Homework 5 - Monte Carlo methods

Quynh Nguyen

December 11, 2015

Note: The zip folder include main c++ code in hw5/main/ and ROOT plot code in hw5/ROOT/. Code is compiled in g++ (clang) in Mac OSX.

1 Problem 1 Ising model

code /hw5/main/1.manyT.cc and /hw5/ROOT/p1root.cc

1.a Metropolis algorithm

A 2 dimensional 50x50 array is used to store spin value (s) of each dipole (with value either -1 or +1). Change in energy is calculated by mean field approximation (a spin only interacts with its direct neighbors). With free boundary condition, dipoles on the boundary have three or two neighbors, the rest have four neighbors.

The array is initialized randomly using an uniformly-distributed random number generator. For any filliping proposal, the change in energy (in unit of J) is

$$\frac{\Delta U}{J} = 2 \times s_{i,j} \times (s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1}) \tag{1}$$

$s_{i,j}$ being the dipole at grid point i,j which run from 1 to 50. If the index is over 50 or less than 1, the corresponding neighbor is set to zero. If $\frac{\Delta U}{J}$ is less than 0, the dipole $s_{i,j}$ is flipped by setting to its negative value. If $\frac{\Delta U}{J}$ is larger than 0, the dipole is flipped if $e^{-\frac{\Delta U}{T}}$ is less than an uniform random number between 0 and 1. Here T is in unit of $\frac{k_B}{J}$

The average number of iteration t_n is chosen by trial and error to be 1000. See Fig. (1) and (2).

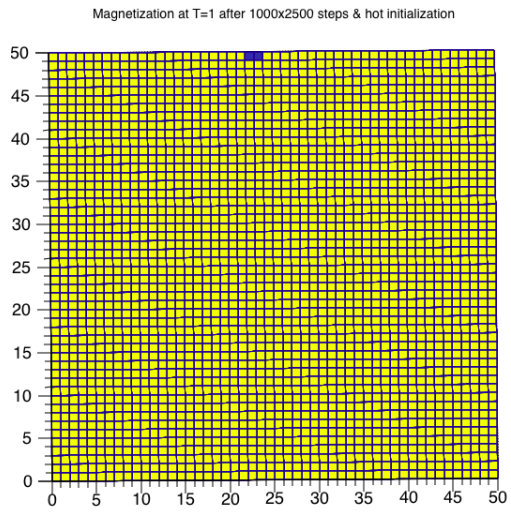

Figure 1: Magnetization at T=1 J/k after 1000x2500 steps. Hot initial condition. Both initial condition converge to the same result.

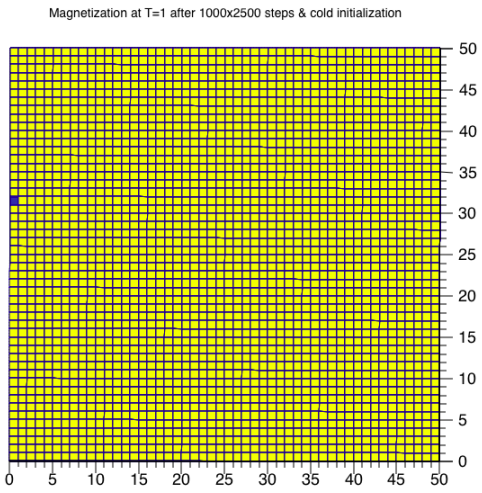

Figure 2: Cold initial condition.

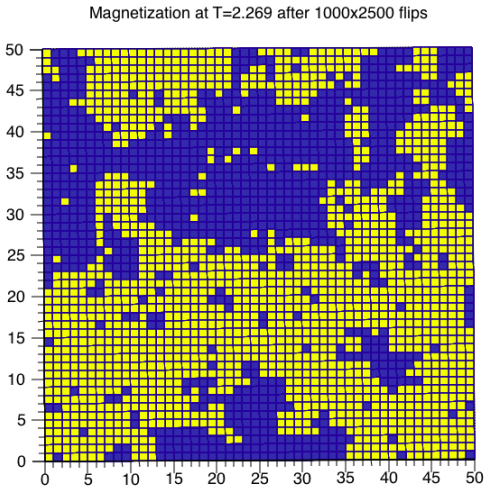

Figure 3: Magnetization at T=2.269J/k. There are clusters of all possible size.

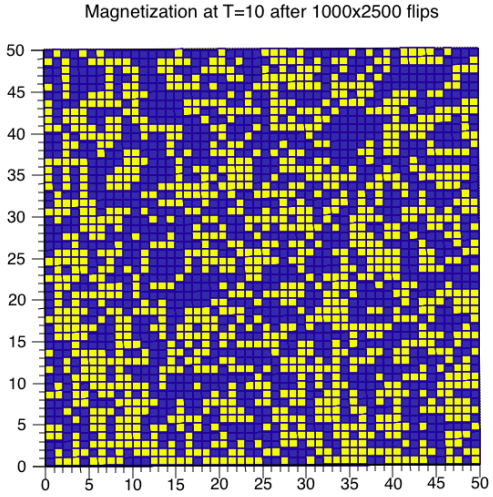

Figure 4: Magnetization at T=10J/k. At high temperature, dipoles are oriented chaostically

1.b Magnetization as a function of time

The Monte-Carlo was run 5 times with different hot initial conditions at each 100 equidistant temperature points between 0 and 5 J/k. The average over initial condition of magnetization is plotted against the temperature in Fig. (5).

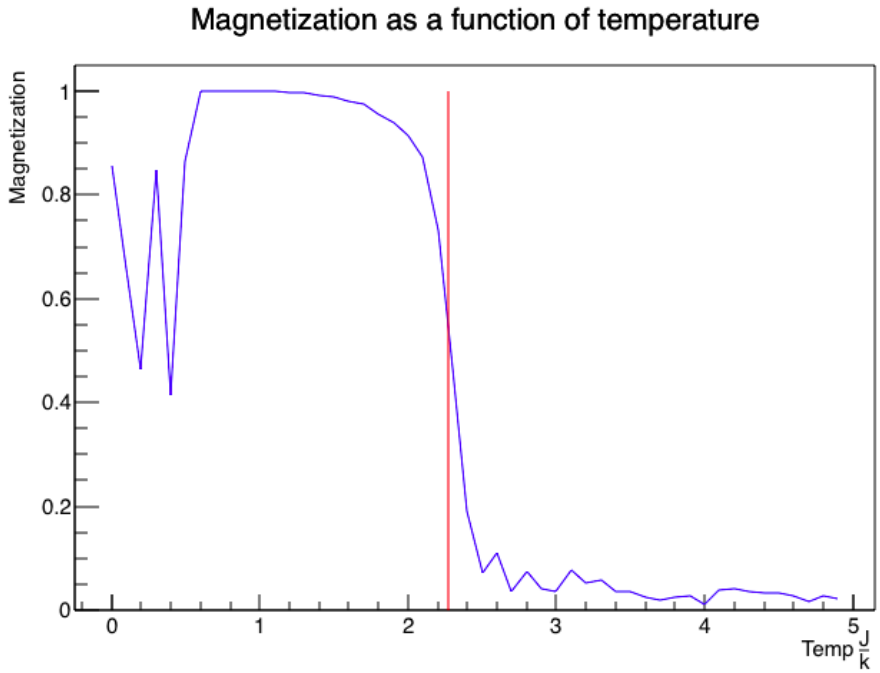

Figure 5: Hot initial condition (5 times average). At around 2.2 J/K, the slope of the plot changes abruptly as expected. The critical temperature is close to theoretically predicted value 2.269. At temperature less than critical, there are metastable states that the dipoles grid is stuck in. This could be solved with an exponentially higher number of iteration and lattice size (here, the number of flip per dipole is 1M). Still, the maximum magnetization approaches 1.

2 Problem 2

code /hw5/main/2.cc and hw5/ROOT/p2root.cc

2.a Units

Choose m=g=1, kT=1/2 thus the change in energy is $\Delta U = \delta x$ and the probability of accepting an energy increasing move is $e^{-\Delta U/kT} = e^{-2\delta x}$

The Metropolis algorithm for this problem is for each iteration, a random particle (position at x) is selected. Propose a move by δx, where δx is a uniformly distributed random number between (-ϵ, ϵ). If ϵ is positive, the proposal is accepted with probability $e^{-2\delta x}$. If ϵ is negative, the proposal is accepted if x+δx is positive. This ensure the boundary condition $x > 0$.

2.b Derivation of ϵ

Any value of ϵ that's not too large or too small, the Metropolis algorithm will converge (albeit at different rate) but ϵ was chosen such that the move is accepted half of the time for a reasonable rate of convergence.

δx is a uniformly distributed random number between (-ϵ, ϵ) thus P($\delta x < 0$)=P($\delta x > 0$)= 1/2. For a randomly chosen particle, the probability for random $\delta x > 0$ AND the move is accepted is P(+) = P($\delta x > 0$) $\times < e^{-\delta x/kT} >$. The probability for $\delta x < 0$ AND the move is accepted is P(-) = P($\delta x < 0$) $\times\alpha$. Here, α is the probability that x+δx is positive to meet boundary condition. ϵ is chosen such that P(+) + P(-) = 1/2 at equilibrium (the stage that dominates the length of the simulation), i.e $< x > = 0.5$.

At equilibrium, ϵ must be larger than $< x >$, other wise, P(-) = 1/2, and P(+) + P(-) > 1/2. Probability for x+δx is positive, i.e. abs(δx) to be less than ϵ, is 0.5/ϵ. The total probability of acceptance equation is then

$$P(\delta x > 0) < e^{-\delta x/kT} > + P(\delta x < 0)\alpha = 1/2 \tag{2}$$

equivalently,

$$\frac{1}{2} \times \frac{1}{\epsilon} \int_0^{\epsilon} e^{-2\delta x} d\delta x + \frac{1}{2} \times \frac{0.5}{\epsilon} = \frac{1}{2} \tag{3}$$

This transcendental equation was then solved in Mathematica to give $\epsilon = 0.920703$.

2.c Equilibrium time

See Fig. (6) for analysis.

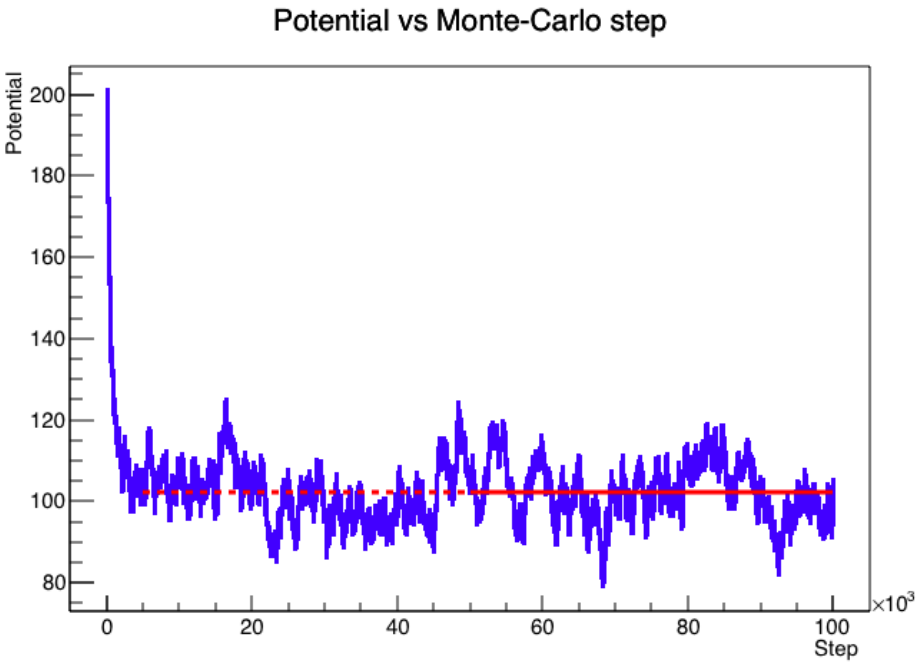

Figure 6: Total potential as number of step increases. The red line shows average of equilibrium potential at 102. Equilibrium time is in the order of 5000 steps (where the red dash line starts). The solid line indicates where data was actually saved to calculate the mean, rms fluctuation, correlation function and histogram.

2.d Mean and RMS

Average equilibrium potential $< U > \approx 102 \approx$ NkT=200 $\times$ 1/2=100, the expected value of U in Boltzmann distribution. Root mean square of fluctuation $\delta U \approx 7$.

2.e Correlation time

See Fig. (7).

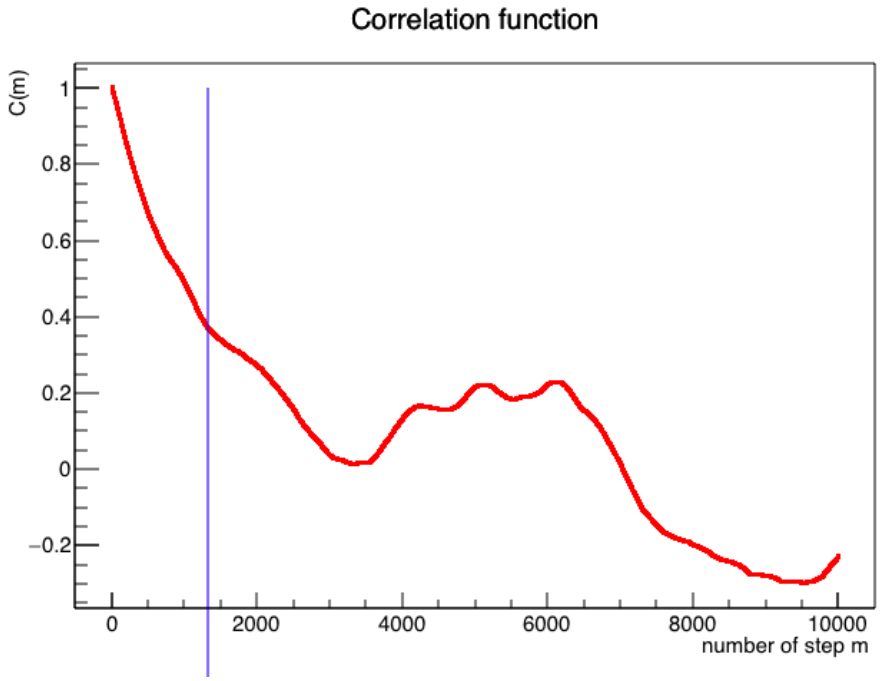

Figure 7: Correlation time, shown at 1323 at the blue line. Depends on the run, this value fluctuates around 1500. Correlation time was found by finding the first minimum value of abs(C[m]-1/e)

2.f Histogram of position

See Fig. (8).

References

[1] Roman Scoccimarro *Lecture notes*

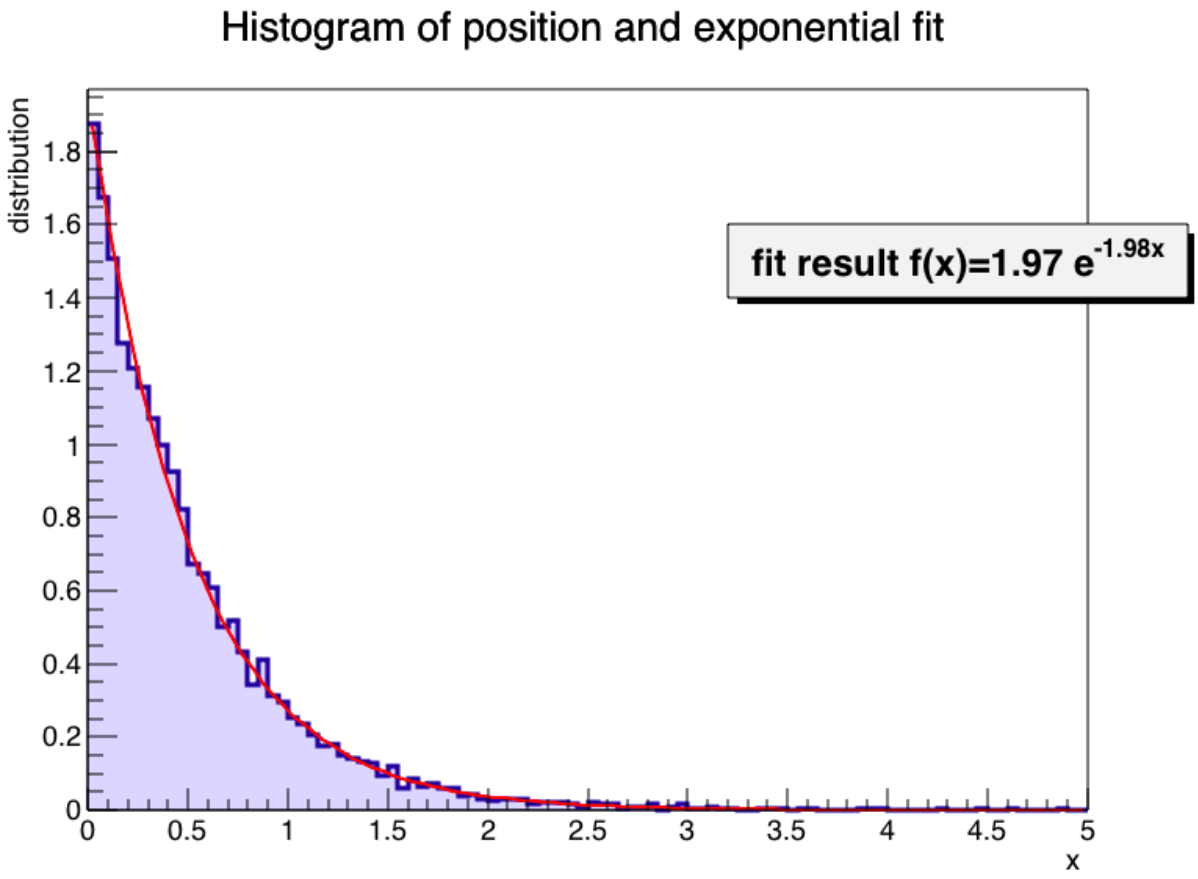

Figure 8: Normalized histogram is fitted to an exponential function, the result is in close agreement with Boltzmann distribution $2e^{-2x}$