Homework 6

link to my github: https://github.com/tanneya/Computational_Physics

Problem 1

1. The initial state of the ising model is completely random, and it looks like this:

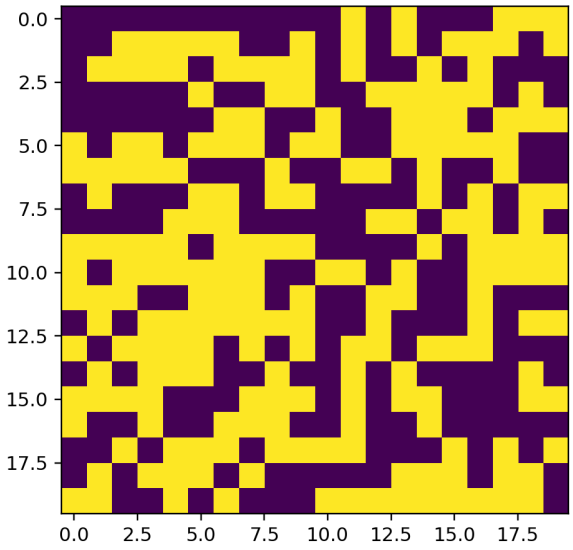

Figure 1: Initial state

Then, by selecting random point and flip its direction, the program will either accept or reject the change by looking at the change in Energy. The probability to accept a change that would increase the total Energy is:

$$P = e^{-\beta \Delta E} \tag{1}$$

where $\beta = \frac{1}{k_B T}$. After 10^6 iterations, the energy converges either to +400 or -400, corresponding to the states which all spins are +1 or -1.

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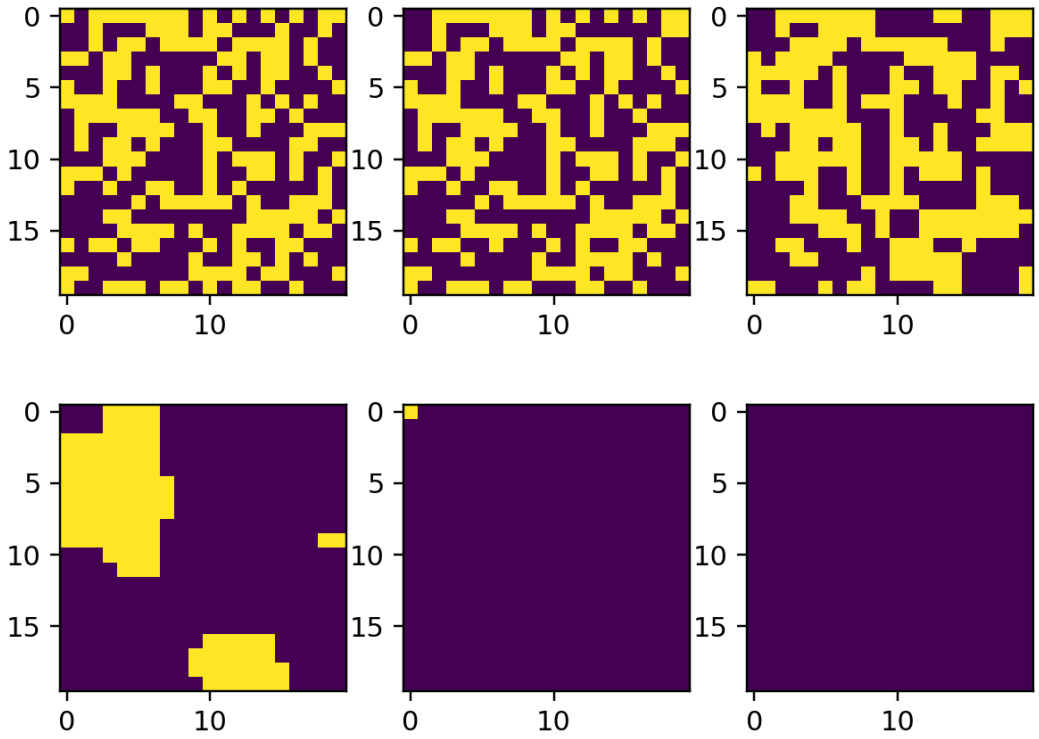

Figure 2: The evolution of the state under Markov chain Monte Carlo simulation, at interation = 1, 15, 251, 3981, 63095, 999999

In this case, the system converged to an all spin down state.

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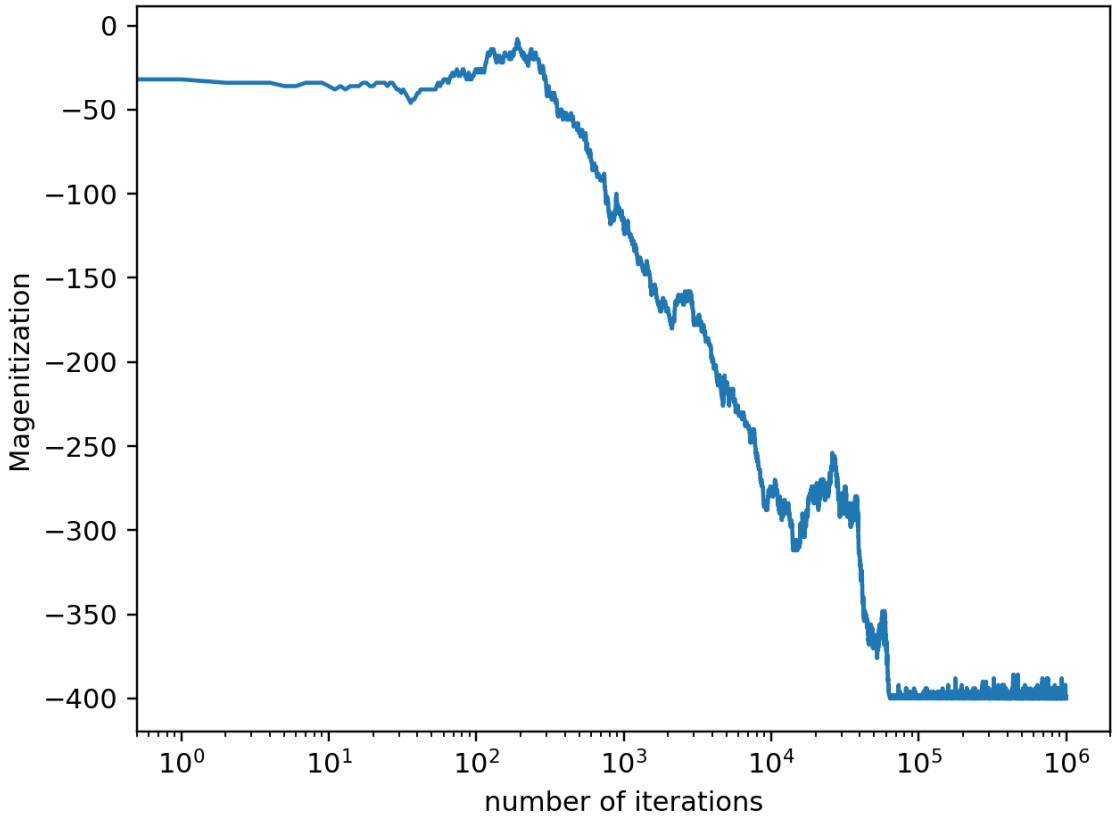

Figure 3: Evolution of the system's Magnetization vs number of iteration

And, if I use different seeds, the system might evolve into an all spin + state. Like shown in the following figure:

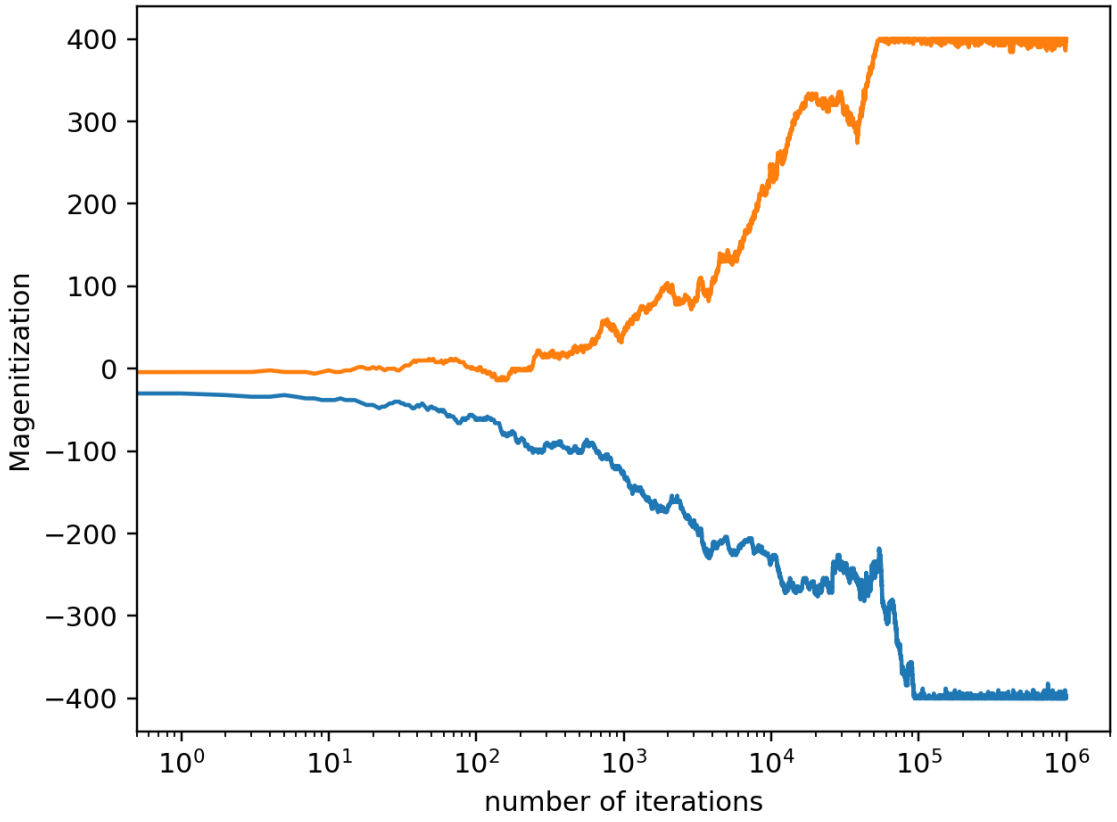

Figure 4: Evolution of the system's Magnetization vs number of iteration

Now let us investigate the influence of T. The following are series of plots for T=1, T=2 and T=3.

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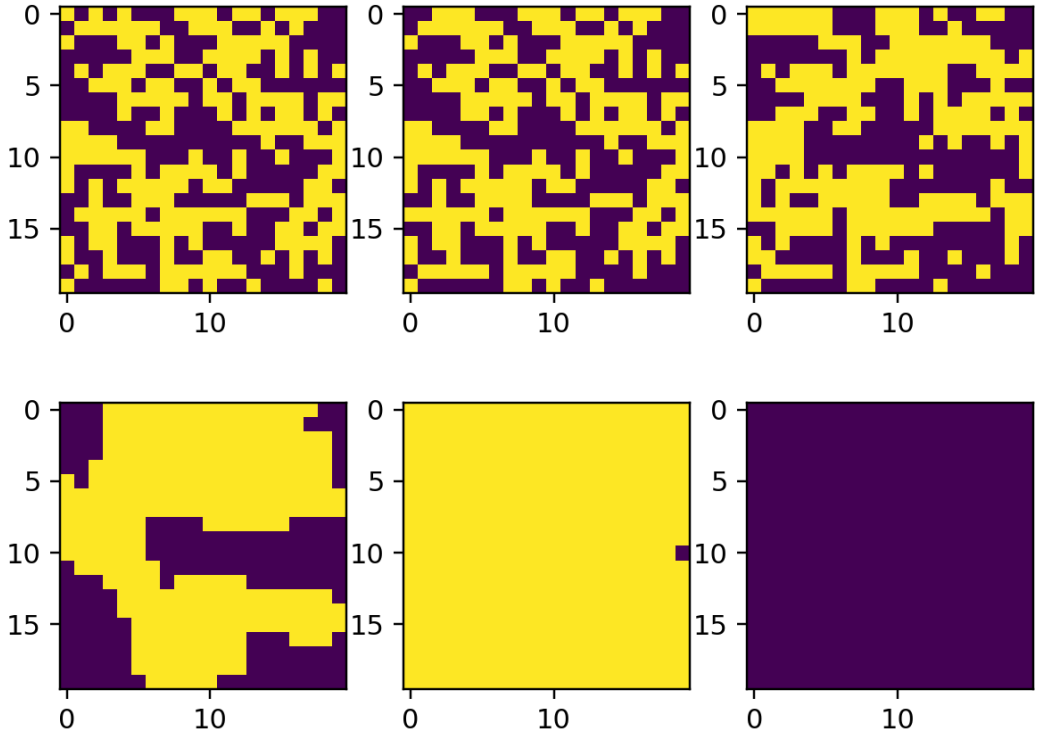

Figure 5: T=1

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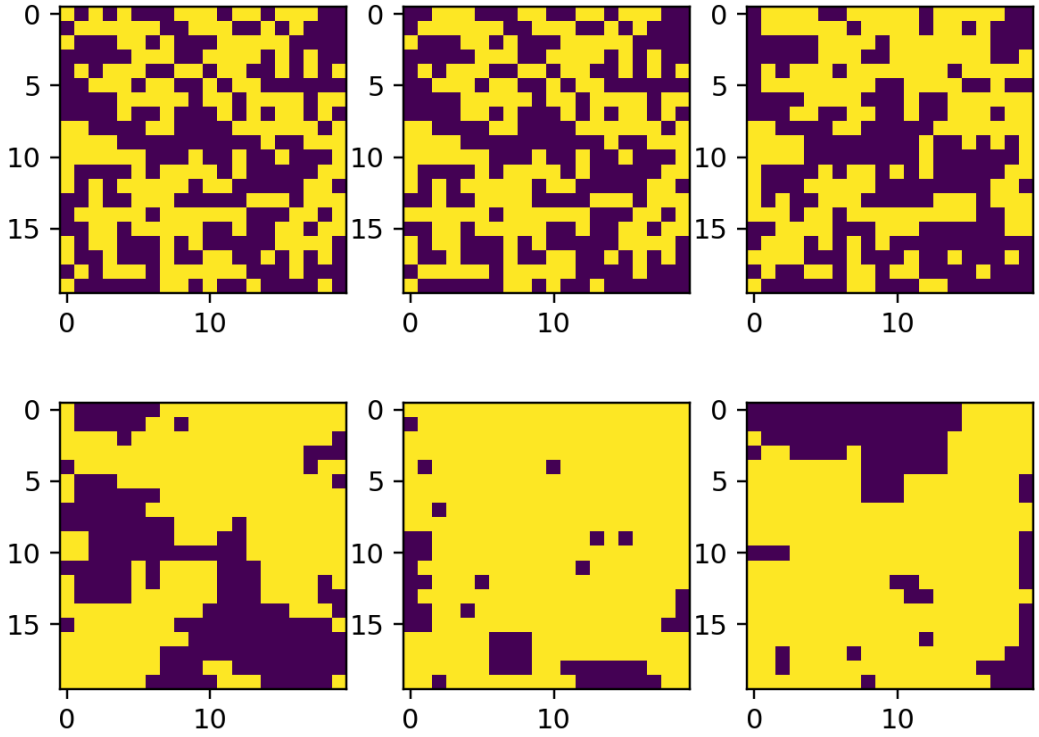

Figure 6: T=2

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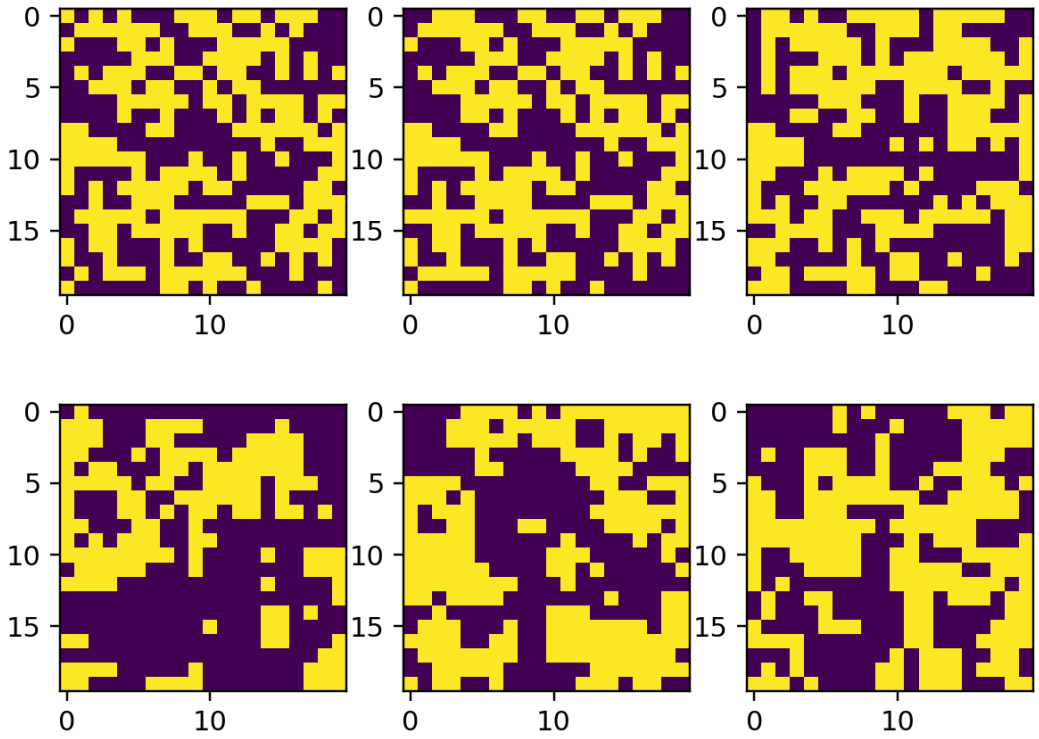

Figure 7: T=3

So as T increases, the probability of accepting an Energy increase also increases. That means it would take more iteration to converge. It is consistent with what we observe, from the above figures. The system converges for T=1, but when T=2 the system could not converge. And for T=3, the system is still disordered.

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Problem 2

1. I have written a code to store the coordinates of the dimers, and by selecting random coordinates, I will either place a new dimer, or remove an existing dimer. The probability of rejecting an existing dimer is:

$$P = e^{-1/T} \tag{2}$$

and T decreases exponentially.

$$T = T_{max} e^{-t/\tau} \tag{3}$$

Comparing an early state ($T = 10$) with the final state ($T = 10^{-5}$) with $\tau = 1000$ and $T_{min} = 10^{-5}, T_{max} = 10$, it is clear that the simulation is working fine.

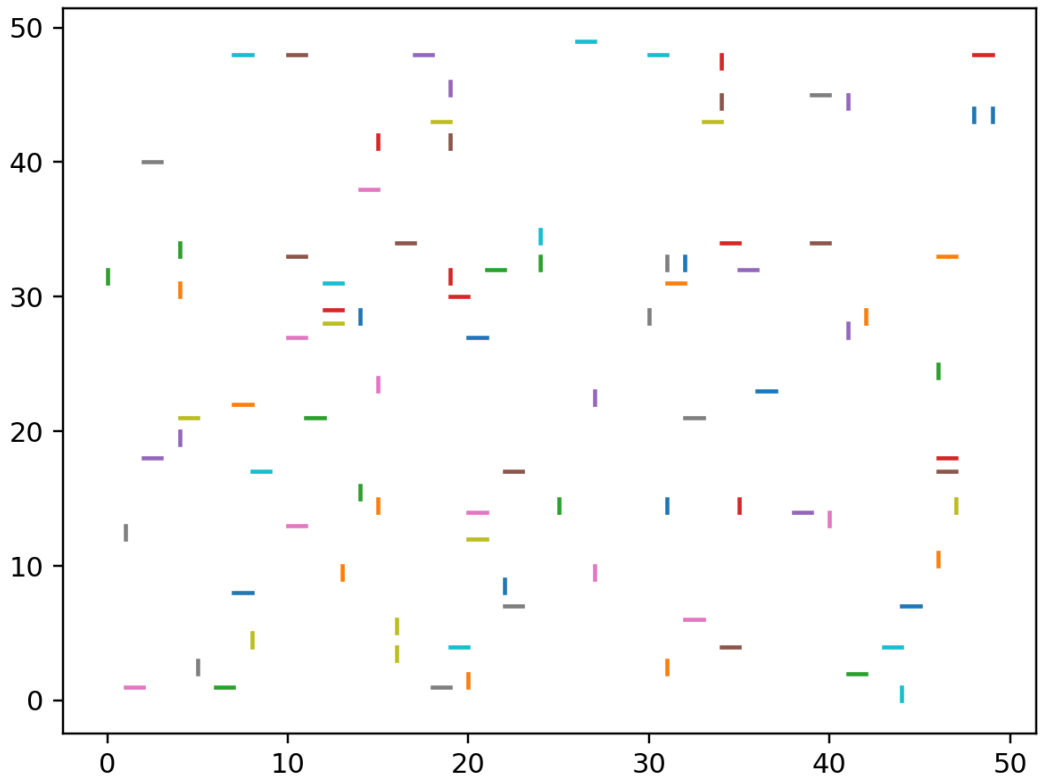

Figure 8: t=100, early state

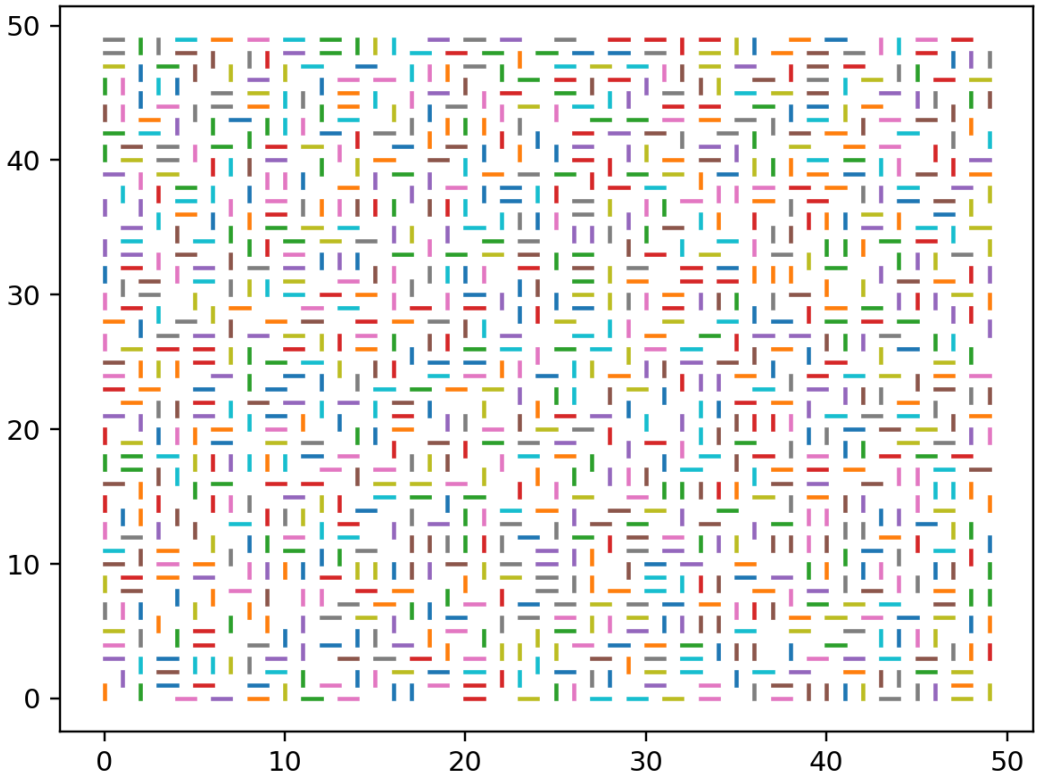

Figure 9: t=13001, final state

It is clear that in the end, the board is almost filled entirely. In fact, 1114 dimers are filled inside. The resulting number of dimers inside the grid is determined by τ and T_max, and the result is shown below:

	τ	number of dimers
1	10^2	656
2	10^3	1108
3	10^4	1175
4	10^5	1225

The result is closer to the optimal value as τ increases. The optimal value is 1250, so as seen, when τ is large enough the result is quite close to the optimal value. However, the system will take a very long time to cool.

Problem 3

1. I have used the linear congruential random number generator from Newman, so:

$$x = (ax + c)\%m \tag{4}$$

and $a = 1664525, c = 1013904223, m = 4294967296$. Using seed x=19, the generated numbers look like:

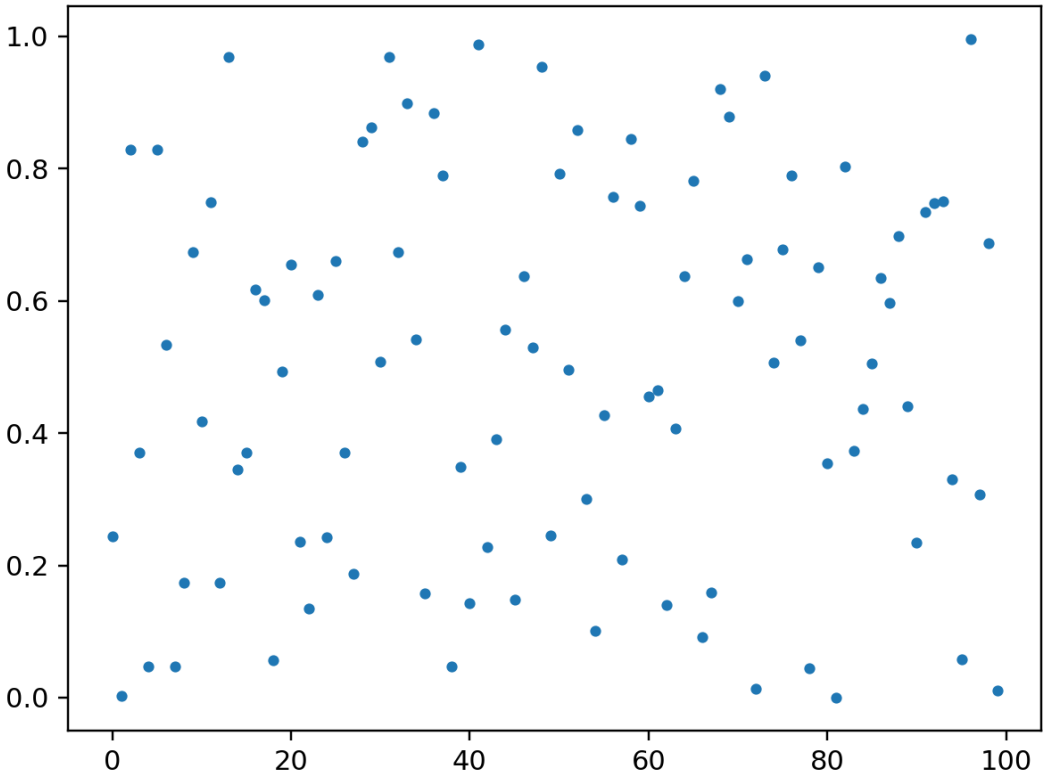

Figure 10: Generated random numbers from uniform distribution

Now according to eq.10.17 and 10.18, Gaussian distribution can be represented by:

$$\theta = 2\pi Z \tag{5}$$

$$r = \sqrt{-2\sigma^2 ln(1-Z)} \tag{6}$$

$$x = rcos(\theta) \tag{7}$$

where Z is an array of 10^4 numbers, randomly generated from an uniform distribution, and σ is the standard deviation.

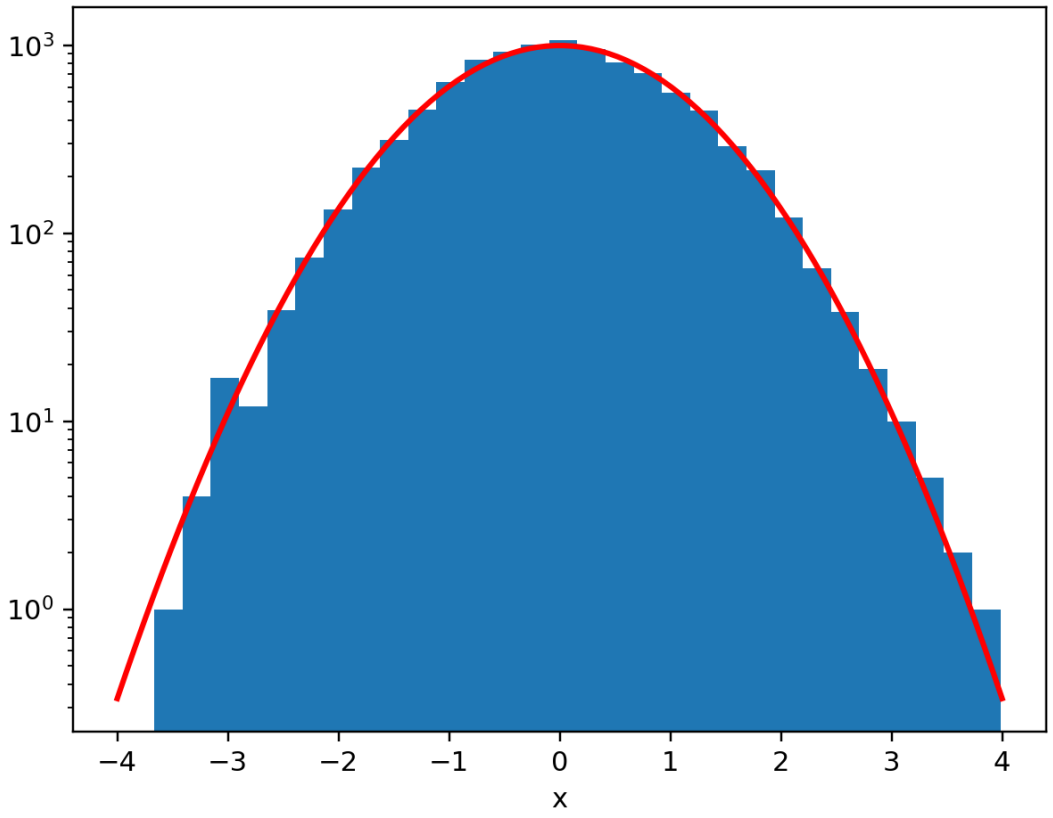

Figure 11: Histogram plot of the generated random numbers from Gaussian distribution with $\sigma = 1.0$. The red line is the theoretical curve for a Gaussian distribution.

Using the DFT code from HW3, I have plotted the power spectrum of the random numbers from Gaussian Distribution:

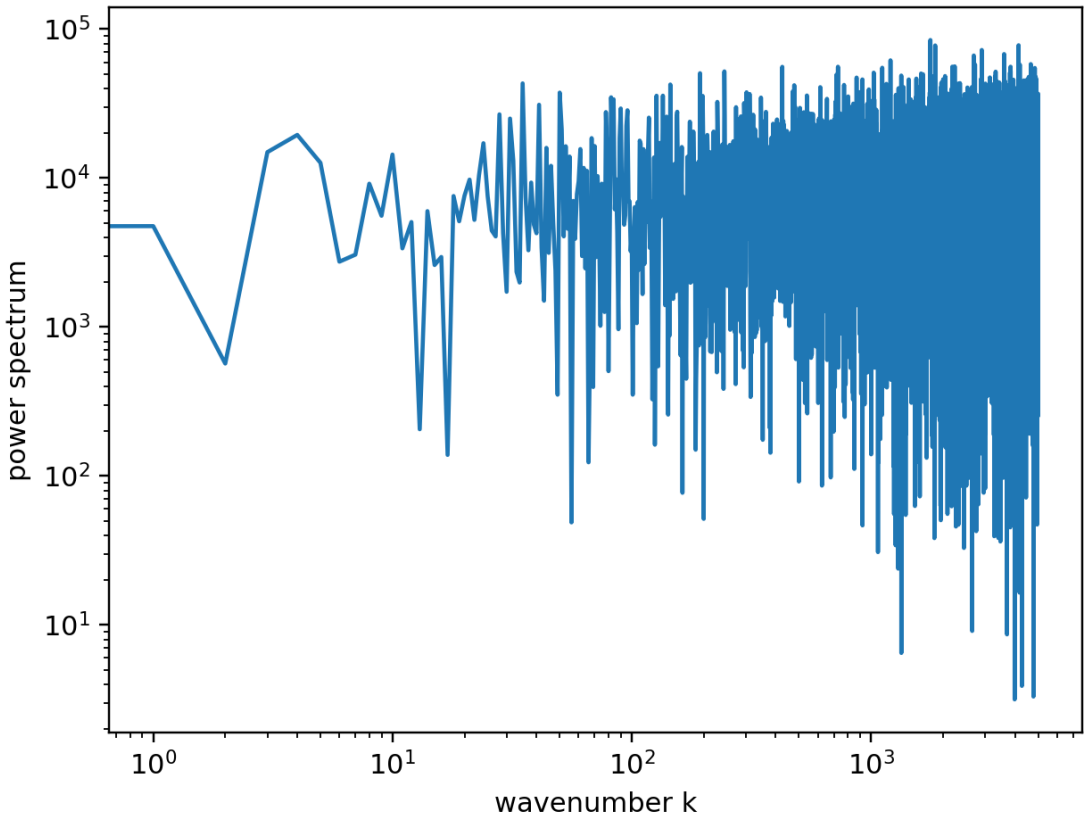

Figure 12: The power spectrum of the randomly generated numbers from Gaussian Distribution

As shown in the graph, the power spectrum is also random, as expected.

Now, applying this random sequence to random walk, the result is shown below:

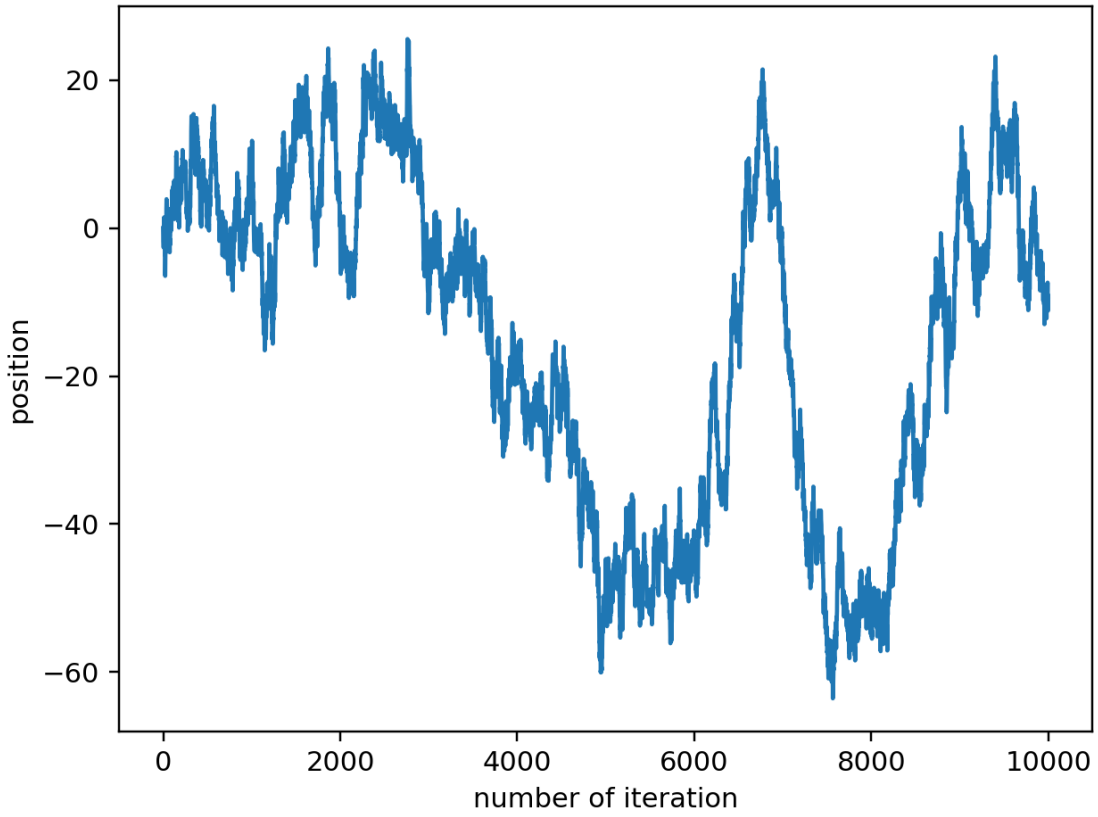

Figure 13: Random walk, position against number of iteration

It is what I have expected, so the particle is walking around x=0.

Next lets look at the power spectrum of the random walk sequence. Below is its figure:

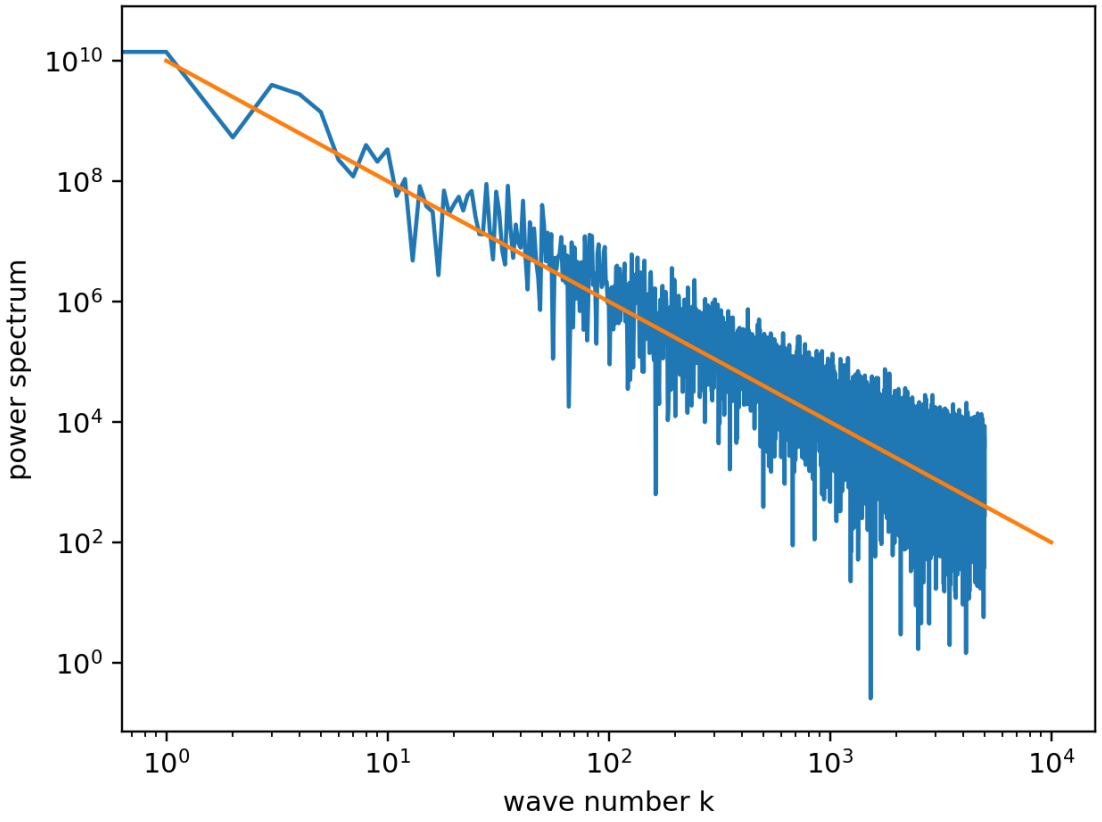

Figure 14: Random walk, power spectrum. The red line is proportional to k^{-2}

As expected, the random walk sequence has a power spectrum proportional to k^{-2}