2D Ising model using the Metropolis algorithm

Michael Dramitinos ph4987

May 2022

1 Introduction

We study the two dimensional Ising model using the Metropolis algorithm. Through the simulation we are able to compute the magnetism m,the total energy E, the heat capacity C and the magnetic susceptibility χ. The results are then compared with the exact solution for $N \to \infty$ and $B = 0$, and seem to approach the correct values.

2 Description of the problem

The relevant Hamiltonian for our problem is:

$$H = -J \sum_{n=1}^{N^2} \sum_{<b=1>}^{4} \sigma_n \sigma_b - B \sum_{n=1}^{N^2} \sigma_n \quad | \quad M = \sum_{n=1}^{N^2} \sigma_n \tag{1}$$

We should note here that the ground state is degenerate. For $J > 0$ the ground state corresponds to all the spins being parallel. However they can all point up or down. Therefore, if the initial state of the system is random, since we are flipping one spin per step, the Metropolis algorithm will likely get stuck in local minima as the energy decreases. In order to avoid this, we will begin our simulations will all spins parallel in the positive direction, thus breaking the symmetry. Thus, the initial energy is $H_0 = -4JN^2 - BN^2 = -(4J + B)N^2$, and the magnetization $M_0 = N^2$.

The program flips all the spins of our lattice before taking a measurement of the energy and the magnetization. Note that we don't need to use (1) every time we flip a spin as the change only affects the four neighbours. More specifically, if we flip $\sigma(i, j)$ then we have:

$$dH = 2\sigma(i, g) \left[J \left(\sigma(i + 1, j) + \sigma(i - 1, j) + \sigma(i, j + 1) + \sigma(i, j - 1)\right) + B\right] \tag{2}$$

as well as:

$$dM = -2\sigma(i, j) \tag{3}$$

These equations alongside the initial energy and magnetization, allow as to run the metropolis algorithm without ever needing to evaluate (1). For our problem we will use periodic boundary conditions. We run the simulation for 200 different temperatures, linearly spaced from 0.01 to $2T_c$, where $T_c = J/0.4406868$ is the critical temperature at which the phase shift happens according to the exact solution:

$$M = \frac{\left(1 + z^2\right)^{1/4} \left(1 - 6z^2 + z^4\right)^{1/8}}{\left(1 - z^2\right)^{1/2}} \quad | \quad z = e^{-2J/T} \tag{4}$$

The whole simulation is repeated for increasing lattice size in order to see if our result approach the exact solution.

3 Results

We now present the results of the program. The first plot shows $<|M|>$ plotted against the temperature. Note that all our results have been scaled with the number of lattice points. The temperature has been scaled with the critical temperature.

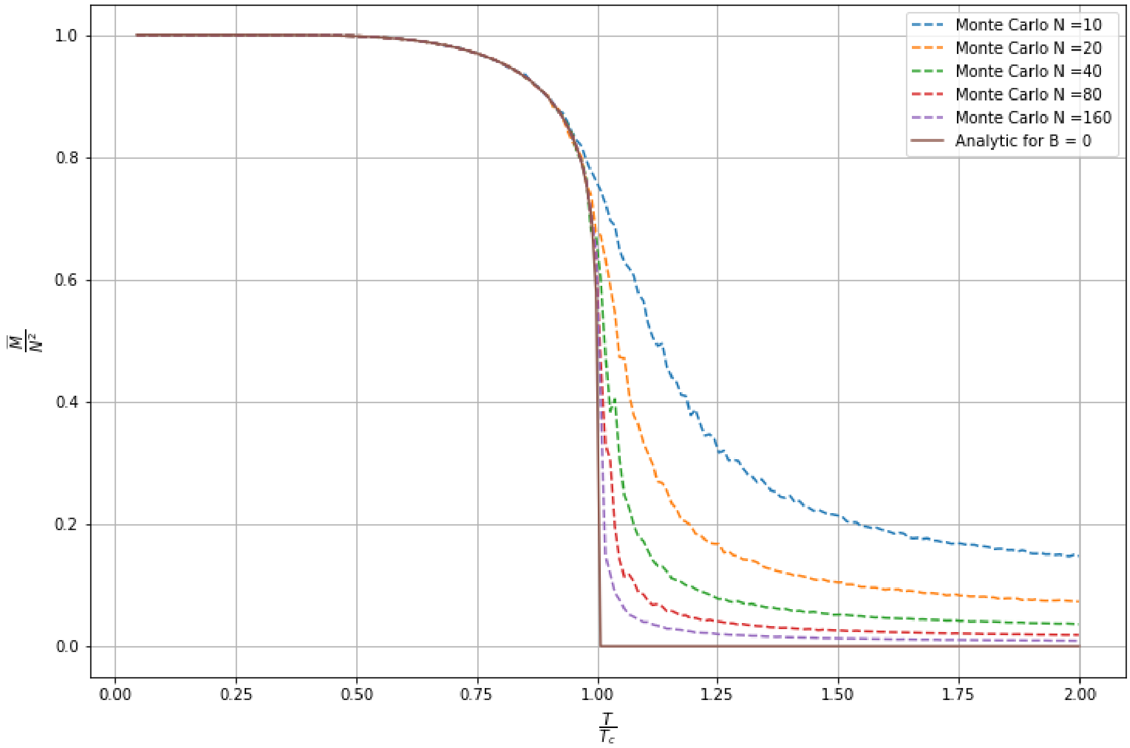

Figure 1: Plot of $<|M|>$ as a function of temperature

We see that there is indeed a phase shift at $T = T_c$ and that our results approach the analytic solution for increasing lattice sizes. Finally we present the plots for the total energy E, the heat capacity $C = \frac{1}{k_b T^2}\left(< E^2 > - < E >^2\right)$ and the magnetic susceptibility $\chi = \frac{1}{k_b T}\left(< M^2 > - < M >^2\right)$.

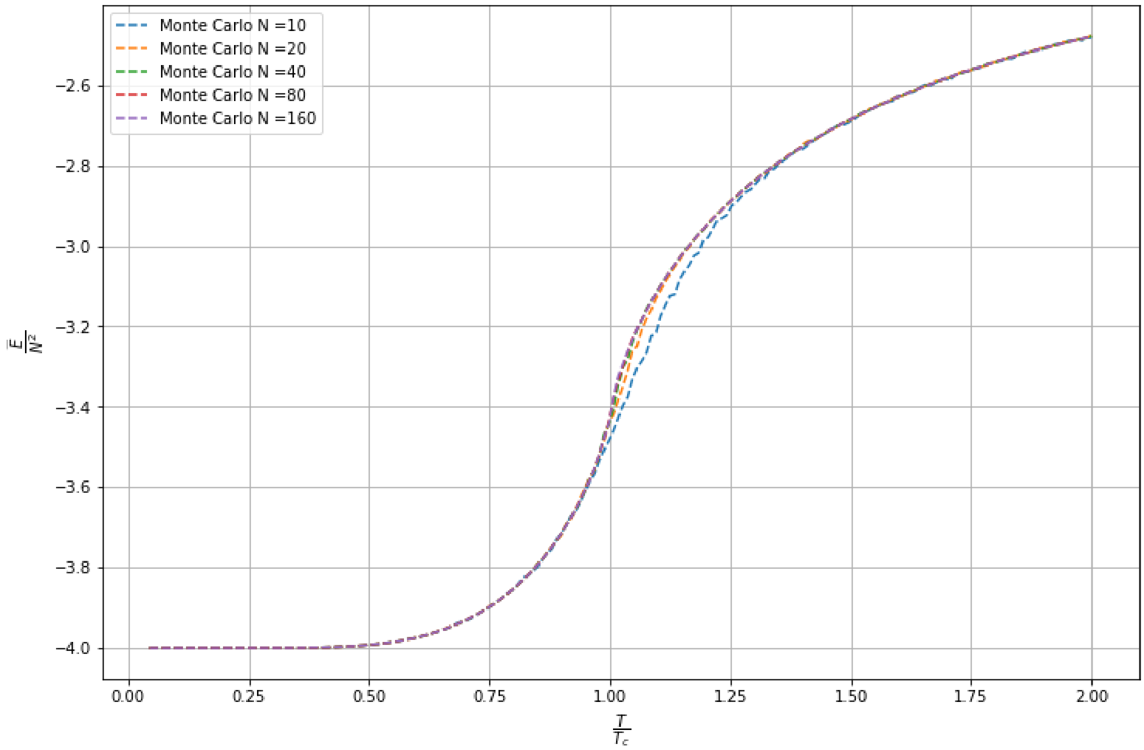

Figure 2: Plot of $<|E|>$ as a function of temperature

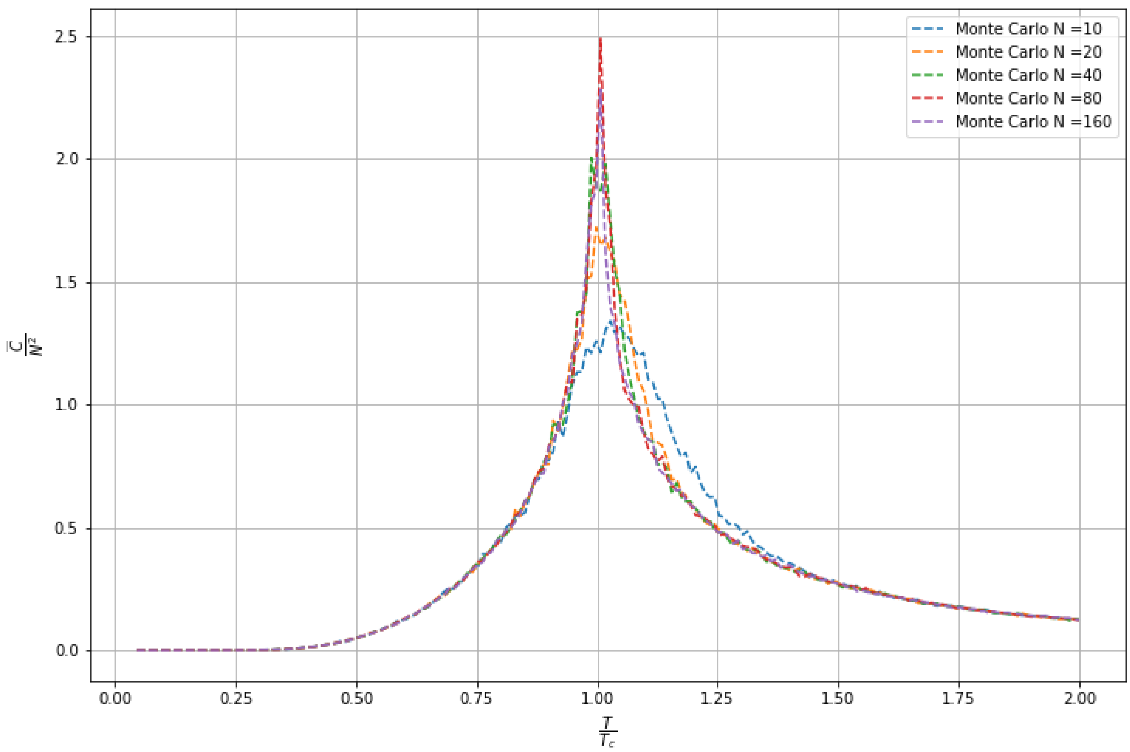

Figure 3: Plot of $<|C|>$ as a function of temperature

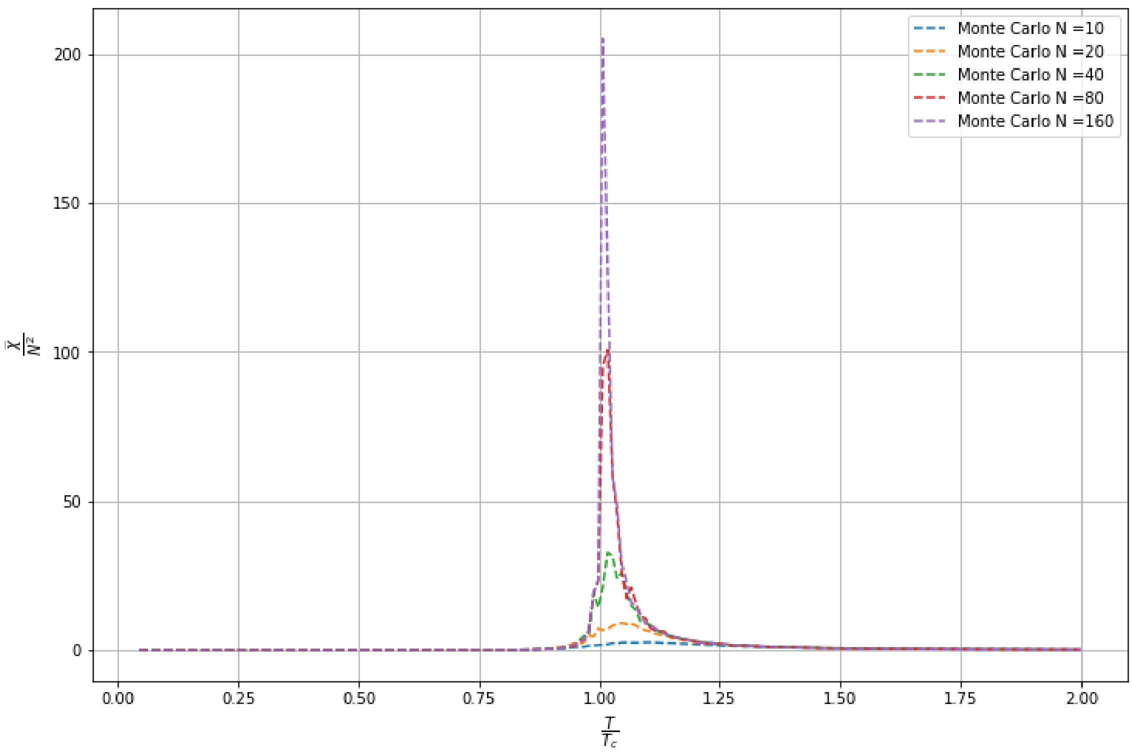

Figure 4: Plot of $< |\chi| >$ as a function of temperature