Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Low-temperature orbital ordering and dynamical frustration of spins in $KCuF_3$: Theoretical model SIDDHARTHA LAL, JAMES C.T. LEE, SHI YUAN, YOUNG IL JOE, YU GAN, SERBAN SMADICI, PAUL GOLDBART, S. LANCE COOPER, PETER ABBAMONTE, University of Illinois, KEN FINKELSTEIN, CHESS, Cornell University, YEJUN FENG, APS, Argonne National Laboratory, ANDRIVO RUSYDI, National University of Singapore — A prototypical orbital ordering material, the charge transfer insulator $KCuF_3$ is believed to undergo orbital ordering at a temperature $T_{OO} \sim 800$ K. Recent Raman and X-ray measurements reveal a low-temperature structural transition just preceding the onset of three-dimensional magnetic ordering at $T_N \sim 40$ K. We present a model of how orbital, structural and magnetic fluctuations are coupled at temperatures between T_{OO} and T_N, leading to the dynamical frustration of in-plane spin order. The low-temperature structural transition quenches the orbital fluctuations, stabilising A-type Néel spin order. A striking implication of our results is that the ground state of $KCuF_3$ lies near a quantum critical point associated with an orbital/spin liquid phase that is obscured by emergent Néel ordering of the spins. This exotic liquid phase might be accessible with the application of pressure.

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Date submitted: 27 Nov 2009 Electronic form version 1.4