PHY 905 Project 1: Monte Carlo simulation of the 2D ferromagnetic Ising model

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Abstract

A simple Fortran implementation of the Metropolis algorithm for Monte Carlo simulation of the Ising model of ferromagnetism is described. Results are presented for energy and magnetization over a range of temperature.

1 Introduction

In statistical mechanics, the Ising model is a mathematical model of ferromagnetism in a d-dimensional lattice.

1.1 Ising model

The energy H of the $N_x \times N_y$ lattice is a sum over all nearest neighbor spin products, multiplied by an interaction strength J:

$$H = -J \sum_{<i,j>} s_i s_j \tag{1}$$

The magnetization M of the lattice in a given state is computed as a sum over all spins in the lattice:

$$M = \frac{1}{N_x N_y} \sum_i s_i \tag{2}$$

2 Implementation Details

At each step of the Monte Carlo iteration, a lattice site i is chosen at random. The spin s_i of this site is negated with probability $e^{-\Delta E_i / k_B T}$. Boltzmann's constant k_B is set equal to 1 for convenience, so that the temperature T is measured in units of k_B.

The change in energy ΔE_i due to negating the spin of a single point i in the lattice is computed as the sum of i's nearest neighbor spins multiplied by the new spin s_i and the interaction strength J:

$$\Delta E_i = J s_i \sum_{<j>} s_j \tag{3}$$

2.1 Algorithm

The Monte Carlo Ising model algorithm comprises the following steps:

1. Choose a temperature T and maximum iteration count N_{iter}
2. Initialize lattice with all spins up
3. Compute initial total energy H and magnetization M
4. Iterate N_{iter} times:
   (a) Select a lattice site i at random
   (b) Compute the change in energy ΔE_i due to negating the spin at lattice site i
   (c) If $\Delta E_i < 0$, retain the flipped spin value at site i, compute the change in magnetization, and update total energy and magnetization
   (d) Otherwise ($\Delta E_i > 0$), retain the flipped spin value at site i with probability $e^{-\Delta E_i / k_B T}$; if retained, update energy and magnetization

3 Results

A Fortran code was written which implements the 2D Ising model. The source code can be found in the GitHub repository. The results in this section were obtained using a $(N_x, N_y) = 50 \times 50$ lattice with all spins up as the initial state. Plots with temperature on the horizontal axis were obtained by averaging the final 50,000 values of energy and magnetization from an iteration with $N_{iter} = 1 \times 10^6$.

4 Conclusion

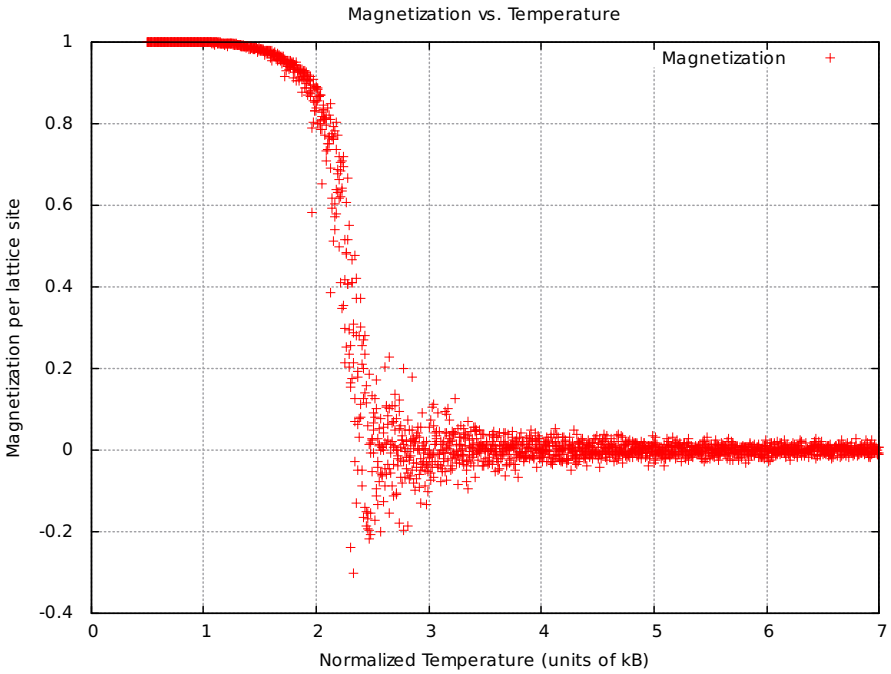


Figure 1: Magnetization per lattice site from $T = 0.5$ to $T = 7$. Values computed by averaging final 50000 Monte Carlo iterations per temperature value.

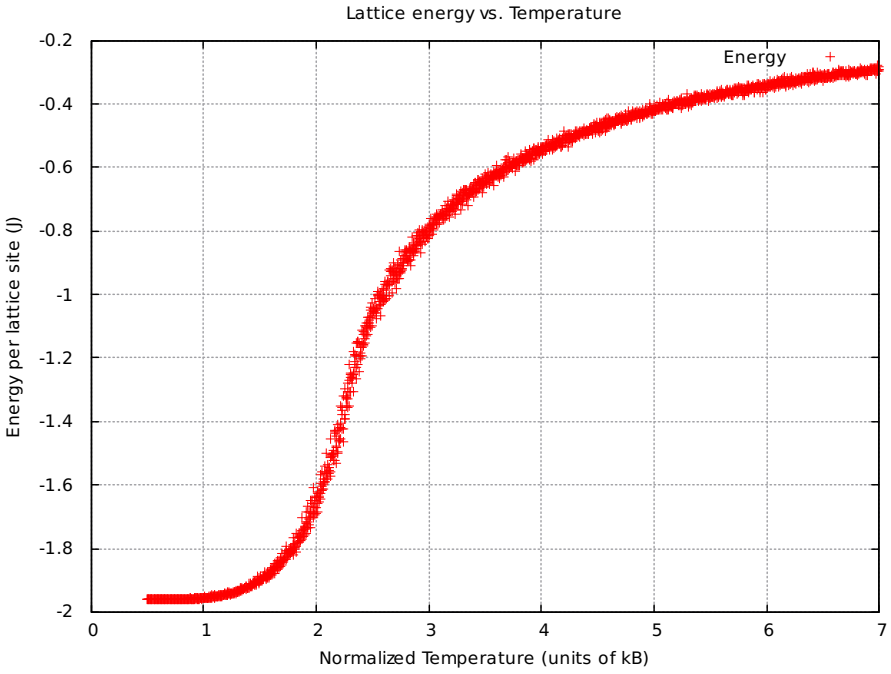
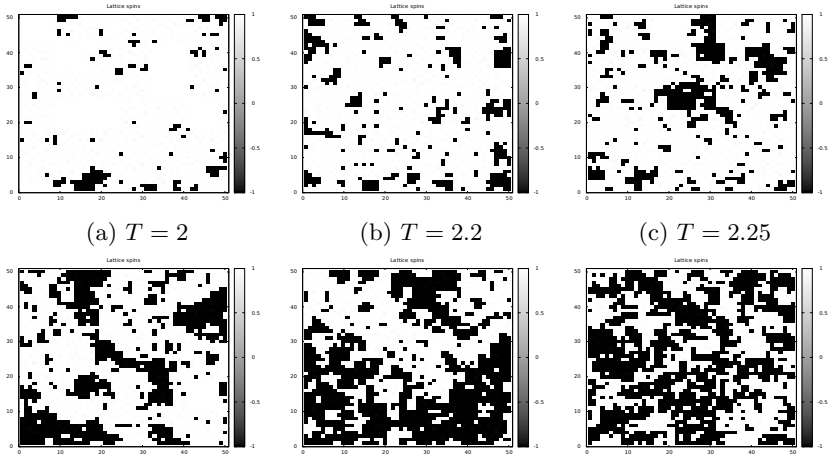


Figure 2: Lattice energy per lattice site from $T = 0.5$ to $T = 7$. Values computed by averaging final 50000 Monte Carlo iterations per temperature value.



(a) $T = 2$ (b) $T = 2.2$ (c) $T = 2.25$

(d) $T = 2.3$ (e) $T = 2.5$ (f) $T = 3$

Figure 3: Spin at each lattice site for various temperatures.