Abstract Submitted
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Orbital 120° model on pyrochlore lattice: MnV_2O_4 GIA-WEI CHERN, University of Wisconsin, Madison, NATALIA PERKINS, University of Wisconsin Madison — Recent first-principles calculation on vanadium spinel MnV_2O_4 reveals a significant trigonal distortion at the vanadium site [1]. Its interplay with other known interactions in this compound, including spin-orbit coupling, Jahn-Teller effect, V-V and Mn-V exchanges, is yet to be understood. To make analytical calculations tractable, we present a theoretical model based on a large trigonal crystal field to describe orbital ordering in MnV_2O_4. At the single-ion level, the trigonal distortion leaves a doubly degenerate ground state and breaks the approximate rotational symmetry of t_{2g} orbitals. We find that the effective interaction between these low-energy doublets is described by a quantum antiferromagnetic 120° model [2] on a pyrochlore lattice. We obtain the classical ground state and show its stability against quantum fluctuations. The corresponding orbital order consists of two inequivalent orbital chains with an additional modulation of electron density within the chain, consistent with experiments and *ab initio* calculations. Furthermore, in the presence of orbital ordering, single-ion spin anisotropy arising from relativistic spin-orbit interaction stabilizes the experimentally observed orthogonal magnetic structure. [1] S. Sarkar, T. Maitra, R. Valentí, and T. Saha-Dasgupta, Phys. Rev. Lett. **102**, 216405 (2009). [2] Z. Nussinov, M. Biskup, L. Chayes, and J. v. d. Brink, Europhys. Lett. **67**, 990 (2004).

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