Markov Chain Monte Carlo approximation of the 2D 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

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

The total spin state or **spin configuration** of a lattice will be represented as $\mathbf{s} = (s_1, s_2, ..., s_N)$. In its simplest form the total energy of the system is expressed as

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle}^{N} s_k s_l - \mathscr{B} \sum_{k}^{N} s_k.$$

Here $\mathscr{B}$ is an external magnetic field. Since we will be looking at the Ising model without an external magnetic field the equation will be simplified to

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle}^{N} s_k s_l, \tag{1}$$

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.

$$M(\mathbf{s}) = \sum_{i}^{N} s_i \tag{2}$$

is the magnetization of the entire system expressed as a sum over all spins. The energy per spin is

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N} \tag{3}$$

and the magnetization per spin is given by

$$m(\mathbf{s}) = \frac{M(\mathbf{s})}{N}. \tag{4}$$

These will be used to compare and analyze results.

$$\beta = \frac{1}{k_B T} \tag{5}$$

describes the "inverse temperature" with the systems' temperature T and the Boltzmann constant k_B.

$$Z = \sum_{\text{all possible } \mathbf{s}} e^{-\beta E(\mathbf{s})} \tag{6}$$

represents the partition function. This, the 'inverse temperature" and the total energy of the system appear in the *Boltzmann distribution*,

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})}. \tag{7}$$

This will be the probability distribution used for random sampling in our Monte Carlo approach.

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	Degeneracy	Total energy	Total magnetization
0	1	-8J	-4
1	4	0	-2
2	4	0	0
2	2	8J	0
3	4	0	2
4	1	-8J	4

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

$$Z = 2e^{\beta 8J} + 2e^{-\beta 8J} + 12 = 4(\cosh(8\beta J) + 3) \tag{8}$$

Additionally we will calculate a few expectation values for which the general formula is given as

$$\langle A \rangle = \sum_{s} A_s p(s). \tag{9}$$

This is a sum over all spin states s_i. Here $p(s)$ is a chosen probability distribution, in our this case the Boltzmann distribution in eq. 7.

$$\langle E \rangle = \frac{16J}{Z}\left(e^{-\beta 8J} - e^{\beta 8J}\right) \tag{10}$$

$$\langle E^2 \rangle = \frac{128ßJ^2}{Z}\left(e^{-\beta 8J} + e^{\beta 8J}\right) \tag{11}$$

$$\langle \epsilon \rangle = \frac{4J}{Z}\left(e^{-\beta 8J} - e^{\beta 8J}\right) \tag{12}$$

$$\langle \epsilon^2 \rangle = \frac{32J^2}{Z}\left(e^{-\beta 8J} + e^{\beta 8J}\right) \tag{13}$$

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

$$\langle M^2 \rangle = \frac{8J}{Z}\left(e^{\beta 8J} + 1\right) \tag{15}$$

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

$$\langle m^2 \rangle = \frac{2}{Z}\left(e^{\beta 8J} + 1\right) \tag{17}$$

NB! Missing analytic C_V and X

The Monte Carlo method will repeatedly require the Boltzmann factor $e^{-\beta \Delta E}$. The energy shift induced by flipping a single spin

$$\Delta E = E_{\text{after}} - E_{\text{before}} \tag{18}$$

can only take five possible values in a 2D-lattice of arbitrary size. This is shown in appendix B. These values are

$$\Delta E = 0, -4J, 4J, -8J, 8J. \tag{19}$$

To avoid repeatedly calling the exponential function we pre-compute the corresponding Boltzmann factors in an array and use the correct one by implementing a set of if-tests.

III. RESULTS

IV. DISCUSSION

V. CONCLUSION

Appendix A: Analytical solutions for a 2×2 lattice

Appendix B: Possible ΔE values

$$\begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$$