Physics 140A Final Project: Ising Model and Block Spin Transformations

Girish Krishnan,* Blase Fencil,† and Zachary Sherman‡
University of California San Diego

(Group A: Ising Model: Yes, willing to present and Yes, you can post on Canvas.)

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I. Motivation

Imagine a ferromagnetic material like iron, made up of many tiny magnetic regions called spins, each of which can point up or down. The Ising model simplifies the study of such materials by placing these spins on a grid, like a chessboard, where each spin interacts only with its nearest neighbors. If neighboring spins point in the same direction, the system is more stable, while opposite directions make it less stable. This interaction determines the overall magnetization of the material.

By focusing on these simple interactions, the Ising model helps us understand complex phenomena such as phase transitions, where a material changes from non-magnetic to magnetic as it cools. Despite its simplicity, the Ising model captures the essential physics, providing valuable insights into how large-scale behaviors emerge from local interactions. This makes it an useful tool for learning about the principles underlying magnetism and other related phenomena in physics.

II. Background

To explain Ising models, we use graphs. A graph G is an ordered pair of a set of vertices V and a set of edges E: $G = (V, E)$. Edges are unordered pairs of vertices. For example, if $V = \{1, 2, 3, 4, 5, 6, 7\}$, the edges E could be $\{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 5\}, \{5, 1\}, \{6, 7\}\}$, indicating connections between vertices.

Graphs model various systems like social networks, transportation, and crystalline lattices. The Ising model is part of n-vector models using graphs to represent materials. The first few models are:

- $n = 0$: self-avoiding walk
- $n = 1$: Ising model
- $n = 2$: XY model
- $n = 3$: Heisenberg model

In the Ising model, edges indicate neighboring vertices, informing how many states to sum over to find the Hamiltonian for each spin-site/vertex. The Hamiltonian is given by:

$$-J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_j \sigma_j$$

where h is the external magnetic field, σ_i and σ_j denote the spin states of adjacent vertices, and J is the spin-spin interaction. If J is positive, the material is ferromagnetic; if J is negative, it is antiferromagnetic; if $J = 0$, the spins are non-interacting.

To simulate the time evolution of spin states in the Ising model, we use the Metropolis-Hastings Monte Carlo algorithm. This algorithm efficiently explores the system's configuration space by probabilistically accepting or rejecting proposed changes to the spin states based on the change in energy.

The process involves:

1. Start with an initial lattice configuration.
2. Randomly select a spin and propose flipping its state.
3. Calculate the change in energy due to the flip.
4. Accept or reject the flip based on a probability threshold.

The selection probability ensures the system is ergodic, meaning it will visit all possible states.

III. Problem

We selected two problems from Schroeder [1]: Problem 8.26 and Problem 8.32.

Problem 8.26: Implement the Ising program and run it for various lattice sizes and temperatures.

(a) Run the program with a 20x20 lattice at T = $10, 5, 4, 3$, and 2.5, for at least 100 iterations per dipole per run. At each temperature make a rough estimate of the size of the largest clusters.

(b) Repeat Part A for a 40x40 lattice. Are the cluster sizes any different? Explain.

(c) Run the program with a 20x20 lattice at T = $2, 1.5$, and 1. Estimate the average magnetization (as a percentage of total saturation) at each of these temperatures.

(d) Run the program with a 10x10 lattice at T = 2.5. Watch it run for 100,000 iterations or so. Describe and explain the behavior.

(e) Use successively larger lattices to estimate the typical cluster size at temperatures from 2.5 down to 2.27 (the critical temperature). The closer you are to the critical temperature, the larger a lattice you'll need and the longer the program will have to run.

* gikrishnan@ucsd.edu
† bfencil@ucsd.edu
‡ zsherman@ucsd.edu

Problem 8.32: Imagine taking a two-dimensional Ising lattice and dividing the sites into 3x3 "blocks", as shown in in Figure 8.11. In a **block spin transformation**, we replace the nine dipoles in each block with a single dipole, whose state is determined by "majority rule". This transformation is one version of a **re-normalization group transformation**, a powerful technique for studying the behavior of systems near their critical points.

(a) Add a routine to the Ising program to apply a block spin transformation to the current state of the lattice, drawing the transformed lattice alongside the original. Have the program execute this routine periodically, so you can observe the evolution of both lattices.

(b) Run your modified program with a 90x90 original lattice, at a variety of temperatures. After the system has equilibrated to a "typical" state at each temperature, compare the transformed lattice to a typical 30x30 piece of the original lattice. The transformed lattice resembles an original lattice at a **different** temperature. When is the transformed temperature greater than the original temperature, and when is it less?

(c) Imagine starting with a very large lattice and applying many block spin transformations in succession, each time taking the system to a new effective temperature. Argue that, no matter what the original temperature, this procedure will eventually take you to one of three **fixed points**: zero, infinity, or the critical temperature. For what initial temperatures will you end up at each fixed point?

IV. Solution

All the code containing our solutions can be found in our GitHub repository [2], which contains detailed Jupyter notebooks with code followed by explanations.

A. Problem 8.26

We implement the Ising model using the structure shown in Algorithm 1. In this code, we perform Markov Chain Monte Carlo simulations using the Metropolis-Hastings algorithm. We perform the Monte Carlo simulations for each time step by calculating the energy difference to flip the spin at each site. If the energy difference is less than or equal to 1, or if a randomly generated number is less than $\alpha = \exp(-\text{energy\_difference}/\text{temperature})$ (Metropolis-Hastings algorithm), we flip the spin at that site.

1. *Part (a)*

Part (a) asks us to run the Ising model program at various temperatures. Our outputs can be seen in Figure 1. Some of the graphs demonstrate more "ordered" clustering behavior, where certain regions are homogeneous in their spin. We notice less ordered clustering behavior for larger temperature values, with more ordered behavior as we approach T=2.5 which is near the critical temperature.

Algorithm 1 Ising Model Simulation

```
size ← lattice size
T ← temperature
steps ← number of steps
B ← external magnetic field
σ ← random(−1, 1, size, size)
for each time step from 1 to steps do
    for i ∈ [0, size) do
        for j ∈ [0, size) do
            spin ← σ[i, j]
            neighbor_sum ← σ[(i + 1)%size, j]
                           +σ[i, (j + 1)%size]
                           +σ[(i − 1)%size, j]
                           +σ[i, (j − 1)%size]
            ΔE ← 2 · spin · (neighbor_sum + B)
            α ← exp(−ΔE/T)
            if ΔE ≤ 0 or random(0, 1) < α then
                σ[i, j] ← −spin
            end if
        end for
    end for
end for
```

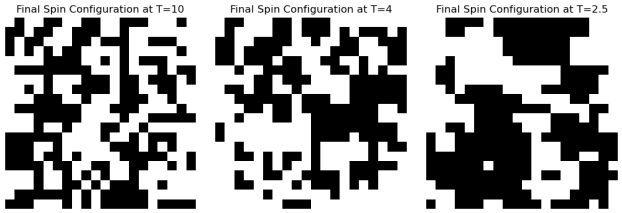

FIG. 1. Final result of 20x20 lattice at T = 10, 4, and 2.5

We can additionally measure the largest cluster size at each temperature as requested in part (a). We estimate the largest cluster size in our code counting the number of connected sites of the same spin orientation. The definition of "cluster" in our code is a group of adjacent dipoles with the same spin. We then plot the largest cluster size at the end of the Ising simulation vs. temperature in Figure 2.

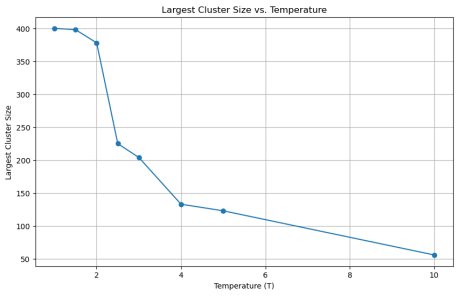

FIG. 2. Largest cluster size in final result of 20x20 lattice vs temperature

FIG. 3. Final result of 40x40 lattice at T = 10, 4, and 2.5

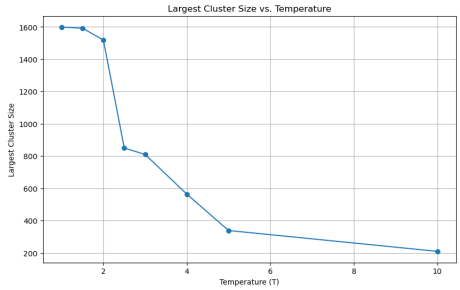

FIG. 4. Largest cluster size in final result of 40x40 lattice vs temperature

2. *Part (b)*

In part (b), we repeat part (a) with a 40x40 lattice. We see the results of final results of the simulation for the 40x40 lattice in Figure 3. We again notice the same trend in disorder increasing at larger values.

We again graph the largest cluster size at the end of the Ising simulation vs. temperature for the 40x40 lattice in Figure 4 and observe similar results to those in Figure 2 for the 20x20 lattice. We can see that the size of the largest cluster increases with decreasing temperature. This is because at lower temperatures, the dipoles are more likely to align with their neighbors, leading to larger clusters of aligned dipoles. The clusters are significantly larger than with a 20x20 lattice, which makes sense due to the larger size of the Ising lattice.

3. *Part (c)*

In part (c), we analyze values of T below the critical temperature, displayed in Figure 5. Again, we notice clustering behavior in agreement with our graph in Figure 2.

For the graphs in Figure 5, we observe a very high magnitude of average magnetization. In python, we calculated the average magnetization at the different temperatures, shown in Table I.

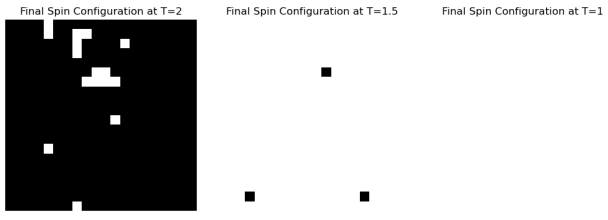

FIG. 5. Final result of 20x20 lattice at T = 2, 1.5 and 1

Temperature (T)	Average Magnetization (M) (%)
2.0	91.07
1.5	-98.62
1.0	-99.74

TABLE I. Average magnetization as a percentage of total saturation at different temperatures.

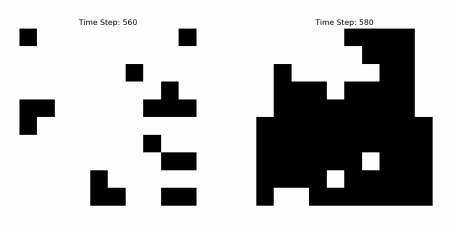

FIG. 6. Time steps 560 and 580 of 10x10 lattice at T = 2.5

4. *Part (d)*

In part (d), we observe the simulation as a GIF scanning across 100000 time iterations. At T = 2.5 and a 10x10 lattice, we can see that the simulation spends a lot of its time in those states where one color is more dominant over the other color. We notice that the 10x10 lattice does not converge to a final state even after many steps. Furthermore, the dominant color reverses quite often. We can see one of these quick reverses displayed in Figure 6. If you tried this at even lower temperatures, the reversal effect would be more prominent, but the time interval between reversals would be longer. This is mainly due to the lattice being very small, only 10x10.

5. *Part (e)*

In part (e), we analyze the typical cluster sizes at temperatures at and slightly above the critical temperature, from around 2.27 to 2.5. As with Figure 2 and Figure 4, we graph our analysis of largest cluster size vs temperature for a various lattice sizes. From our plots in Figure 7, we notice that the cluster size increases as the temperature approaches the critical temperature, and the cluster size is limited by the size of the lattice. It is plausible that the cluster size goes to infinity with lattice size as the temperature approaches the critical temperature, as the system becomes more ordered and the clusters become larger, as we see our graph rises very sharply when approaching critical temperature for the larger lattice sizes.

For further analysis, we recreate a result similar to Fig. 8.10 in Schroeder [1]. In Figure 8, a 400x400 lattice at T = 2.27 is run for 100,000 iterations. We note that for this simulation, we ended with approximately -33% average magnetization and the largest cluster having a size of approximately 121000.

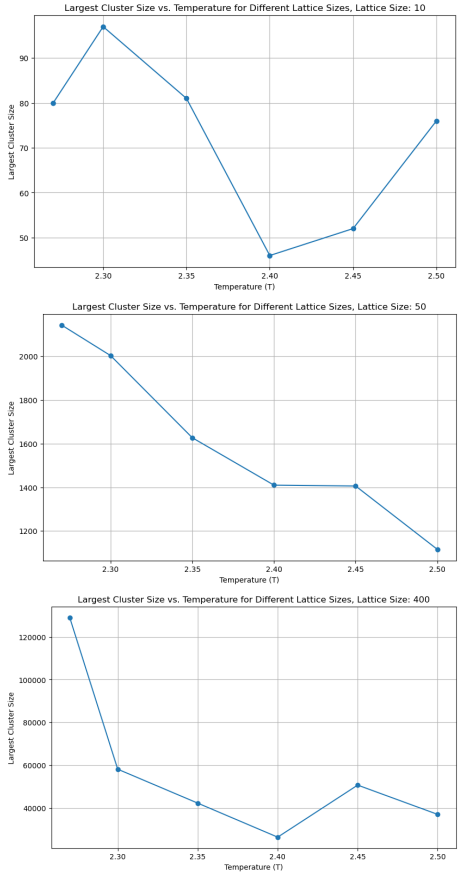

FIG. 7. Analysis of Cluster Size vs Temperature for different lattice sizes 10,50, and 400

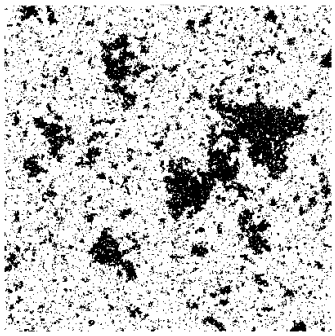

FIG. 8. 400x400 lattice at critical temperature T=2.27 after 100000 iterations

B. Problem 8.32

1. *Part (a)*

The **block spin transformation** reduces the original lattice's width to one-third by considering 3×3 blocks. The new spin state of each block is determined by the majority rule:

- If more than half of the original dipoles in the block point up, the new dipole points up.

FIG. 9. Final result of 90x90 lattice at T = 2.5 after 100000 steps, alongside its block-transformed lattice, which is 30x30.

- If more than half of the original dipoles in the block point down, the new dipole points down.

Mathematically, given a lattice σ of size $N \times N$ and a block size $b = 3$, the new lattice σ' of size $\frac{N}{3} \times \frac{N}{3}$ is defined as:

$$\sigma'_{i,j} = \begin{cases} 1 & \text{if } \sum_{k=0}^{2} \sum_{l=0}^{2} \sigma_{3i+k,3j+l} > 0 \\ -1 & \text{otherwise} \end{cases}$$

where i and j are the indices of the blocks in the new lattice.

The following algorithm outlines the block spin transformation procedure:

Algorithm 2 Block Spin Transformation

$N \leftarrow$ lattice size
$b \leftarrow 3$
$new\_size \leftarrow N//b$
$\sigma' \leftarrow$ zero matrix of size $new\_size \times new\_size$
for $i \leftarrow 0$ to $new\_size - 1$ **do**
  for $j \leftarrow 0$ to $new\_size - 1$ **do**
    $block \leftarrow \sigma[i \cdot b : (i+1) \cdot b, j \cdot b : (j+1) \cdot b]$
    if $\sum block > 0$ **then**
      $\sigma'[i, j] \leftarrow 1$
    else
      $\sigma'[i, j] \leftarrow -1$
    end if
  end for
end for
return σ'

The transformation was applied to a simulated Ising lattice, and the simulation was run over several steps to produce a video showing the evolution of the original and the transformed lattice over the steps. A visualization showing the original and transformed lattice at T = 2.5 for an original lattice of size 90 and 100000 steps is shown in

2. *Part (b)*

We ran simulations on a 90×90 Ising lattice at various temperatures to investigate the effects of the block spin transformation. After equilibrating the system at each temperature, we applied the block spin transformation and compared the results to a typical 30×30 piece of the original lattice.

The temperatures used were: 1, 2, 2.27, 2.5, 3, 3.25,

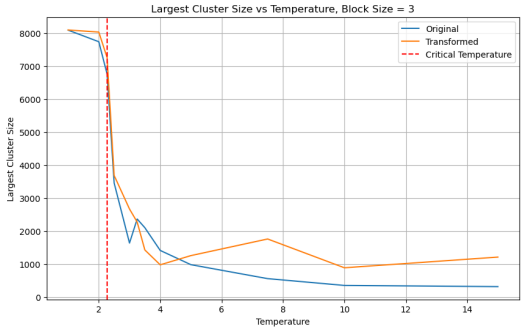

FIG. 10. A plot showing the size of the largest cluster against the temperature for the original and transformed lattices.

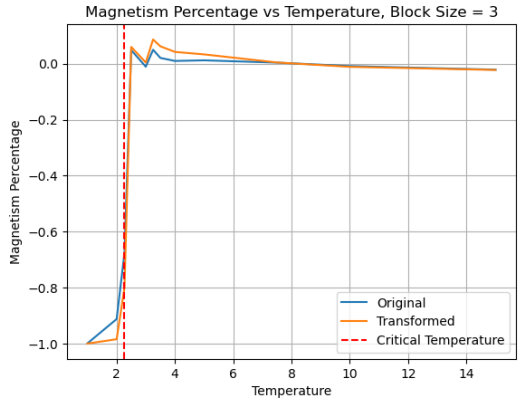

FIG. 11. A plot showing the net magnetization against the temperature for the original and transformed lattices.

3.5, 4, 5, 7.5, 10, and 15, with 50000 simulation steps per temperature. We computed the magnetism percentage and the largest cluster size for both the original and transformed lattices. Figures 10 and 11 present this data.

The plots show a sharp change in magnetism percentage near the critical temperature. Below the critical temperature, the lattice approaches saturation, while above it, the magnetism percentage drops to zero due to random spin orientations. The transformed lattice shows higher magnetization below the critical temperature and behaves as if at a higher temperature above the critical temperature, displaying greater randomness. Additionally, the cluster size for the transformed lattice is larger than the original lattice below the critical temperature and approximately equal at the critical temperature. Above the critical temperature, the transformed lattice indicates greater randomness, suggesting an effectively higher temperature.

3. *Part (c)*

Consider an initial temperature T_0 and apply successive block spin transformations to the lattice. Each transformation maps the system to a new effective temperature, analyzed relative to the critical temperature T_c.

If $T_0 = T_c$, the system exhibits scale invariance, making the critical temperature a fixed point:

$$T_{n+1} = T_c \quad \text{if} \quad T_n = T_c$$

Thus, starting at T_c, the system remains at T_c.

If $T_0 > T_c$, each block spin transformation increases the system's temperature, as block averaging above T_c increases disorder:

$$T_{n+1} > T_n \quad \text{for} \quad T_n > T_c$$

Consequently, the temperature moves towards infinity. Thus, for $T_0 > T_c$, the system converges to infinity.

If $T_0 < T_c$, each block spin transformation decreases the system's temperature, as block averaging below T_c increases order:

$$T_{n+1} < T_n \quad \text{for} \quad T_n < T_c$$

Hence, the temperature moves towards zero. Therefore, for $T_0 < T_c$, the system converges to zero.

In summary, an Ising model lattice converges to one of three fixed points: zero, infinity, or the critical temperature. The final fixed point depends on the initial temperature relative to T_c. Starting at T_c keeps the system at T_c, starting above T_c drives it towards infinity, and starting below T_c drives it towards zero.

[1] D. V. Schroeder, *Introduction to Thermal Physics* (Addison Wesley Longman, 1999).

[2] B. Fencil, G. Krishnan, and Z. Sherman, UCSD PHYS 140A Group A (Ising Model) GitHub (2024).