Computational Physics: Project 3
2D Ising Model

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1 Introduction

The statistics and collective phenomena of many systems across physics and elsewhere can be effectively described by the Ising model, such as brain activity [Schneidman *et al.*, 2006], social segregation [Schelling, 1971], and mechanical metamaterials [Plummer *et al.*, 2022]. The Ising model describes a collection of binary variables on a lattice. These variables are allowed to interact with their near neighbours, where the interaction switches between the two allowed values of the variables to decrease the system's overall energy. External noise, or thermal fluctuations, disturbs these switches. The result is that different structural phases emerge as a function of the fluctuations. For example, an ordered-like phase at low noise can be *scrambled* as the noise increases. Although originally proposed to study ferromagnetism, where the variables are up-down spins and the temperature plays the role of noise [Kardar, 2007], nowadays, it is well understood that such behavior across systems is a consequence of an underlying universality. Namely, all previously mentioned systems belong presumably to the same universality class. Here, we employ a Monte Carlo Markov Chain (MCMC) approach to compute classical physical features of the Ising model. We cluster spins based on the Swedsen-Wang scheme [Frenkel, 2023] and employ the Metropolis algorithm on the clusters. Our key result is a confirmation of the predicted phase transition in the magnetization of the system, where it is known that the system becomes magnetized at a critical temperature as the temperature is decreased. Finally, to validate our results, we show that we can recover analytical results of the system at zero magnetic field.

2 2D Ising Model of Ferromagnetism

Consider a square lattice with a spin variable σ_i on i^{th} lattice site. The variables are only allowed to take two values, $\sigma_i \in \{-1, +1\}$, where -1 means spin down and $+1$ spin up. The configuration state of the system is determined by fixing values to all $\{\sigma_i\}$ on the lattice. In the presence of an external magnetic field of magnitude h acting on all spins, the energy of the system is given by the Hamiltonian,

$$\mathcal{H} = -\sum_{i,j} \mathrm{J}_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i \tag{1}$$

where we consider a near-neighbour interaction parameterized by the interaction matrix, J_{ij}. Ferromagnetic interactions correspond to $\mathrm{J}_{ij} > 0$ where the spins want to align with each other, while the antiferromagnetic interaction is $\mathrm{J}_{ij} < 0$, where the spins want to misaligned. The choice of the square lattice is important to guarantee the ground state of system corresponds to the minimum of the Hamiltonian (1) at zero temperature. It is well known that the system cannot do so for some lattices, such as the triangular lattice. These frustrated systems may show different phenomenology, such as forming vortices with binding-unbinding transitions [Zhiling *et al.*, 2021], the so-called Berezinskii–Kosterlitz–Thouless (BKT) transition originally discovered in the two-dimensional XY model [Kardar, 2007].

To study the behavior at finite temperature T, we consider the partition function of the system

$$\mathrm{Z} = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}[\sigma_i]} \tag{2}$$

where $\beta = \frac{1}{k_b\mathrm{T}}$ and the sum is over the allowed values of each spin, σ_i. The probability of a configuration of spins is given by

$$\mathrm{P}(\{\sigma_i\}) = \frac{1}{\mathrm{Z}} e^{-\beta\mathcal{H}[\sigma_i]} \tag{3}$$

Lastly, we validate our results when the external field is turned off, $h = 0$, for which there is an analytical solution in the case of homogeneous ferromagnetic interactions, $\mathrm{J}_{ij} = \mathrm{J} > 0$ famously obtained by Lars Onsager [Onsager, 1944]. This analytical result predicts the critical temperature,

$$k_b \mathrm{T}_c = \frac{2\mathrm{J}}{\ln(1+\sqrt{2})} \approx 2.27\mathrm{J} \tag{4}$$

at which the average magnetization goes to zero, the correlation length of the system goes to zero, and the specific heat of the system shows a cusp.

3 Implementation - Monte Carlo Method

To compute equilibrium quantities from the probability distribution specified by eq. (3), we employ the Metropolis algorithm [Frenkel, 2023]. We label all our spins with an integer from 0 to N where N is the total number of spins. Then, we follow the steps,

1. Sample uniformly an integer in the interval $[0, \mathrm{N}]$.
2. Flip the sign of the spin corresponding to the number sampled in the previous step.
3. Calculate the energy of the new configuration, $\mathcal{H}_{\text{new}}$.
   (a) If $\mathcal{H}_{\text{new}}$ is smaller than the energy of the system before the flip, keep the change.
   (b) If $\mathcal{H}_{\text{new}}$ is larger than the energy of the system before the flip, calculate the transition probability, $p = e^{-\beta(\mathcal{H}_{\text{new}} - \mathcal{H}_{\text{old}})}$ and sample uniformly a number q in $[0, 1]$.
      i. If $p < q$, keep the change.
      ii. if $p > q$, do not keep the change.
4. Return to step 1.

Our choice of transition probability, motivated by the canonical ensemble of statistical mechanics, ensures that the entire configuration space of the spins is sampled to prevent the algorithm from getting stuck in local minima. However, if the size of the system is large, the configuration space is also extremely large, and this algorithm will require a lot of time to explore the space. Of particular concern is when the system is closed to the critical temperature, where it is well-known that the dynamics slow down because the auto-correlation time becomes infinitely large exactly at the critical point. To deal with these difficulties, we employ a cluster algorithm, a non-local operation to change the energy of the configuration by flipping entire clusters of spins at a time. We define clusters of spins as follows,

1. Pick two spins on the lattice.
   (a) If the nearest neighbours are antiparallel, do not connect them.
   (b) If the nearest neighbours are parallel, connect them with probability p and disconnect them with probability $1 - p$.

Once the connected bonds have been chosen, we define a cluster as a set of spins at least singly connected by bonds. Once the clusters are chosen, we can treat them as single spins and run the metropolis algorithm.

4 Results

We ran the algorithm for 500 interactions using the following parameters:

- 20×20 lattice sites
- Temperature $\mathrm{T} \in [1.5, 6]$
- $\mathrm{J}_{ij} = \mathrm{J} = 1$
- Magnetic field magnitude $h = 0.1$

for which the critical temperature is $\mathrm{T}_c = 2.27$.

Fig. (1) shows a representative configuration of spins below the critical temperature. We obtain a highly ordered state as expected since we are below the critical point.

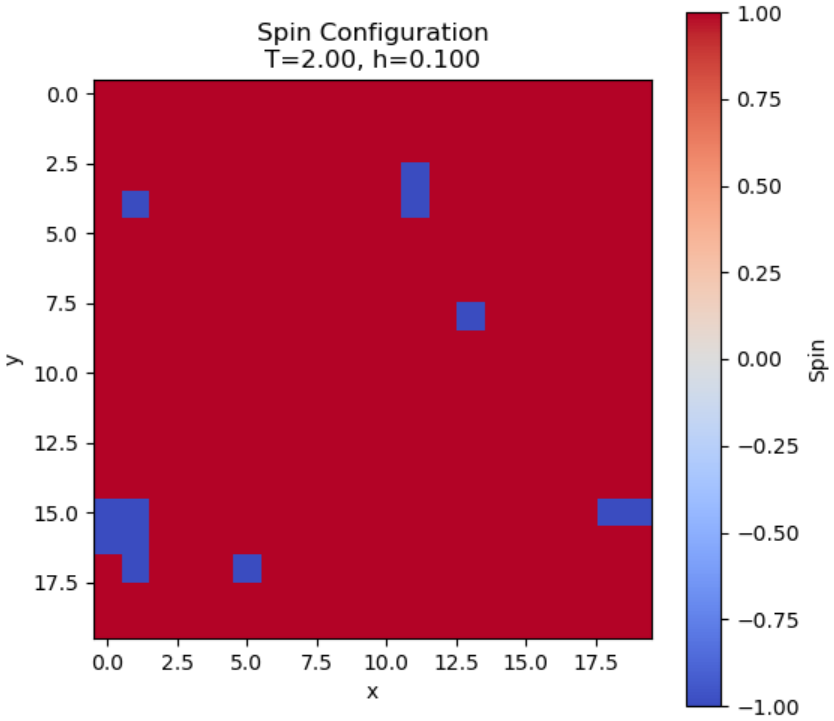

Figure 1: Representative spin configuration below critical temperature.

Fig. (2) shows our computed averaged quantities in the presence of a magnetic field. We consistently see that expected quantities decay past the critical temperature, which we marked in red as a visual aid. We remark that, even for a small system size as the one chosen, we can still see the signatures of the phase transition taking place.

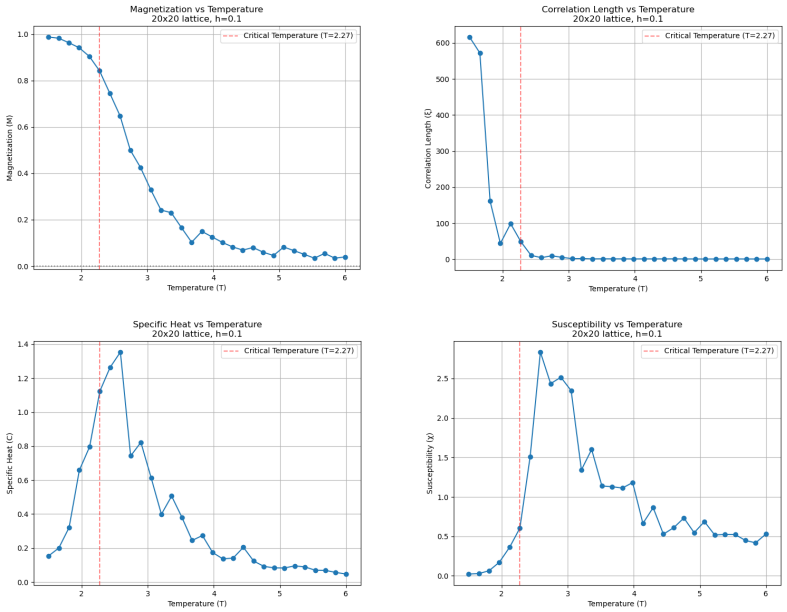

Figure 2: Average quantities computed in the presence of a magnetic field.

5 Validation

To validate our results, we turned off the magnetic field and checked our numerical results against analytical results. Fig. (3) shows our results at zero magnetic field. The susceptibility and correlation length are expected to increase at the transition due to the ordered phase appearing when the average magnetization increases. The specific heat is predicted to diverge around the critical temperature, a hallmark of a second-order phase transition as expected in the two-dimensional Ising model. Our numerical results agree with these predictions, particularly the specific heat showing a cusp around the transition, presumably becoming a true divergence as we approach the thermodynamic limit.

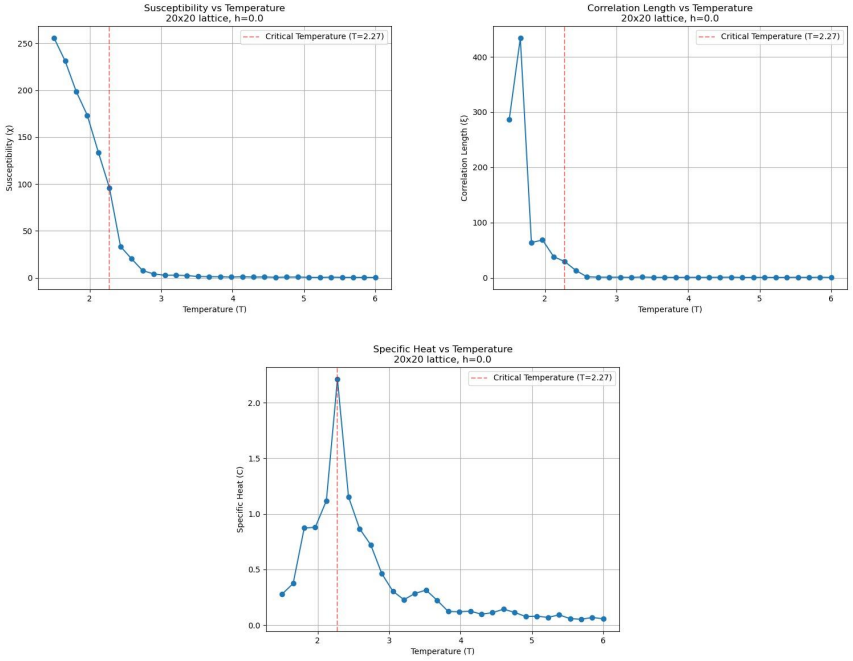

Figure 3: Computed quantities to validate the numerical implementation.

Finally, we checked the MCMC burn-in by computing the thermalization of the energy per spin and average

magnetization as a function of the steps in Fig. (4). Both quantities fluctuate about a clear mean value, implying that the algorithm has reached equilibrium and is sampling the desired probability density from eq. (3).

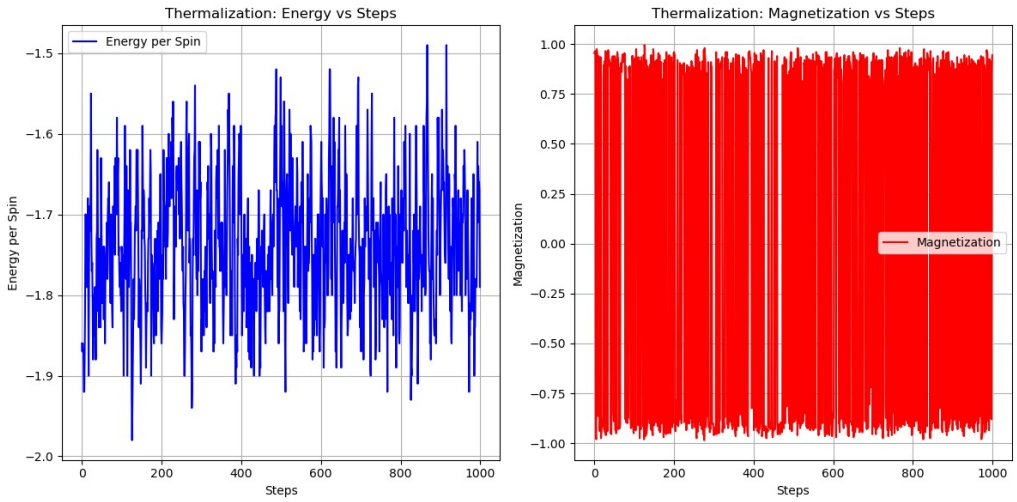

Figure 4: Thermalization of two representative quantities.

6 Conclusion

We have shown a Metropolis algorithm with non-local moves of clusters of spins can produce numerical results of the statistical mechanics of the two-dimensional Ising model. Moreover, we can compare to analytical predictions in the absence of a magnetic field with good agreement, validating our results.

7 References

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