Monte Carlo Simulation 3 State 3D Potts Model

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Introduction

Monte Carlo simulations is a class of simulations which uses random sampling to study different types of systems such as fluids and crystalline, it is used in the area of condensed matter physics (and other areas such as astrophysics and biology). For the specific task studying crystalline lattices the potts model is widely used. The method has its strength in the way it is possible to simulate large system where it is practically hard (or even impossible) to use other mathematical methods. However, some statistical error is introduced using Monte Carlo methods.

The method was developed at Los Alamos Laboratory during the second world war in the US while doing research on nuclear weapons.

The model and simulation

The simulation here presented is a 3 state 3D potts model which is a model of interacting spins in a crystalline lattice using the Metropolis-Hastings algorithm. Every site on the lattice is represented by a state $\mathbf{0}$, $\mathbf{1}$ or $\mathbf{2}$. The interaction between neighboring sites is defined by the hamiltonian

$$H = -J \sum_{<i,j>} \delta_{\sigma_i,\sigma_j} + h \sum_i \delta_{\sigma_i,o} \tag{1}$$

where $J = \mathbf{1}$ here for ferromagnetic coupling [1]. $h = \mathbf{0}$ defines no external magnetic field applied to the lattice. The hamiltonian can be viewed as the summation over the neighboring sites, where the dirac is one if a neighbor is in the same state as the site examined.

The idea is to walk over the lattice calculating the hamiltonian. A new state at a given site is sampled with equal probabilities. A new hamiltonian is calculated, if the energy of the new hamiltonian is lower than the preceding a change in state will occur. If not the change in state will only be accepted with a certain probability.

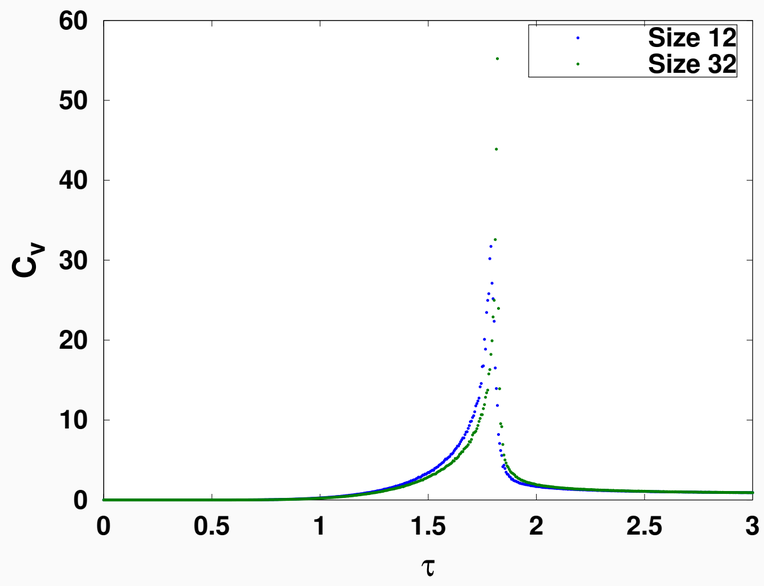
The simulation was ran by first having $\mathbf{10^4}$ thermalization MCS's (Monte Carlo Sweeps). Measurements on the system is then taken by $\mathbf{10^5}$ MCS's for temperatures between $\mathbf{0}$ and $\mathbf{3}$ with $\mathbf{0.005}$ increase in temperature.

Specific heat C_v

The specific heat C_v is calculated from

$$C_v = \frac{1}{L^3}(< E^2 > - < E >^2). \tag{2}$$

The energy E comes from the hamiltonian H where the sum is over all the interactions in the lattice.



Using the specific heat and studying for which the maxima occurs the critical temperature τ_c can be found at $\tau_c = \mathbf{1.820}$ for the $\mathbf{32}$-sized lattice.

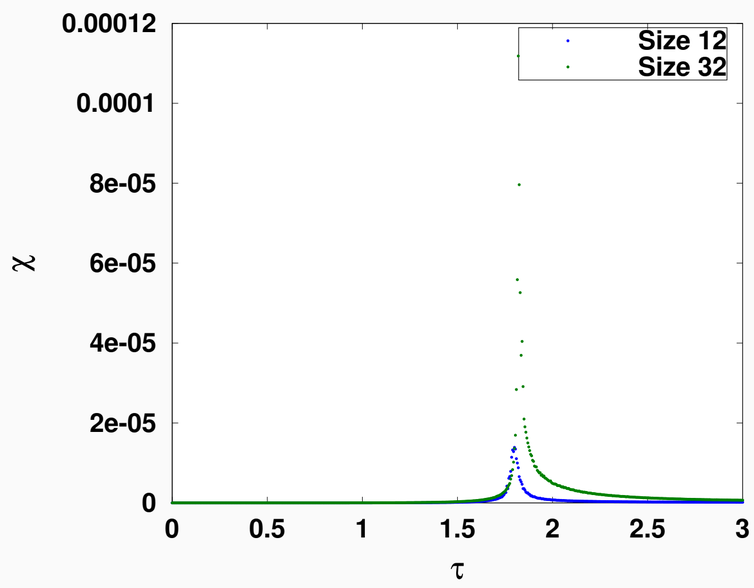
Magnetizaion m and magnetic susceptibility χ

The magnetization M (for the lattice) is calculated by

$$M = n_{i,max} - \frac{(L^3 - n_{i,max})}{2}, \tag{3}$$

where $n_{i,max}$ is the number of sites with the most states in the lattice. M can be scaled by L^3 for the magnetization per site m. The magnetic susceptibility χ is

$$\chi = \frac{1}{L^3}(< M^2 > - < M >^2). \tag{4}$$



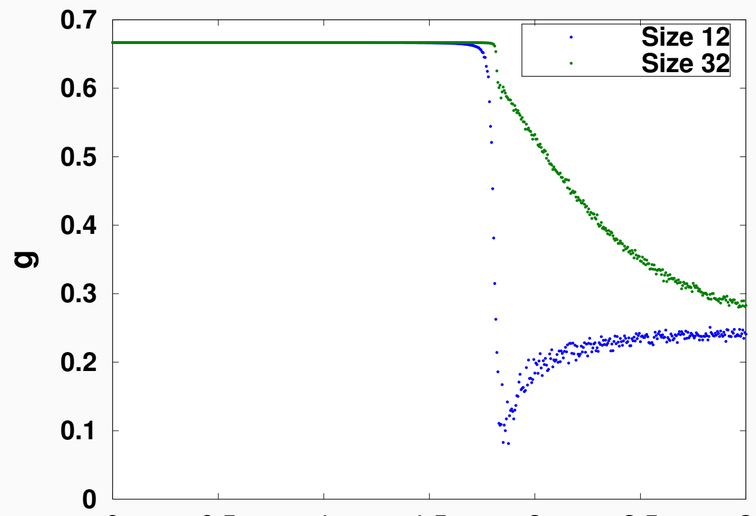
The magnetic susceptibility for the $\mathbf{32}$-sized lattice have been scaled up by $\mathbf{10^3}$ to fit graph.

Binder cumulant g

The binder cumulant g is calculated by

$$g = \mathbf{1} - \frac{< m^4 >}{\mathbf{3} < m^2 >^2}. \tag{5}$$

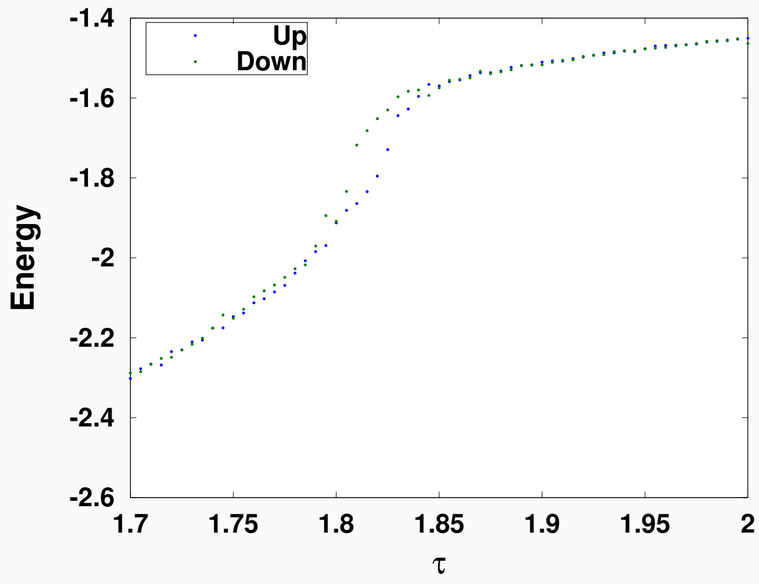
For a second order transition there will an intersect between the different sizes on the lattice. The point where the intersect occurs is where the critical temperature is to be found (and thus is independent of the lattice size).



No intersection occurs and one could thus expect that the transition is of first order.

Hysteresis

Considering any possibly hysteresis a test was done by first raising the temperature and then lowering the temperature over the span around the critical temperature simulating supercooling and superheating. For a first order transition one should expect this to yield a metastable state resulting in hysteresis [2]. The simulation was done by first having a thermalization of $\mathbf{5000}$ MCS's and then rasing the temperature by $\mathbf{0.005}$ for $\mathbf{250}$ MCS's for every temperature with measuring after $\mathbf{50}$ MCS's. The result for the $\mathbf{32}$-sized lattice is presented.



The hysteresis is shown, indicating a first order transition since the simulation shows that metastable states occur. The reader should also be appraised with the fact that the expectation value for the energy per lattice of the model will be $-\mathbf{3}$ when the temperature is low ($\mathbf{0}$) and the lattice is in ground state, all the sites will be in the same state. For high (infinite) temperature the energy per lattice will be $-\mathbf{1}$ due to the fact that on average one state per site will be equal to a neighbor.

Discussion

Only continious phase transitions (as a second order transition) are characterized by the critical exponents, finite size scaling are not done in the first order transition found here. The first order phase transition involves latent heat compared with continious phase transitions which does not.

Furthermore, one may considering running the simulation on larger lattices and study the transition. Due to limited computational power (running Ubuntu 14.04 @ Intel Core i3, 2.30GHz x 4), this, however have been restricted to run on $\mathbf{12}$ and $\mathbf{32}$-sized lattices. One may also consider to utilize parallel computation using Monte Carlo algorithms. This was however achieved in a somewhat ad-hoc way by starting four instances of the software for different temperatures. This would not apply to the hysteresis analysis since the simulation depends on the preceding temperature for the metastable state.

The simulation was done in C and the results are plotted using Octave. The source files can be found at https://github.com/olundberg/MC.

References

[1] H. G. Katzgraber. *Introduction to Monte Carlo Methods.* arXiv:0905.1629v3, 2011.
[2] P. Chaddah. *Studies on Magnetic-field induced first-order transitions.* arXiv:cond-mat/0602128v1, 2006.

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