Complex Physics
Mid Term Exam1

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Contents

1 Question1

First, I initialize the lattice and set the model parameters. The exchange coefficient is set as $J = 1$. To simplify the problem, in this report, the temperature T is actually interpreted as $k_B T$, where k_B is the Boltzmann constant. The lattice size is set to 5000, which approaches the thermodynamic limit. Additionally, there is no external magnetic field, so the Hamiltonian is given by:

$$H = -\sum_{\langle i,j \rangle} s_i s_j$$

where s_i and s_j represent the spins of neighboring sites, and the summation is taken over two nearest neighbors(for model1a) or four neighbors (for model1b).

Next, Monte Carlo sampling is performed, using the stability of the average magnetization as a reference indicator to determine n_0 (the warm-up stage). In this program, n_0 is set to 1,000, although our simulation results (see the accompanying notebook) indicate that such a large value may not be necessary.The maximum number of iterations $n_{\max}$ is set to 100,000. As shown below, discard the first n_0 data points when calculating the average spin.

```
    # Compute the average spin after transient (for n > n0)
    if n_steps > n0:
    return np.mean(magnetization_list[n0:])  # Compute after n0 steps
```

1.1 1a Model

Core Procedure of Metropolis

```
    def metropolis_step(lattice, J, T):
    N = lattice.size
    for i in range(N):
    # Randomly select a site
    site = np.random.randint(0, N)

    # Calculate energy difference
    delta_E = 2 * J * lattice[site] * (lattice[(site - 1) % N] + lattice[(
   site + 1) % N])

    # Metropolis algorithm: accept or reject the spin flip
    if delta_E < 0 or np.random.rand() < np.exp(-delta_E / T):
    lattice[site] = -lattice[site]

    return lattice
```

When attempting to flip a spin at a randomly selected site, say site i, we need to calculate the energy difference ΔE before and after the spin flip. For this 1D Ising model,

each spin interacts with its two nearest neighbors, i.e., the spin to its left s_{i-1} and the spin to its right s_{i+1}.

For a given spin s_i, the interaction energy with its neighbors before the flip is:

$$E_{\text{before}} = -J \cdot s_i \cdot (s_{i-1} + s_{i+1})$$

After flipping the spin s_i to $-s_i$, the interaction energy becomes:

$$E_{\text{after}} = -J \cdot (-s_i) \cdot (s_{i-1} + s_{i+1})$$

The energy difference ΔE is the difference between these two energies:

$$\Delta E = E_{\text{after}} - E_{\text{before}} = -J \cdot (-s_i) \cdot (s_{i-1} + s_{i+1}) - (-J \cdot s_i \cdot (s_{i-1} + s_{i+1}))$$

Simplifying:

$$\Delta E = 2J s_i \, (s_{i-1} + s_{i+1})$$

This is the formula used in the code to calculate the energy difference when attempting to flip the spin at site i.

Simulation Results

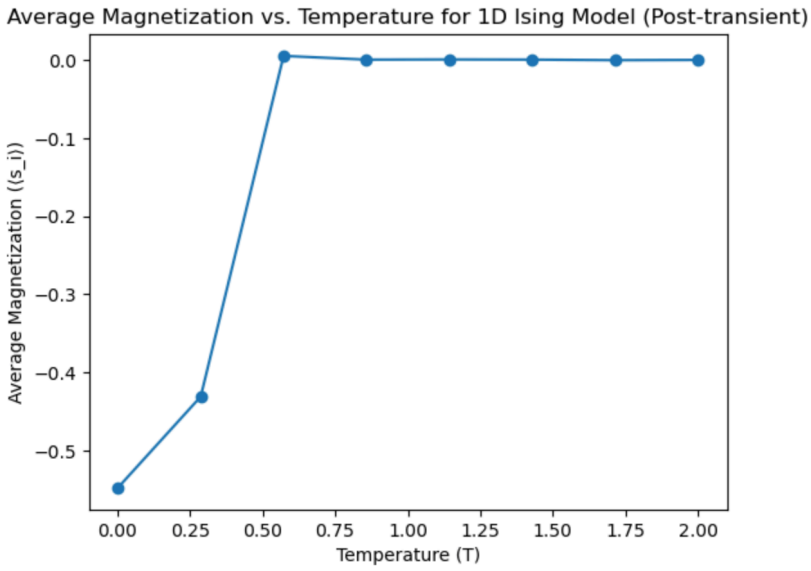

Figure 1: N=5000,1D Ising Model

The figure1 shows the average magnetization $\langle s_i \rangle$ as a function of temperature T for the 1D Ising model .In the plot, we observe that there is a small region before $T = 0.5$,where the system retains some non-zero magnetization, This is due to the finite system size $N = 5000$, which, while large, does not reach the thermodynamic limit (infinite size).

However,as the temperature slightly increases, the magnetization quickly approaches zero. This behavior indicates that thermal fluctuations dominate, leading to a disordered state where spins are randomly oriented.For temperatures above approximately $T = 0.5$, the magnetization remains close to zero, indicating that the system is in a disordered phase, with no net magnetization.

In fact, if I set the number of steps to 500,000 and the number of lattice sites to 50,000(approaching thermodynamic limit), we can observe from figure2 that even at very low temperatures, the average magnetization only shows a slight positive value. Then, as the temperature increases slightly, it quickly becomes zero. To some extent, this confirms the theoretical result for the 1D Ising model(infinite size): there is no true phase transition (or spontenous magnetization) at any finite temperature.

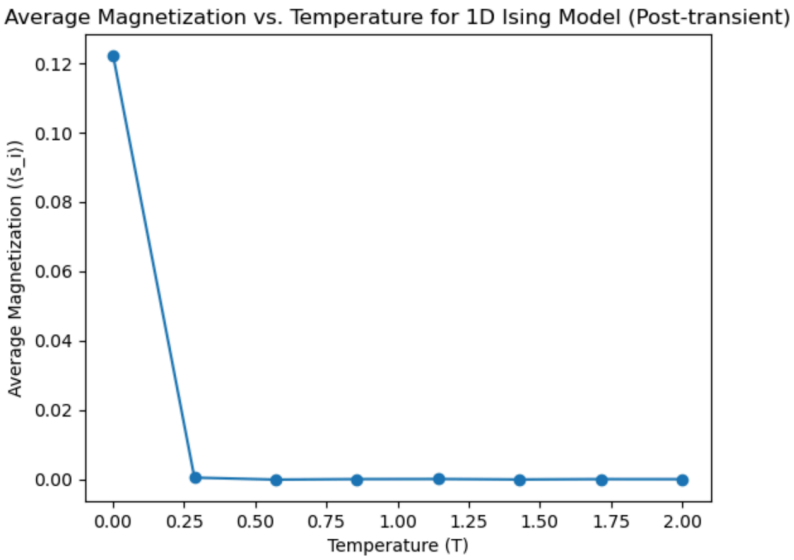

Figure 2: N=50000,1D Ising model

1.2 1b Model

Method

Given the specific requirements of this problem, I adopted the following strategy to determine neighboring nodes during initialization.

```
    # 2. Generate two random neighbors for each site
    @nb.njit
    def generate_random_neighbors(N):
    random_neighbors = np.zeros((N, 2), dtype=np.int64)  # Use NumPy array
    for i in range(N):
    neighbors = set()
    while len(neighbors) < 2:
```

```
    candidate = np.random.randint(0, N)
    # Exclude nearest neighbors and itself
    if candidate != (i - 1) % N and candidate != (i + 1) % N and candidate !
= i:
    neighbors.add(candidate)
    random_neighbors[i] = list(neighbors)
    return random_neighbors
```

Simultaneously update the corresponding Metropolis algorithm steps (with the additional energy changes brought by the random neighbors).

```
    # Calculate energy difference (left and right nearest neighbors)
    delta_E = 2 * J * lattice[site] * (lattice[(site - 1) % N] + lattice[(
site + 1) % N])

    # Calculate the energy difference for random neighbors
    for neighbor in random_neighbors[site]:
    delta_E += 2 * J * lattice[site] * lattice[neighbor]
```

Simulation Result

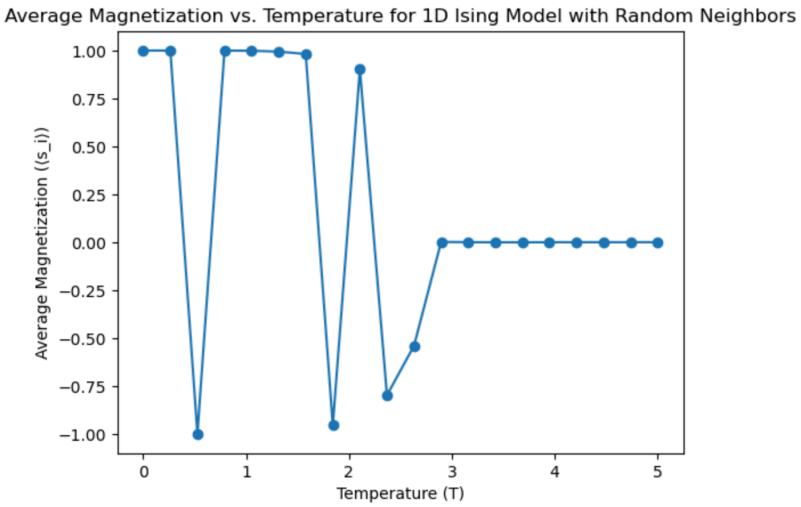

Figure 3: 1D with additional neighbors,N=5000

In 1D Ising models, spins only interact with their immediate neighbors, but with the addition of random neighbors, the system gains additional connections, making it somewhat resemble a two-dimensional system where spins interact with more neighbors.
In figure3, we also observe a critical temperature (around T≈2.7,after which the system reaches a disordered state, and the magnetization stabilizes around zero . However, before this critical temperature, the absolute value of the average spin magnetization of the Ising model system is always 1 (although sometimes it is 1 and sometimes -1), indicating that

before the critical temperature, one type of spin can dominate. Unlike the 1D Ising model, this critical temperature is not close to zero.This is indicative of a phase transition-like behavior, similar to what is observed in higher-dimensional Ising models.

2 Question2

I tried different values of N, transitioning from a finite grid size to an infinite size.

```
N_values = np.array([50,100,500,1000,5000,10000])
```

In order to better present the variation of average magnetization with temperature for different values of N, I adopted the following visualization approach: For each system size N, a set of vertical rectangular blocks (bars) is drawn. The height of each block represents the temperature, and the color of the block reflects the magnetization value at that temperature. A color mapping (using the Viridis color map) is employed to indicate the magnitude of the magnetization. The color gradient helps easily distinguish different magnetization values, with cooler colors representing lower magnetization and warmer colors representing higher magnetization.

2.1 1a Model

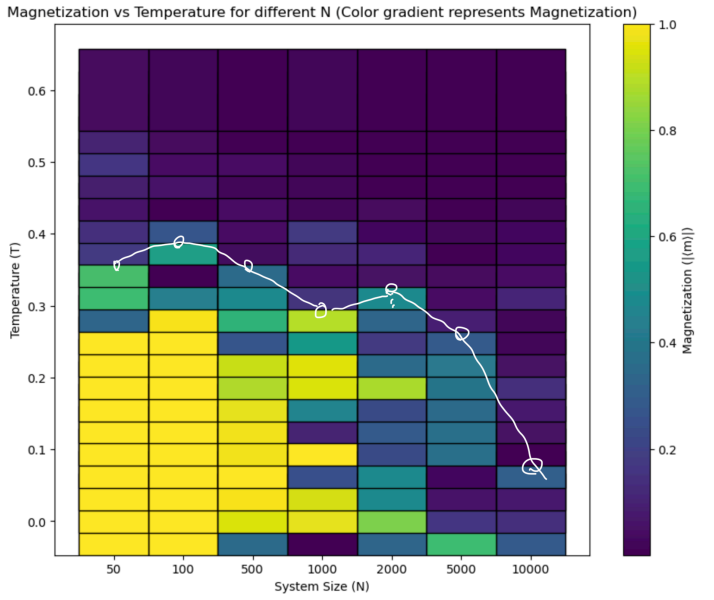

Figure 4: 1D Ising model |<s>| T for different N

In figure 4 it seems less difficult to identify the phase transition temperature for smaller N, while for larger N, it becomes more difficult to pinpoint the phase transition temperature(the colors gradually transition within the cooler color spectrum). I still manage to

mark a curve based on the color change, and from the overall trend of the curve, we can roughly judge that as N increases, the phase transition temperature gradually decreases. Furthermore, as discussed in Q1, when N becomes particularly large (e.g., $N = 50000$), even at very low temperatures, the average magnetization is low, and with only a slight increase in temperature, the average magnetization drops to zero. Therefore, we can conclude that for the model in 1a, as N increases, the critical temperature T_c decreases until it eventually reaches zero.
Based on the lecture notes, the exact solution of the one-dimensional Ising model, when $N \to \infty$, the average spin $\langle s_i \rangle$ is given by:

$$\langle s_i \rangle = \frac{\sinh(\beta h)}{\left[\sinh^2(\beta h) + e^{-4\beta J}\right]^{1/2}}$$

When $h \to 0$, for any fixed choice of $J > 0$ and $\beta > 0$, $\langle s_i \rangle$ tends to 0. This means that for an infinitely large system, the one-dimensional Ising model does not exhibit any spontaneous magnetization. However, when N is not infinite, we cannot conclude that the critical temperature is zero. (Further analysis will be done in extra question using domain wall and free energy)

2.2 1b Model

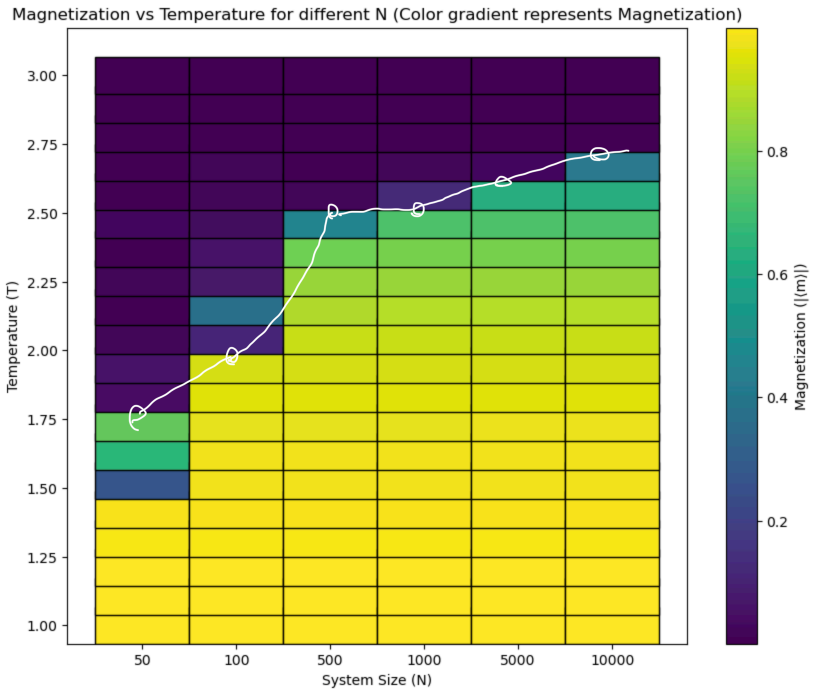

Figure 5: 1D Ising model with additional random neighbors |<s>|-T relation for different N

In figure 5, the situation is different. It is easy to identify a critical phase transition temperature T_c for most values of N, as there is a sudden shift from warm to cool tones. Moreover, from the graph, we can observe that initially, as N increases, the phase transition temperature also increases. Then, when N becomes very large, the increase in the phase transition temperature becomes less significant and the phase transition temperature become stable.

In fact, as mentioned in Q1, this one-dimensional Ising model with additional random neighbors resembles a two-dimensional Ising model. The range that a node can influence might be even broader than in two dimensions, because it can randomly connect to a distant node. This leads to stronger connections between the nodes compared to a simple one-dimensional Ising model.

Based on Onsager's exact solution for the two-dimensional Ising model, when the system approaches the thermodynamic limit, i.e., when the system size tends to infinity, the critical temperature approaches a fixed value, approximately $k_B * T_c/J \approx 2.269$. This value represents the critical temperature in an infinite system for the 2D Ising model.Now, let's compare this with the data from the figure 5. When the system size N is quite large (for example, around 10,000 or more), the critical temperature appears to be close to $T \approx 2.5$.

3 Extra Question:Domain Wall, Free Energy and Finite Scaling

First, recall the formula for free energy: $F = U - TS$, where U is the internal energy of the system, T is the temperature (including the Boltzmann constant), and S is the entropy. A system always tends to reach equilibrium by moving in the direction that reduces its free energy.

3.1 1D Ising model

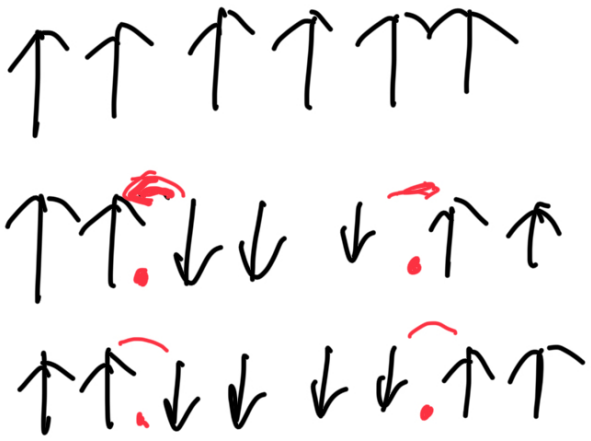

Figure 6: from top to bottom: one of the two microstates with a single spin domain one of N(N-1)equally probable micro states with two spin domains(different seperated spins n=3,or n=4,but same energy)

There are two possible microstates with a single spin domain, each with energy $-NJ$. The entropic contribution to the free energy is $-k_B T \ln 2$. Hence, the associated free energy for a single spin domain is

$$F_{1-\text{dom}} = -NJ - k_B T \ln 2,$$

To create two domains of oppositely aligned spins, two domain walls need to be inserted, with an energy cost of $4J$(which does not depend on the seperated spinsn). There are $N(N-1)$ equally probable microstates with two domain walls. The free energy for this case is:

$$F_{2-\text{dom}} = -NJ + 4J - k_B T \ln N(N-1).$$

The difference between the free energies is:

$$F_{2-\text{dom}} - F_{1-\text{dom}} \approx 4J - 2k_B T \ln N \quad \text{for large } N.$$

A single domain of aligned spins becomes unstable against thermal fluctuations if $F_{2-\text{dom}} < F_{1-\text{dom}}$, or equivalently if

$$\frac{2J}{k_B T} < \ln N.$$

Thus, at any finite temperature, it becomes energetically favorable to insert at least two domain walls(and thus average spin will tend towards zero) as $N \to \infty$ which again support the conclusion of the exact analytical solution of 1D Ising mode and our simulation results.

For two spin domains, the free energy difference is $4J - 2k_BT \ln N$, meaning larger N increases the entropy term, making the system more prone to thermal fluctuations that introduce domain walls and destabilize spin alignment. In contrast, for smaller N, the system requires a higher temperature to become prone to such fluctuations and domain wall formation. Therefore, the critical temperature scales as $T_c \sim \frac{2J}{k_B \ln N}$, decreasing as N increases and approaching zero when $N \to \infty$.This is consistent with the rough trend of the fitted line in figure 4.

3.2 1D Ising model with two additional next nearest neighbours

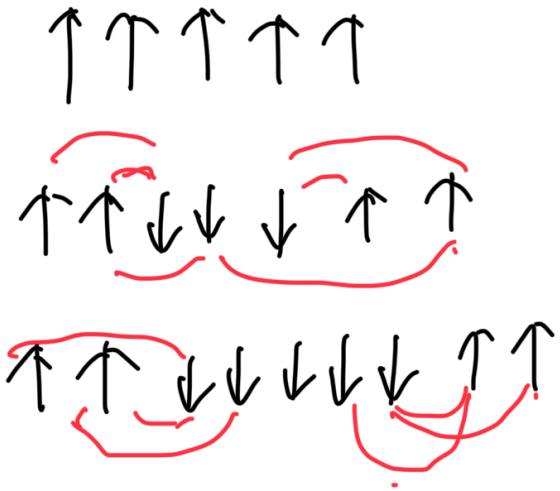

Figure 7: from top to bottom: one of the two microstates with a single spin domain
one of N(N-1)equally probable micro states with two spin domains(different seperated spins n=3,or n=5,but same energy

If a 1D Ising model includes two additional next-nearest neighbors at positions i-2 and i+2 as illustrated in figure 7, the energy required to insert two domain walls becomes 6*2=12J. Notably, similar to the case with only two neighbors, the energy required to insert two domain walls remains independent of the number of separated spins, n. From previous analyses, the critical temperature T_c is proportional to $\frac{2J}{k_B \ln N}$ in 1D Ising Model and should triple to $T_c \sim \frac{6J}{k_B \ln N}$ in this model. But the nature of the no-phase-transition 1D Ising model will not change. Furthermore, numerical simulation result depicted in figure 8 indicate that the overall critical temperature has indeed tripled compared to the previous case shown in figure 4, yet the trend of decreasing with increasing N persists.This result has confirmed our analysis.

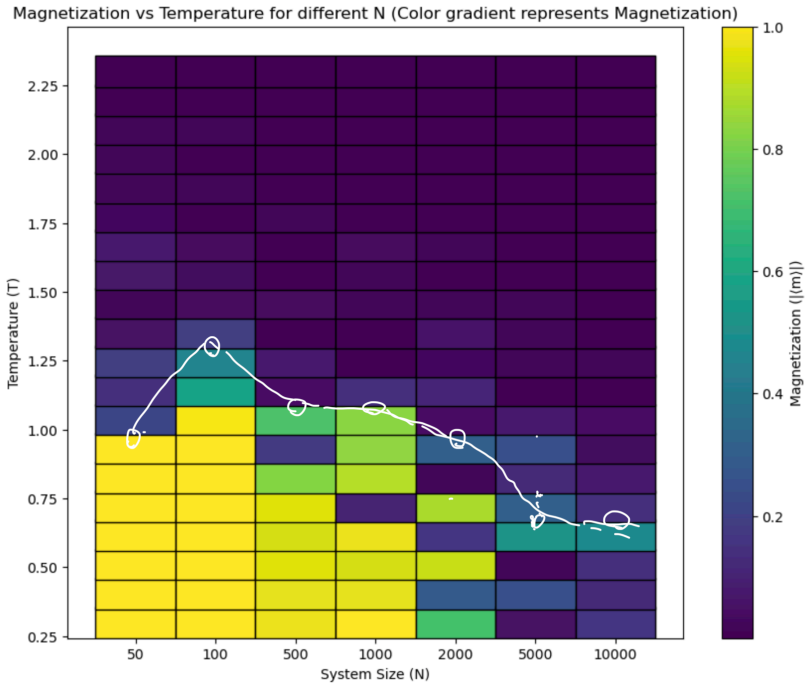

Figure 8: |<s>|-T relation for different N for 1D two additional next nearest neighbours

3.3 1D Ising model with two additional random neighbours

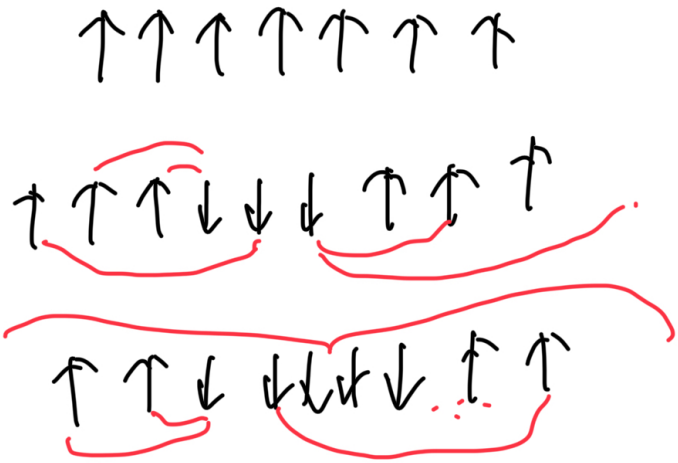

Figure 9: "From top to bottom: one of the two microstates with a single spin domain; one probable microstate with two spin domains (with different separated spins, $n = 3$ or $n = 5$, and varying energy,

In this model with two domains and 2 additional random neighbors, the energy required to create a domain wall depends on the number of spins it separates, represented by n because each spin in the separated group may influence another random distant spin
As discussed in Q1 and Q2, we can analyze this situation using ideas similar to the two-dimensional Ising model. For a compact, two-dimensional shape, the boundary scales with the square root of the area. So for two domains that are roughly the same size, the length of the domain wall generally scales as $\sqrt{N}$, where N is the total number of spins in the system.Therefore, the energy difference from adding walls to become two domains is approximately $2J\sqrt{N}$.

To estimate the upper bound of entropy, we think of the boundary of the domain wall as a self-avoiding walk of length n on a square grid. For each step, there are up to three possible directions to move without retracing the path, resulting in a maximum of 3^n possible configurations. Additionally, there are N different locations where the center of mass of the wall could start, suggesting fewer than $N \times 3^n$ total possible configurations.

This leads to the following inequality for the difference in free energy between the two-domain and one-domain cases:

$$F_{\text{2-dom}} - F_{\text{1-dom}} > 2J\sqrt{N} - k_B T \ln(N \times 3^{\sqrt{N}}).$$

For the two-domain case to be more favorable, the following inequality must hold, giving the lower bound for the critical temperature:

$$k_B T > \frac{2J}{\ln 3 + \frac{\ln N}{\sqrt{N}}}.$$

In the thermodynamic limit, as $N \to \infty$, we find a lower bound for the critical temperature:

$$k_B T_c > \frac{2J}{\ln 3} \approx 1.820.$$

As N increases, $\frac{\ln N}{\sqrt{N}}$ becomes smaller, raising the lower bound for T_c. This suggests that the critical temperature increases with N, eventually leveling off. This could explain the trend of our earlier simulation results (as seen in figure 5).

Now, let's compare this with a one-dimensional Ising model. In the 1D case, the energy required to create a domain wall does not depend on the size of the domains, so the entropy gain becomes much more significant at any non-zero temperature, meaning there is no spontaneous magnetization for $T > 0$. However, in the 2D Ising model (and this 1D Ising model with additional random neighbors), the energy needed to create a domain wall increases with its length, making energy more important than entropy at low temperatures. This is why the 2D Ising model and the 1D Ising model with random neighbours can exhibit spontaneous magnetization when $T < T_c$.

Appendix

References:

Kim Christensen, Nicholas R. Moloney. *Complexity and Criticality* (English reprint).