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Metastability and Instability in a Model Spin-crossover Material: Free-energy Landscapes Explored by a Constrained Wang-Landau Monte Carlo Method[1]

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Spin-crossover materials present an interesting example of systems with competing interactions on different length scales. Here I present a toy model of such a system: a square-lattice Ising model with nearest-neighbor antiferromagnetic and mean-field like long-range ferromagnetic interactions. Using standard importance sampling Monte Carlo (MC) methods, we have recently obtained rather complex phase diagrams for this model in several parameter regimes [PAR, G. Brown, S. Miyashita, C. Omand, M. Nishino, PRB 93, 064109 (2016)]. One question that cannot easily be answered by these methods, is that of the structure of the free-energy landscape in the space of the two macroscopic order parameters: magnetization and staggered magnetization. We have therefore developed a new method to directly obtain the density of states (DOS) of such a model, using the Wang-Landau MC (WLMC) method. I will briefly discuss our modifications to the original WLMC method to obtain DOS constrained to specific values of the two order parameters, and show the resulting numerical free-energy landscapes and phase diagrams for several parameter values [C.-H. Chan, G. Brown, PAR, unpublished]. Comparison with phase diagrams by standard MC raises some new questions about the nature of metastable phases in models with competing short- and long-range interactions.

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