# Complex Physics - Midterm Exam 1

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**Consider the two different lattice geometries in Fig. 1a and b. The schematic in Fig. 1a displays a one-dimensional periodic closed ring consisting of N sites, where each site has two nearest neighbors. The schematic in Fig. 1b shows a modification of the closed ring, where each of the $N$ sites on average has two additional links to random sites so that each site now has an average of four nearest neighbors.**

**In each of these two cases place an electron of spin $\frac{1}{2}$ on each site - modeled as our usual Ising model with $s_i = \pm 1$. Let the energy of any configuration of spins be described by the familiar ferromagnetic zero-field Ising model ($J > 0, h = 0$), i.e.**

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j,$$

**where $\langle ij \rangle$ denotes any bond that exists between sites $i$ and $j$ in the geometries shown.**

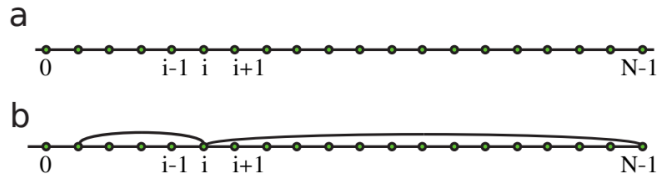



Figure 1: **(a)** Basic lattice, where any given site $i$ is connected with $i - 1$ and $i + 1$. **(b)** Each node has the same links as in (a) but with two additional random links.

## Question 1

**Implement the Ising model for both geometries. Using a Metropolis algorithm, plot the order parameter $\langle s_i \rangle$ vs. $T$. How does the order parameter depend on $T$ in each case? You will need to simulate various values of $T$ and you will need to ensure that you have simulated for a sufficiently long time. 5pt**

### Geometry a)

For this case, the geometry is quite simple, we have a straight line with spins only connected to their nearest neighbors. To implement the Metropolis algorithm, the code goes through the following steps:

1. Define a function "*create_array*" to create an array of $N$ numbers randomly assigned the values of one of minus one.
2. Define functions "energy" and "mag" that calculate the total energy $\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j$ and the magnetization density $m = \frac{1}{N} \sum_i s_i$ of the array.
3. Define the function "update", which randomly chooses a point in the array and calculates the energy difference $\Delta E$ of flipping it. If $\Delta E$ is negative, it accepts the flip and if not, it accepts it with probability $e^{-\beta \Delta E}$. The function does this procedure $N$ times.
4. Define the function "montecarlo", which implements the function "update" a total of $n_{max}$ times and calculates the energy and magnetization in every iteration after the first $n_0$ iterations.

Before trying to calculate any expected values, we need to see the amount of iterations needed for the system to thermalize. To do that, I ran the algorithm with $n_{max} = 1000$, $N = 500$ spins and $k_B T/J$ ranging from 0.1 to 10 in 20 equally sized steps.

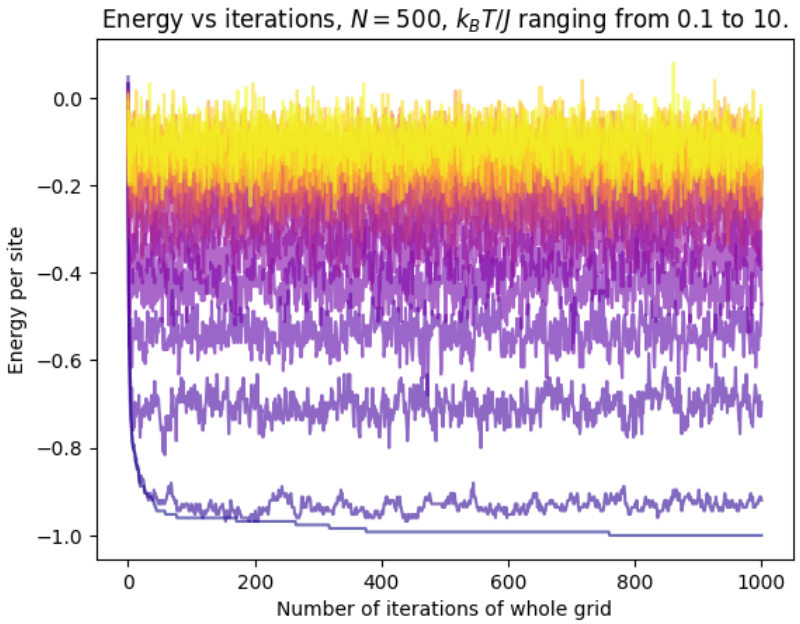



Figure 2: Energy vs iterations for temperatures $k_B T/J$ going from 0.1 to 10, $N = 500$ and $n_{max} = 1000$ total iterations. Notice that an iteration is counted as trying $N$ spin flips, not as a single try of a spin flip. The change in color shows different temperatures, going from purple to yellow.

We can see that for all temperatures, the energy converges pretty quickly (after around 100 iterations) to an almost stable value and then just fluctuates around said value. Therefore, when taking averages, running a warmup of around 500 iterations should be more than enough time for the system to thermalize.

Given this, we can now calculate the expected value of the magnetization $|\langle s \rangle|$ for different temperatures. To do it, we take 20 temperatures in a range from 0.1 to $10 k_B T/J$. Since we know that the systems thermalize after about 100 iterations, we can comfortably use $n_0 = 500$ iterations and we will use a total of $n_{max} = 25000$ iterations, so that the averages are calculated with 24500 values.

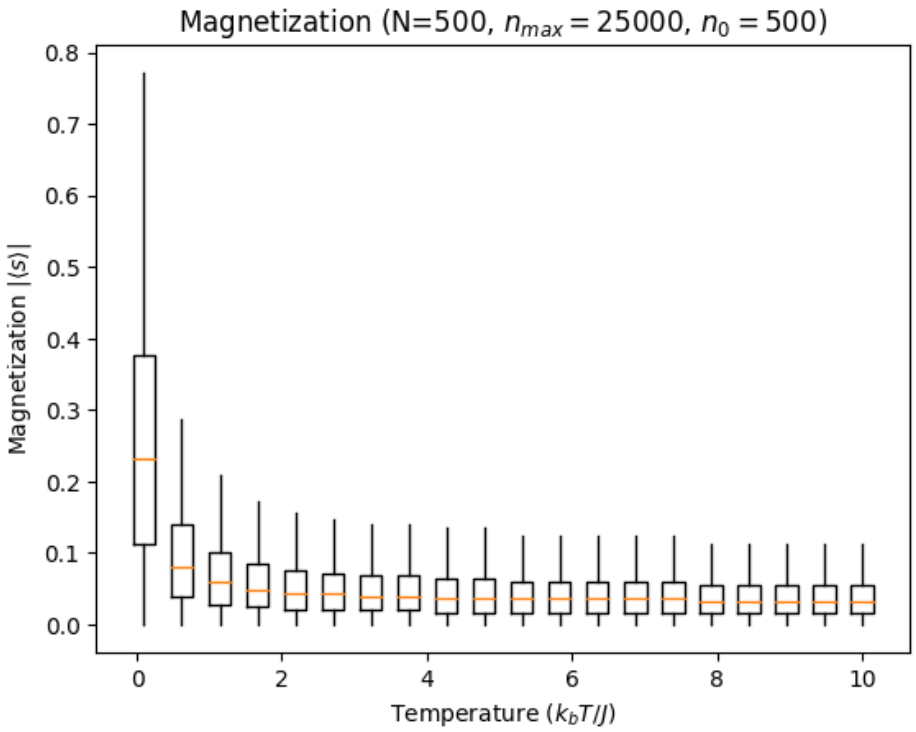



Figure 3: Mean magnetization as a function of temperature. For any temperature, we have $n_{max} - n_0$ values of magnetization, the mean of which is shown with the orange line, while the boxes show the interquartile range and the line shows where the extreme data falls in. The graph was made with $N = 500, n_{max} = 25000, n_0 = 500$.

### Geometry b)

Now we follow the same procedure as before, but with the geometry of figure 1 b), where each spin has two added random links to other spins.

To create the additional random connections, I followed the next procedure:

1. Create a random permutation $P$ of the numbers $\{1, \cdots, N\}$. We will use this permutation to link the spins $i$ and $P(i)$ together.
2. Check that the permutation has the following properties, and if not create a new random permutation:
   - $P(i) \neq i$ for every $i$: This is done so that we don't add a connection of a spin to itself.
   - $P(i) \neq i - 1 (mod\ N)$ and $P(i) \neq i + 1 (mod\ N)$ for every $i$: This is done so that the new connections are not the same as the old ones.
   - $P(P(i)) \neq i$ for every $i$: With this, we make sure that the new links $(i, P(i))$ and $(P(i), P(P(i)))$ are different.

3. If the permutation fulfills these requirements, we create links between $i$ and $P(i)$ for every $i$. That way, we will add a total of $N$ new links, and therefore every spin will have in average 2 new links. Furthermore, the links will be different between themselves and different from the old ones.

As before, we begin by doing the metropolis algorithm with $n_{max} = 1000$ iterations just to see if the energies reach an equilibrium value. The results are show in the following figure.

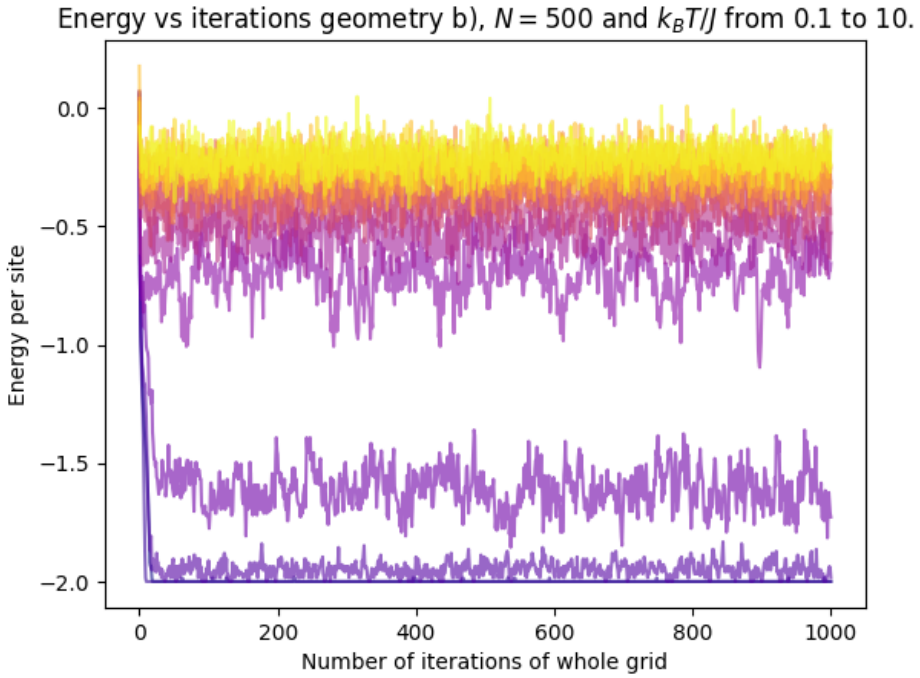



Figure 4: Energy vs iterations for the geometry b), with temperatures $k_BT/J$ going from 0.1 to 10, $N = 500$ and $n_{max} = 1000$ total iterations. Notice that an iteration is counted as trying $N$ spin flips, not as a single try of a spin flip. The change in color shows different temperatures, going from purple to yellow.

We can see that 100 iterations seem to be enough for thermalization. Therefore, we will use $n_0 = 300$ iterations before taking averages, which should be more than enough to reach thermalization. Given this, we can now calculate the expected values of the magnetization for different temperatures. We'll use $n_{max} = 5000$ total iterations, $N = 500$ spins and temperatures ranging from 0.5 to $10k_BT/J$.

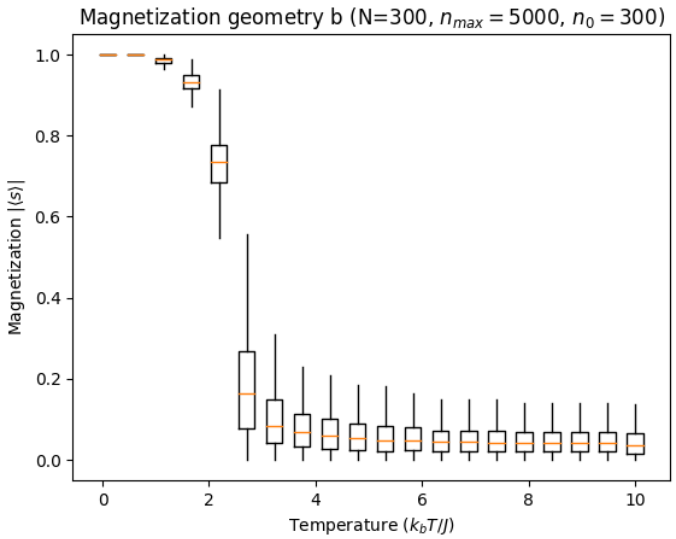



Figure 5: Mean magnetization box plot as a function of temperature for geometry b. The graph was made with $N = 500, n_{max} = 5000, n_0 = 300$.

Since in this case there seems to be some interesting behaviour at around $2k_BT/J$, we'll make another plot zooming in on that section.

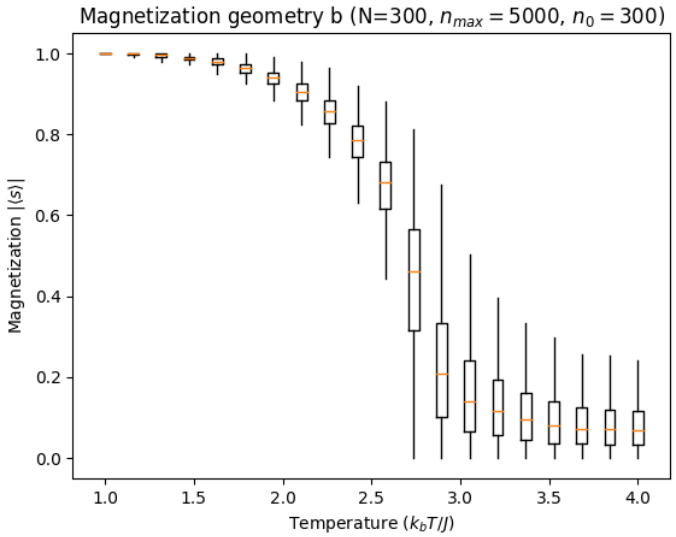


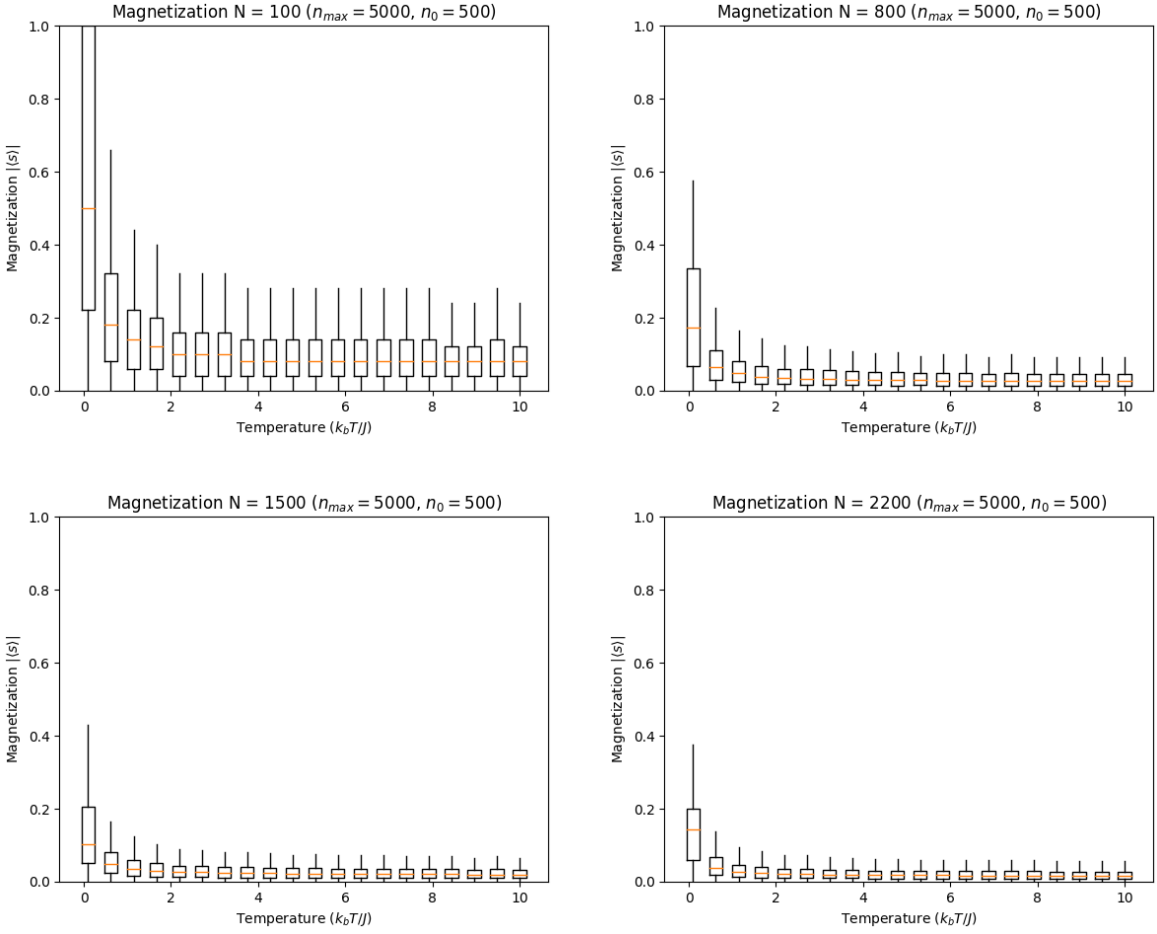

Figure 6: Mean magnetization box plot as a function of temperature for geometry b. The graph was made with $N = 500, n_{max} = 5000, n_0 = 300$.

## Question 2

**Explore possible phase transition behavior of each system. In particular, try to assess if a critical temperature $T_c$ can be found for either of these two cases. Keep in mind that $T_c$ relates to the behavior in the thermodynamic limit, so, besides choosing a sufficiently long simulation time, you will need to extrapolate to infinite system size (i.e., $1/N \to 0$). Hint: Try plotting the absolute value of average magnetization $|m|$ vs. $T$ for various $N$ and visually inspect the plots. Optionally, you can even try to automatize the identification of $T_c$ for each finite system and then plot $T_c vs. 1/N$, to obtain a finite-size scaling. Try to interpret your findings w.r.t. the value of $T_c$ in the thermodynamic limit. 5pt**

### Geometry a)

As mentioned in the hint, we will plot the absolute value of average magnetization $|m|$ vs. $T$ for various values of $N$ and inspect the plots visually to find if there is a critical temperature and where is it. We did that for 8 values of $N$ ranging from 100 to 5000 and the results are shown below.



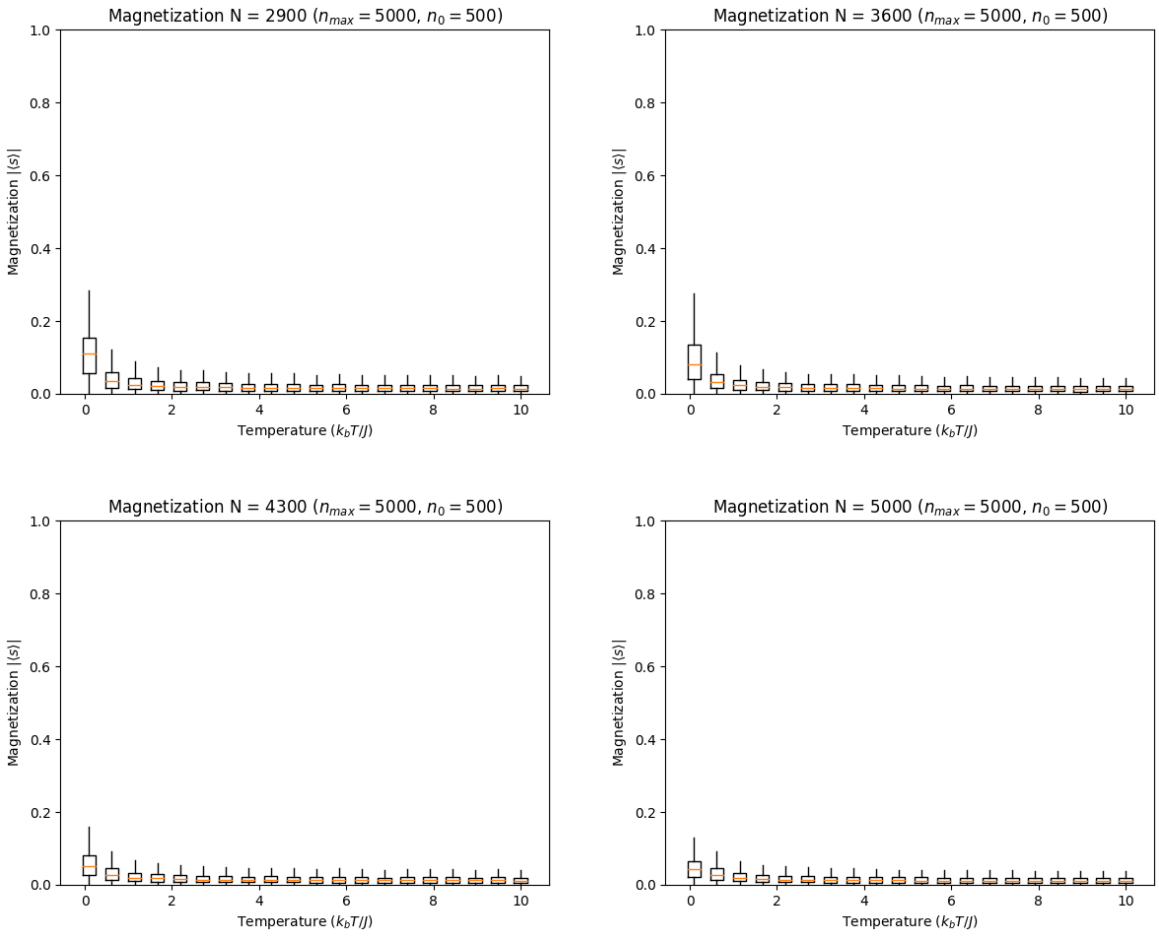



Figure 7: Mean magnetization box plots as a function of temperature for many different values of $N$ ranging from 100 to 5000.

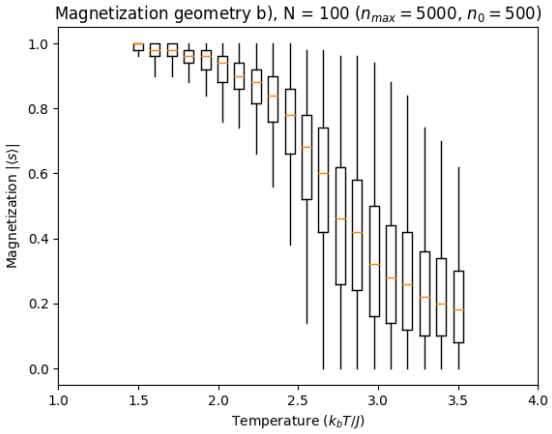
The first few plots show a rather high value of magnetization at low temperatures, that decreases quickly for higher temperatures. However, as we make $N$ bigger, this effect disappears and the magnetization is always low, even at small temperatures.

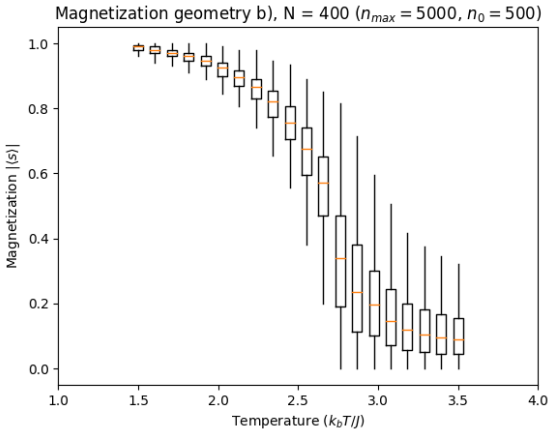
The need of a high $N$ is explained in the answer to question 3 and basically follows from the fact that even at low temperatures, there is a high enough $N$ such that the energy needed to create a domain wall is smaller than the entropy generated by said wall. Therefore, generating a domain wall is more favorable to reduce $F = E - TS$ than having all the spins aligned.

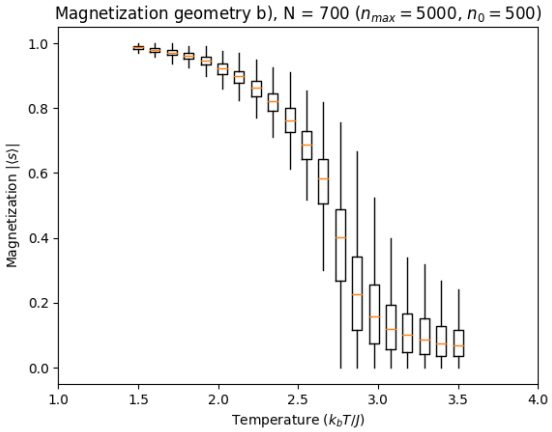
This shows that there is no phase transition, since the system is always on the disordered state (at least for high enough $N$). This coincides with what we saw in class, where we showed that the $1D$ ising model has no phase transition. At most, we could say that there is a phase transition at $T_c = 0$, since at that point all spins would align, the magnetization density would be equal to 1 and there wouldn't be thermal fluctuations. We can't really simulate the $T_c = 0$ point, but the closeness to the critical point explains why we have trouble converging and big fluctuations for values of $k_BT/J$ near 0.

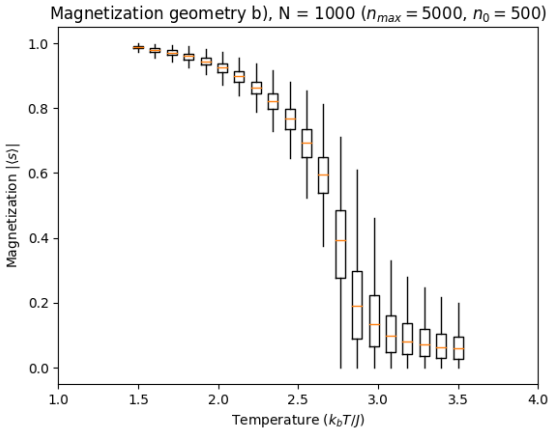
### Geometry b

Now we do the same procedure but for geometry b, which has on average two additional random links per spin. As before, we will plot the absolute value of average magnetization $|m|$ vs. $T$ for various values of $N$ and inspect the plots visually to find if there is a critical temperature and where is it. We did that for 7 values of $N$ ranging from 100 to 1900 and the results are shown below.



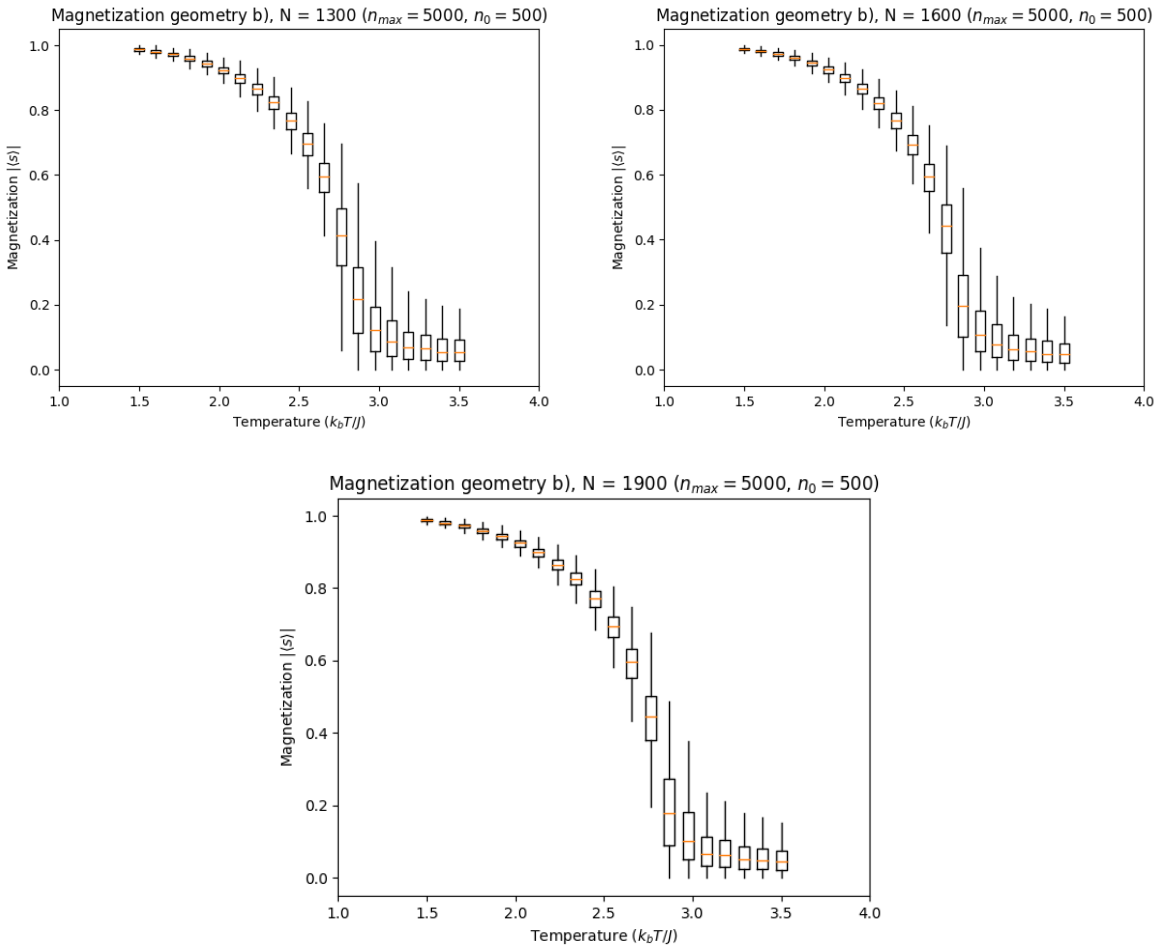



Figure 8: Mean magnetization box plots in geometry b as a function of temperature for different values of $N$ ranging from 100 to 1900.

In this case, there is a clear jump between an ordered state at low temperatures and the disordered state at higher temperatures. In opposition to the case of geometry a), this jump is clear at low values of $N$ and gets even clearer as $N$ grows higher, instead of disappearing as in geometry a).

This behaviour can be explained by the fact that the introduced random connections give the possibility of having long range interactions. Consider a domain of the array in which all spins are aligned together. In the case of geometry a), this domain only interacts with two other spins (the ones next to the extreme points of the domain) and the size of the domain is not important to this interaction, only the spins at the extreme points count. This is in big contrast to the case of geometry b), where this domain would have interactions with many other spins all over the array, and the amount of interactions grows as the size of the domain grows. Therefore, in geometry b), a domain can easily spread to the rest of the chain (as long as the temperature is low enough so that there are no significant thermal fluctuations). Meanwhile, in geometry a), a domain can't spread as easily.

The graphs show that there is a phase transition between the ordered and disordered

state and we can visually inspect that it happens at around $k_B T_c/J = 2.7$. And although the phase transition looks clearer as we take higher values of $N$, the value $T_c$ does not seem to change much.

We can try to obtain the actual value of the critical temperature simulated. To do it, we can calculate the magnetic susceptibility $\chi_T = \dfrac{1}{k_B T}(\langle m^2 \rangle - \langle m \rangle^2)$, which we know that diverges at $T_c$. Therefore, for each value of $N$, I calculated $\chi_T(T)$ this way and found the value of $T$ in which it takes the highest value. The result for different values of $N$ didn't change and in all of them I got $\boxed{k_B T_c/J = 2.76}$. Of course this depends on the array of values of $T$ I simulated. I chose an array from 1.5 to 3.5 with 25 values, and always got that the maximum of $\chi_T$ happened at the point with $k_B T_c/J = 2.76$.

## Question 3

**Extra Credit: In the case of Fig. 1a, try to support your reasoning about $T_c$ by discussing the introduction of a domain wall and the associated free energy change. How would this reasoning change if you modified Fig. 1a so that each sites i has two further links to $i-2$ and $i+2$? 2pt**

Suppose we have a 1D array of $N$ spins at temperature $T$. We will consider two states of this system:

1. Consider the case where all spins are aligned up. The energy of this state is $E_1 = -J\sum_{\langle ij\rangle} s_i s_j = -J\sum_{\langle ij\rangle} 1 = -NJ$ (since $N$ is the total number of links between spins). On the other hand, there is only one way of having all spins aligned up, so the entropy is $S_1 = k_B \ln(1) = 0$. Therefore, the free energy is:

$$F_1 = E_1 - TS_1 = -NJ$$

2. Now consider the case in which we have many spins aligned up, until some domain wall where the rest of spins are aligned down. In this case, $N-1$ of the links contribute an energy of $-J$, while the one connecting the two domains contributes an energy of $J$, to give us a total energy of $E_2 = -NJ + 2J$. On the other hand, there are $N$ total ways of setting up this state (the $N$ choices of where to put the domain wall), so that the entropy is $S_2 = k_B \ln N$. Therefore:

$$F_2 = E_2 - TS_2 = -NJ + 2J - k_B T \ln N$$

Then, the difference in free energy between states 2 and 1 is:

$$\Delta F = F_2 - F_1 = 2J - k_B T \ln N$$

We can notice that if $N$ is big enough (bigger than $e^{2J/k_B T}$), then $\Delta F$ is negative, showing that the second state has a lower free energy than the first. This means that the system would favor the second state over the first one, leading to the formation of a domain wall.

In conclusion, for large enough $N$, the system won't align into an ordered phase no matter how small we make the temperature, and it will always be preferable to create domain walls. This explains why we see no ordered phase and therefore no phase transition for the 1D Ising model (except at $T = 0$, where $\Delta F = \Delta E$ and the system would reach the ordered state).

Now, for the case of interactions with $i-2$ and $i+2$, now the energy cost between states 1 and 2 mentioned earlier is no longer $2J$, but becomes $6J$ (since now a total of 3 links are being changed between one state and the other). Therefore, the change in free energy becomes:

$$\Delta F = F_2 - F_1 = 6J - k_B T \ln N$$

Just as before, for big enough $N$ (bigger than $e^{6J/k_B T}$), $\Delta F$ would be negative. Therefore, the system still favors the creation of a domain wall rather than having all the spins aligned. However, now the minimum value of $N$ is much higher than before, since the exponent changed from $2J/k_B T$ to $6J/k_B T$. Again, there is no phase transition, but now we would need much higher values of $N$ to really see the lack of a phase transition in a simulation.

Finally, I believe that the reason we still see no phase transition in this case is that the interaction that a domain can have with the rest of the system is still very small. Concretely, no matter the size of our domain, the amount of interactions it has with the rest of the system is 4 (with the two nearest neighbors at each extreme point of the domain). That is the reason why we see no phase transitions.

In contrast, for the geometry b) studied in the other questions of this assignment, the situation is very different. In that case, the number of interactions that a domain has with the rest of its environment is very big, since each spin in the domain has two additional random interactions (that may be connected to the outside of the domain). Notably, the amount of interactions of a domain with the rest of the system now grows bigger as the domain gets bigger. This means that a domain can spread easier, leading to the possibility of aligning all the spins in one direction and therefore creating an ordered phase.