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Finite temperature phase diagram of the classical Heisenberg-Kitaev model. NATALIA PERKINS, CRAIG PRICE, Physics Department, UW Madison — We study finite-temperature properties of classical version of the Heisenberg-Kitaev model on the honeycomb lattice. This model is a prominent example of anisotropic spin-orbital models, which can possibly describe the low-energy physics of Na_2IrO_3 and Li_2IrO_3 . In these compounds, Ir^{4+} ions are in a low spin $5d^5$ configuration and form weakly coupled hexagonal layers. Our main result is a finite-temperature phase diagram obtained by classical Monte Carlo simulations. Because of highly anisotropic Kitaev interaction, the spin symmetry of the model is reduced to the discrete symmetry, which may be regarded as $Z_3 \times Z_2$. As the discrete symmetry can be broken at finite temperature even at 2D, the model undergoes phase transitions as a function of temperature. At low temperature phase, thermal fluctuations induce order-by-disorder, just as the quantum fluctuations do at zero temperature. As a result, magnetically ordered ground states of the Heisenberg-Kitaev model persist up to a certain critical temperature. Finally, we discuss the relevance of obtained results for experimental findings in real compounds.

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