

Inhomogeneous Classical Systems: A Mean Field and Monte Carlo Study

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Master Thesis in Physics

In this research, the Ising model and the Lennard-Jones fluid are studied using Monte Carlo simulations and mean field theory. The objective is to elucidate the structure of inhomogeneous systems and systems in disequilibrium, for which the acquisition of exact statistical mechanical solutions is intractable.

On the two-dimensional lattice, I investigate the critical behaviour of the Ising model, calculating the heat capacity and correlation length. I investigate the effect of a wall of positive spins on a one-dimensional and two-dimensional lattice, in presence and absence of a negative magnetic field.

I propose a modification of Weiss mean field theory for the Ising model, which allows for spatial variation in the magnetic field and the magnetisation: varying mean field theory (VMFT). I compare the behaviour of this model with the Monte Carlo simulations and find that it qualitatively agrees well. Then I investigate some of the critical behaviour of this model, and calculate critical exponents for the surface tension (1.504) and the width of the interface (-0.4999) between the positive and the negative phase at zero field. I investigate the stability of the metastable phase when an external field is applied, and define regions in temperature-magnetic-field space where spontaneous breakdown occurs, where nucleation is possible and where phases can coexist stably.

Finally, I present results of coexisting gaseous and liquid phases from Monte Carlo simulations of a Lennard-Jones fluid. The interface width expands with temperature, like in VMFT, but I failed to observe critical phenomena.

As a future direction, I propose to compute expected magnetisation of an inhomogeneous Ising model based on the convolution inserted values from respective homogeneous solutions with the correlation function appropriate for the temperature.

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