Ising Model in 2D solved using Metropolis Monte Carlo Algorithm

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PROBLEM 1

Calculate the internal energy per lattice site $U(T) = \langle H \rangle / N$ and the specific heat per lattice site, $C = (\langle H^2 \rangle - \langle H \rangle^2)/(T^2 N)$, for the 2D ferromagnetic Ising 4×4 model with periodic boundary conditions, for T in range $0.2 - 5$(in units J/k_B). Explore the following methods:
a) using explicit generation of all 2^{16} configuration (ie, exact evaluation)
b) Metropolis Monte Carlo simulation.
Compare the results.

Solution

The internal energy and the specific heat per a lattice site for 4×4 lattice of spins are evaluated exactly and using the Metropolis Monte Carlo method. The internal energy and specific heat per lattice site computed using the following formulas.

$$U(T) = \frac{< E >}{N}, \tag{1}$$

$$C(T) = \frac{< E^2 > - < E >^2}{N k_B T^2}, \tag{2}$$

where the thermal average of a physical quantity A taken over the all possible configurations $\{\alpha\}$ as $< A >= \sum_\alpha A_\alpha e^{-\beta H_\alpha}$. In the MC simulations, the spin configuration is changed 20000 times to thermalize before the average of the physical quantities are calculated by taking 10000 measurements. It is seen from the first figure that they are comparable although the MC simulation shows some fluctions around the exact values. At low temperatures, because each site interacts with four nearest sites and taking into account the double counting we would obtain $-2J$ energy per site which is seen from the figure. And this corresponds to all the sites having aligned spins. With heating the lattice the inernal enerrgy increases as expected.

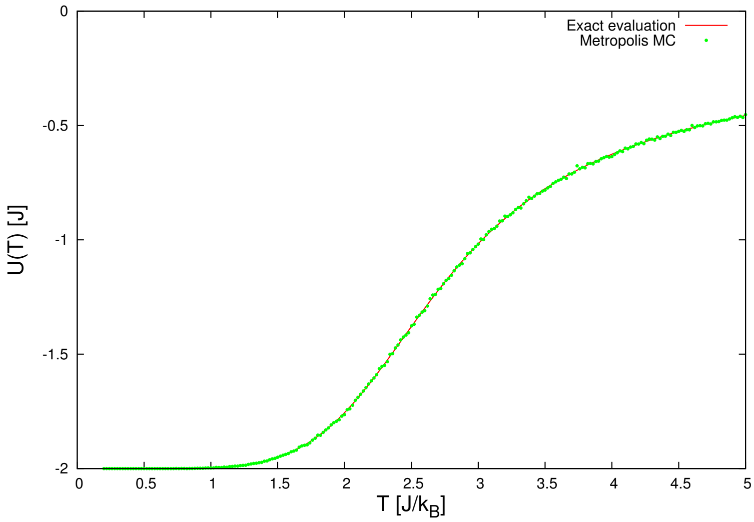

FIG. 1. The internal energy per lattice site as functions of temperature computed exactly and using Metropolis algorithm

From the specific heat graphs it is observed that there is a critical point around in temperature where the behaviour of the system changes drastically. This charachteristic temperature point becomes more pronounced with more lattice sites as it will be seen in the next graphs. From the agreement of the results just for 4×4 spin lattice we can conclude that MC calculations are much better alternative to the exact calculation which becomes computationaly expensive, even imposible, for the larger lattices.

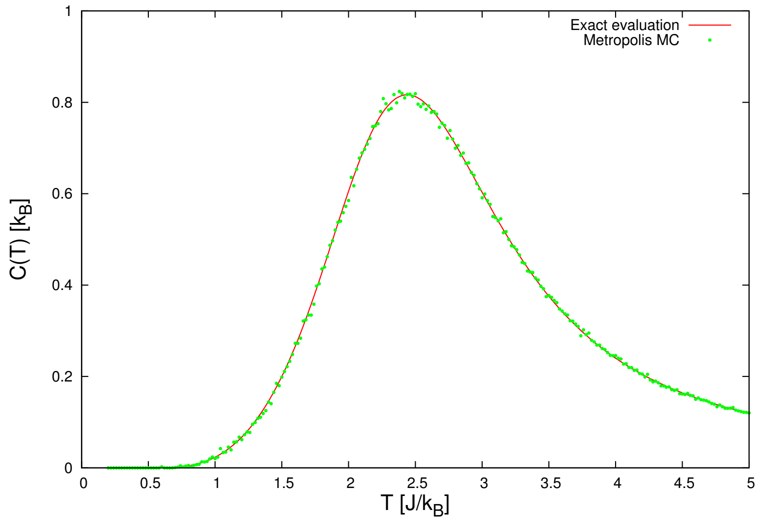

FIG. 2. The specific heat per lattice site as functions of temperature computed exactlyi and using Metropolis algorithm

PROBLEM 2

Using Metropolis algorith simulate 10×10 and $20 \times 20 2D$ Ising models.
a) Evaluate the internal energy $\langle H \rangle / N$ and the specific heat per site in the range of T $0.2 - 5$(in $J/k_B T$). Estimate approximately the value of the critical temperature (think about which approach to use.)
b) For each temperature estimate approximately the magnetization $\langle s \rangle$. Interperet your results.

Solution

The same physical quantities are simulated in 2D Ising model for the 10×10 and 20×20 lattices. The first thing to notice that the MC simulations yield better results for the larger lattices. Now the critical point becomes more apparent from the graphs of internal energies and the specific heat.

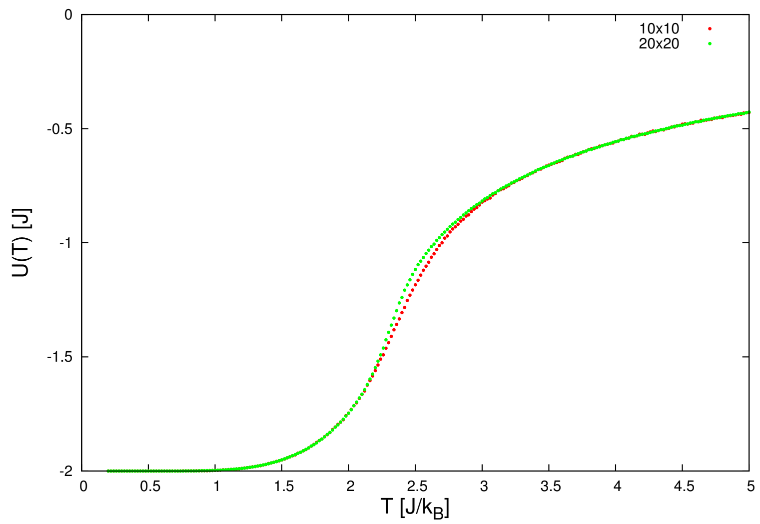

FIG. 3. The internal energy per lattice site as functions of temperature in 2D Ising model for 10x10 and 20x20 lattices

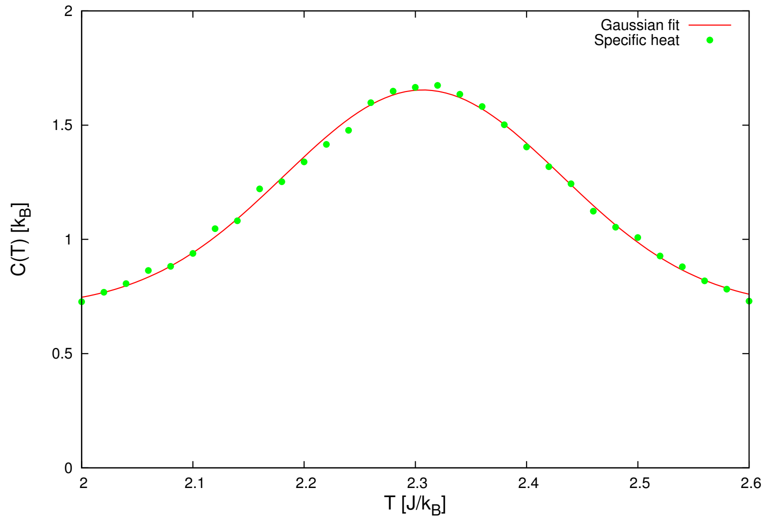

FIG. 5. The critical temperature is found by fitting the specific heat per latiice site curve to a gaussian fucntion for 20×20 lattice

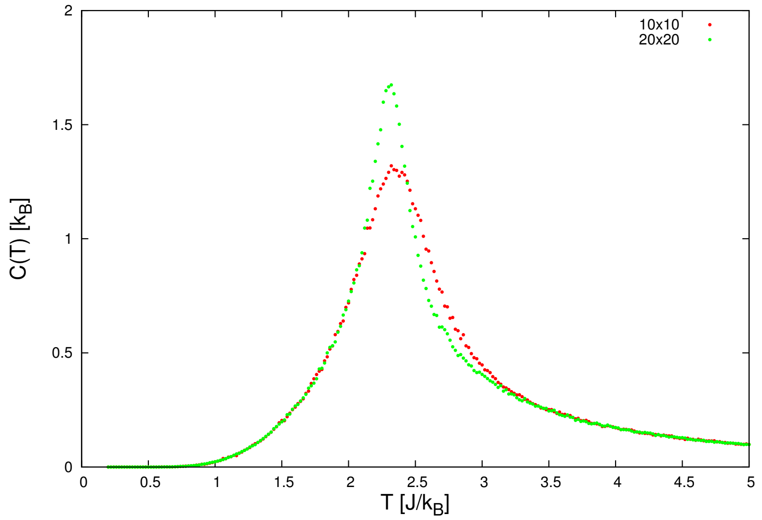

FIG. 4. The specific heat per lattice site as functions of temperature in 2D Ising model for 10x10 and 20×20 lattices

The critical temeparature is found by fitting the specific heat curve per lattice site for the 20×20 lattice with the gaussian function which is shown in the FIG.5. The fitted critical temperature is $T_c = 2.307 \pm 0.001$. In the limit the number of lattice sites going to infinity it is $T_c \approx 2.27$. If we increase the number of sites, T_c would decrease toward this value; we can see that the T_c decreases with the incsrease of the number of sites in the previous figure comparing the spesific heat of lattices 10×10 and 20×20.

Finally, the magnitization for both lattices shown in the figures. When the system cooled down to low temperatures, one can guess that all spins are aligned either up or down. The choice essentially depends on the initial conditions. We can see this from FIG.6 for magnitizations. It is almost 1 or -1 untill the critial point. Around the critical point one can see very noticable fluctuations. These can be improved by increasing the number of thermalization steps which would take a longer time. Of course, the obvius way is to increses the number of lattice sites, but we are just looking the given number of lattice sites. After passing the vicinity of the critical point the magnetizions drops to zero, where we call the a phase transition occured from the ferromagnetic to a paramagnetic state, where no more spontaneous magnetization. Another observation is that 20×20 has a closer critical temperature to the ideal $T_c \approx 2.27$ point, again pointing out that the Ising model works better for the lattices with more sites.

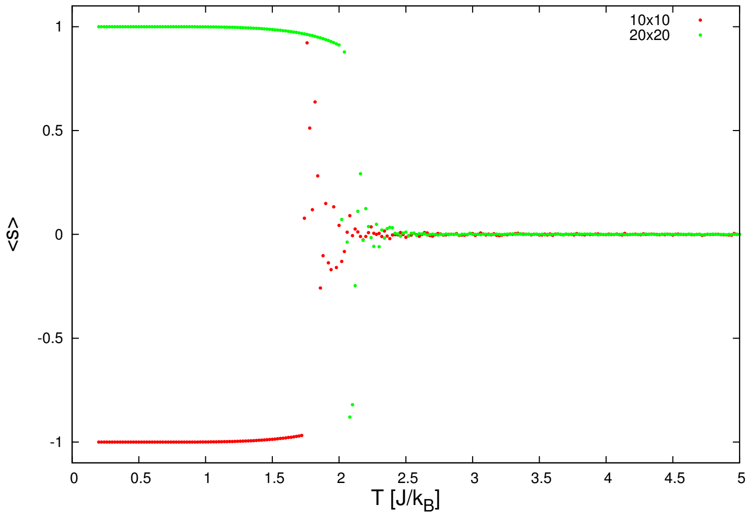

FIG. 6. The magnitization per lattice site as functions of temperature for 10x10 and 20x20 lattices in Ising model

[1] N. J. Giordano and H. Nakanishi, **Computational Physics** (2nd edition, Prentice Hall, New Jersey, 2005).