Monte Carlo Simulations of the 3-State Potts Model in 2D

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Author
Teun Zwart (10499873)

Supervisor
dr. Phillipe Corboz

Second Assessor
dr. Edan Lerner

Instituut voor Theoretische Fysica Amsterdam
Faculteit der Natuurwetenschappen, Wiskunde en Informatice
Universiteit van Amsterdam

Abstract

Populaire Samenvatting

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Chapter 1

Theory

1.1 The Two-Dimensional Ising Model

The two-dimensional Ising model in zero-field was first solved exactly in 1944 by Lars Onsager.[3] It describes a square lattice with nearest neighbour interactions, where each lattice point has with it associated a number (which we'll refer to as spin) which may either be +1 or -1 and was originally meant as a model for magnets. The Hamiltonian is[1]

$$H = -J_1 \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j,k+1} - J_2 \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j+1,k}, \tag{1.1}$$

with $\mathcal{M}$ and $\mathcal{N}$ the extent of the lattice in the x- and y-directions respectively and J_1 and J_2 the interaction strength between neighbours in respectively the x- and y-directions. In the case where the interaction strength in both directions is the same the Hamiltonian becomes[2]

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j, \tag{1.2}$$

where the bracket denotes summation over nearest neighbours.[1] In the ferromagnetic ground state ($J > 0$) all spins on the lattice are aligned in one of two possible directions (the direction is chosen when the mirror symmetry in the lattice plane is spontaneously broken). The Hamiltonian is subject to toroidal boundary conditions in both directions, meaning $\sigma_{1,k} = \sigma_{\mathcal{M}+1,k}$ and $\sigma_{j,1} = \sigma_{j,\mathcal{N}+1}$. We are interested in the thermodynamic properties of the Ising Model. To that end we define the partition function

$$\begin{aligned} Z &= \sum_{\sigma=\pm 1} e^{-\beta H} &(1.3)\\ &= \sum_{\sigma=\pm 1} \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} e^{\beta J_1 \sigma_{j,k}\sigma_{j,k+1}} \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} e^{\beta J_2 \sigma_{j,k}\sigma_{j+1,k}}, &(1.4) \end{aligned}$$

with $\beta = 1/T$ (throughout this work we set the Boltzmann constant k_B equal to 1) and the sum running over every possible orientation of the spins on the lattice. To get an exact solution for this partition function some work is required.

[1] Note that naively applying this Hamiltonian to calculate the lattice energy overcounts the energy by a factor of 2 since each bond is counted twice.

Bibliography

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[3] L. Onsager. Crystal statistics. I. a two-dimensional model with an order-disorder transition. *Physical Review*, 65(3):117–149, February 1944.