# A CURSORY STUDY OF THE THERMODYNAMIC AND MECHANICAL PROPERTIES OF MONTE-CARLO SIMULATIONS OF THE ISING MODEL

Abstract

by

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The Ising model has been very successful in simulating ferromagnetic and antiferromagnetic materials. It is, in fact, the pedagogical explanation for the behavior of magnetic materials. Researchers have adapted the Ising model to simulate materials as disparate as foams, cell aggregates and metallic crystals.

In this research, I used different modifications of Metropolis algorithms to simulate phase separation and Brownian motion in the Ising model. One of the algorithms (Algorithm Three in the text) is a choice popular with many researchers. My goal is to illuminate the differences in the dynamical and equilibrium properties of various algorithms and model parameters.

I found that the most popular choice is not always the right choice. It produces a non-Boltzmann equilibrium and its simulated droplets diffuse much slower than other near-Boltzmann algorithms. In fact, the non-Boltzmann algorithm does not have a critical point, while the others do.

In my phase separation simulations, I investigated a number of thermodynamical properties of the two-dimensional Ising model, including the surface energy, surface tension, partition function, free energy and entropy as a function of model parameters and algorithms.

To obtain a functional form for analyzing phase-separation, I developed a second-nearest neighbor *Solid-On-Solid* (*SOS*) model. I found that the SOS model agrees well with the Ising model up to about one-half the critical temperature. I also used heuristic arguments to create a modified SOS model and compared it to simulation results for up to fourth-nearest-neighbor interactions.

I discovered unexpected behavior when I used the model to simulate Brownian motion. For all the algorithms, droplets diffuse slower than predicted at low temperatures, which I explain by assuming that the underlying lattice is sticky.

One could devise more tests to further distinguish and delineate the limitations of the algorithms, like simulating Stoke's flow. When one modifies or add more terms to the Ising Hamiltonian to simulate different phenomena, one needs to modify the algorithm's acceptance probabilities accordingly in order to preserve detailed balance and Boltzmann equilibrium. I have presented a clear method to create algorithms that obey detailed balance and produce near-Boltzmann equilibria.