Markov Chain Monte Carlo approximation of the infinite lattice Ising model

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NB! Abstract here

I. INTRODUCTION

This report will explore temperature-dependent behavior in ferromagnetism using the two-dimensional **Ising model**. The main purpose is determining a numerical estimation of the **critical temperature** at which the system transitions from a magnetized to a non-magnetized phase.

... more about Ising model and phase transitions + Mote Carlo methods and Markov chains.

II. METHODS

The square 2D lattices for our Ising model will have a length of L containing N spins with the relation $N = L^2$. Each spin s_i will have two possible states of

$$s_i = -1 \text{ or } s_i = +1. \tag{1}$$

The total spin state or **spin configuration** of a lattice will be represented as $\mathbf{s} = (s_1, s_2, ..., s_N)$. The following equations will be used:

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle}^{N} s_k s_l \tag{2}$$

E is the total energy where $\langle kl \rangle$ denotes the sum going over all *neighboring pairs* of spins avoiding double-counting. J is the **coupling constant** simply setting the energy associated with spin interactions. *Periodic boundary conditions* will be implemented allowing all spins to have four neighbors.

$$M(\mathbf{s}) = \sum_{i}^{N} s_i \tag{3}$$

Here M is the magnetization of the entire system expressed as a sum over all spins.

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N} \tag{4}$$

$$m(\mathbf{s}) = \frac{M(\mathbf{s})}{N} \tag{5}$$

ϵ is the energy per spin and m the magnetization per spin. These will be used to compare results.

$$\beta = \frac{1}{k_B T} \tag{6}$$

β describes the “inverse temperature” with the systems' temperature T and the Boltzmann constant k_B.

$$Z = \sum_{\text{all possible } \mathbf{s}} e^{-\beta E(\mathbf{s})} \tag{7}$$

Z is the partition function. This, the ‘inverse temperature” and the total energy of the system appear in the *Boltzmann distribution* given bellow. This will be the probability distribution used for random sampling in our Monte Carlo approach.

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})} \tag{8}$$

For comparison with early numerical implementations we will fist consider an analytical solution. The following table I summarizes all sixteen possible **spin configurations** of a 2×2 lattice with *periodic boundary conditions*.

TABLE I. Analytic values for the sixteen **spin configurations** of 2×2 Ising model lattice.

Nr. of spins in state +1	Total energy	Total magnetization	Degeneracy
0	-8	-4	1
1	0	-2	4
1	0	-2	4
1	0	-2	4
1	0	-2	4
2	0	0	4
2	0	0	4
2	8	0	2
2	0	0	4
2	0	0	4
2	8	0	2
3	0	2	4
3	0	2	4
3	0	2	4
3	0	2	4
4	-8	4	1

Based on the values in table I we derive the specific analytical expressions bellow for the 2×2 lattice case. More comprehensive calculations of the analytic solutions can be found in appendix ??. The specific partition function becomes

$$Z = 2e^{\beta 8} + 2e^{-\beta 8} + 12 \tag{9}$$

Additionally we will calculate a few expectation values. The general formula sis given as

$$\langle A\rangle = \sum_s A_s p(s) \tag{10}$$

which is a sum over all spin states s_i. Here $p(s)$ is a chosen probability distribution, in our this case eq. 8.

$$\langle E\rangle = \frac{16J}{Z}\left(e^{-\beta 8} - e^{\beta 8}\right) \tag{11}$$

$$\langle E^2\rangle = \frac{128J^2}{Z}\left(e^{-\beta 8} + e^{\beta 8}\right) \tag{12}$$

$$\langle \epsilon\rangle = \frac{4J}{Z}\left(e^{-\beta 8} - e^{\beta 8}\right) \tag{13}$$

$$\langle \epsilon^2\rangle = \frac{32J^2}{Z}\left(e^{-\beta 8} + e^{\beta 8}\right) \tag{14}$$

$$\langle |M|\rangle = \frac{8}{Z}\left(e^{\beta 8} + 2\right) \tag{15}$$

$$\langle M^2\rangle = \frac{8}{Z}\left(e^{\beta 8} + 1\right) \tag{16}$$

$$\langle |m|\rangle = \frac{2}{Z}\left(e^{\beta 8} + 2\right) \tag{17}$$

$$\langle m^2\rangle = \frac{2}{Z}\left(e^{\beta 8} + 1\right) \tag{18}$$

III. RESULTS

IV. DISCUSSION

V. CONCLUSION