the crystal field plays the role of the itinerant fermions; the observed $\sqrt{3} \times \sqrt{3}$ type order is indeed, close to half filling, the optimum state according to our model (out of the commonly considered alternatives) . In contrast, the limit of strong J_H favors the cuboc1[1] state over the $\sqrt{3} \times \sqrt{3}$ state[3], giving a bound on the possible value of the J_H in FeCrAs. Additionally, for weak J_H, cuboc1[1] is selected instead of $\sqrt{3} \times \sqrt{3}$ close to 5/12 filling. The complete phase diagram as a function of filling can be found using Monte Carlo (MC) minimization with the RKKY Hamiltonian. [1] Messio et al PRB 83, 184401 (2011) [2] W. Wu et al EPL 85, 17009 (2009) [3] Shivam Ghosh, Contributed talk, March Meeting 2013

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