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Numerically estimating the two-point correlation function in spin systems

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1 Introduction

The Ising model or Lenz-Ising [1], named after german physicists Ernst Ising and Wilhelm Lenz, is a mathematical model for ferromagnetism in statistical mechanics. It consists of discrete variables which represent the magnetic dipole moments of atomic "spins" and can take on values of either +1 or -1. These spins are arranged on a lattice, and the model defines the interactions between these spins.

This lattice structure repeats periodically in all directions, allowing each spin to interact with its neighboring spins. The key aspect of the model is that neighboring spins with the same orientation (either both +1 or both -1) have lower energy than those with opposing orientations. This setup allows the model to capture the fundamental behavior of ferromagnetic materials.

One of the intriguing aspects of the Ising model is the way it balances energy minimization and thermal disturbance [2]. While the system naturally tends towards a state of lowest energy, thermal fluctuations can disrupt this tendency, leading to two structural phases namely the paramagnetic phase and the ferromagnetic phase. The paramagnetic phase is characterized by a random orientation of spins and the ferromagnetic phase is characterized by a uniform orientation of spins. The transition between these two phases is known as the phase transition. The Ising model is one of the simplest models to exhibit a phase transition however, it is still a non-trivial problem to solve analytically. It is important to note that 1D Ising model does not exhibit a phase transition. The phase transition occurs only in 2D [3] and higher dimensions. This dynamic is crucial for understanding phase transitions in physical systems.

The concept of the Ising Model dates back to 1920 when Wilhelm Lenz proposed it, later tackled by his student Ernst Ising. In his 1924 thesis [1], Ising solved the one-dimensional version of the model, demonstrating the absence of a phase transition in this case. The more complex two-dimensional square-lattice version remained unsolved until 1944, when Lars Onsager provided a groundbreaking analytic solution [3], marking a significant advancement in statistical mechanics.

2 Motivation

2.1 Why study The Ising Model?

1. Significance in Understanding Phase Transitions

The Ising model is a quintessential tool in the study of phase transitions. It demonstrates key phenomena such as:

- *Symmetry Breaking in Low-Temperature Phase*: As previously discussed, the Ising model showcases how symmetry is broken in the low-temperature phase, a fundamental concept in understanding phase transitions [4; 5].
- *Existence of a Critical Point*: The model features a distinct critical point

at a well-defined temperature, analogous to the critical point in the phase diagram of water [6].

- *Richness of Features*: Besides these, the Ising model harbors other rich features that deepen our understanding of phase transitions in various systems [7].

2. Utility in Thermodynamics

The Ising model stands out as one of the few exactly solvable models in statistical mechanics. This is significant because:

- *Calculation of Thermodynamic Quantities*: Computing thermodynamic quantities in general involves summing over a large number of terms. Recall from introductory thermodynamics [8; 9; 10] that an equilibrium system can be viewed as an ensemble of many states s, each with a probability P_s. The observable thermodynamic quantities are averages over this ensemble. For an observable $A(s)$, its ensemble average is $\langle A \rangle = \sum_s A(s) P_s$. However, the challenge arises because the number of states scales exponentially with the number of particles in a system. For a system with N particles, where N is on the order of 10^{23}, this becomes computationally infeasible.

- *Importance of Exactly Solvable Systems*: Thus, the ability to exactly solve the Ising model [1; 3] and compute its partition function is a significant achievement. It allows for precise calculations and predictions in a field where such precision is often unattainable.

3. Universality and Applicability

Lastly, the Ising model's simplicity belies its wide applicability:

- *First Encounter with Universality*: The Ising model introduces us to the concept of universality in critical phenomena. The same theoretical framework can describe a variety of different phase transitions, whether in liquids, gases, magnets, superconductors, or other systems.

- *A Reflection of Deeper Order*: Such universal behavior is particularly intriguing to physicists as it suggests an underlying order in the seemingly chaotic natural world.

In conclusion, the Ising model is not just a theoretical construct but a vital tool that offers profound insights into the complex world of phase transitions and critical phenomena. Its simplicity, exact solvability, and universality make it a cornerstone in the field of statistical mechanics and beyond.

2.2 Why 1D Models?

- *Testing Ground for Approximate Techniques*: One-dimensional (1D) models serve as a testing ground for the validity of approximate techniques developed for higher-dimensional systems.

- *Insights into Higher-Dimensional Systems*: They help in guessing properties of higher-dimensional systems.
- *Representation of Quasi 1D Systems*: Some materials behave as quasi one-dimensional systems [11] [12] due to dominating inter-particle interactions along a chain of particles.
- *Mapping to 1D Ising-like Models*: There are classes of problems that can be mapped onto one-dimensional Ising-like models, such as the conformational equilibria of a linear polymer. [13]
- *Applicability of Mathematical Techniques*: The mathematical techniques employed to solve one-dimensional problems are often applicable to other types of problems.
- *Ordering at Absolute Zero*: Even the one-dimensional spin system must become ordered at $T = 0$. Therefore, understanding the behavior of the system as $T \to 0$ will be important in our treatment of spin systems via renormalization group methods.

3 Theoretical Background

3.1 Mathematical Formulation of the 1D Ising Model

The Ising Model is a theoretical construct representing a lattice of sites, each of which can exist in one of two states: -1 or +1. These states are denoted as σ_i, where i is the site index. For instance, $\sigma_i = -1$ indicates that the i-th site is in the state -1.

3.2 The Hamiltonian

The Hamiltonian of the Ising Model includes two main components: the interaction energy between nearest neighboring spins and the individual energy of each spin due to an external magnetic field. Mathematically, it is represented as:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{1}$$

Here, the first term sums the interactions of adjacent spins, denoted by $\langle i, j \rangle$, indicating summation over nearest neighbors. The second term sums the individual spin energies, with h representing the external magnetic field's strength. The coupling constant J determines the interaction strength between neighboring spins, being positive for ferromagnetic and negative for antiferromagnetic interactions. This mathematical representation is central to understanding the physical implications and behaviors modeled by the Ising model.

3.2.1 The Partition Function

The partition function Z is a central concept in statistical mechanics. It represents the sum of all possible states of a system, weighted by their respective Boltzmann factors. For the Ising model, the partition function is given by:

$$Z = \sum_{\{\sigma_i\}} e^{-\beta H} \tag{2}$$

Here, $\beta = \frac{1}{k_B T}$, where k_B is the Boltzmann constant and T is the temperature. The sum is over all possible states of the system, denoted by $\{\sigma_i\}$. Boltzmann factor $e^{-\beta H}$ is a measure of probability of a state occurring, with lower energy states being more probable. The partition function is a central concept in statistical mechanics [9] [10], as it allows us to calculate the thermodynamic properties of a system.

3.2.2 Exact Solution of the 1D Ising Model

The 1D Ising Model can be solved exactly, as demonstrated by Ernst Ising in his 1924 thesis [1]. In case of periodic boundary conditions, we can use the transfer matrix method, where partition function is formulated as a product of matrices. The partition function for the 1D Ising Model is then given by:

$$Z = \sum_{\{\sigma_i\}} e^{-\beta H} = \sum_{\{\sigma_i\}} \prod_{i=1}^{N-1} e^{-\beta H_i} \tag{3}$$

where N is the number of sites on the lattice, and the Hamiltonian for the interaction between the i-th and $(i+1)$-th site is:

$$H_i = -J\sigma_i\sigma_{i+1} - \frac{h}{2}(\sigma_i + \sigma_{i+1}) \tag{4}$$

The partition function can be expressed as a product of matrices using the transfer matrix method. The transfer matrix T for each pair of adjacent spins is given by:

$$T = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix} \tag{5}$$

The partition function in terms of the transfer matrix is:

$$Z = \sum_{\{\sigma_i\}} T^{N-1} = \mathrm{Tr}(T^N) \tag{6}$$

where Tr denotes the trace of the matrix. This expression shows that the partition function can be calculated by raising the transfer matrix to power of N and taking its trace, providing a complete solution to the 1D Ising model.

To solve this, we diagonalize the matrix T. The Eigenvalues λ_1 and λ_2 of T are found by solving the characteristic equation, which is the determinant of $T - \lambda I$, where I is the identity matrix. The characteristic equation is:

$$\det(T - \lambda I) = \begin{vmatrix} e^{\beta(J+h)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} - \lambda \end{vmatrix} = 0 \tag{7}$$

Solving this equation gives us the eigenvalues λ_1 and λ_2. The partition function Z can then be expressed as:

$$Z = \mathrm{Tr}(T^N) = \lambda_1^N + \lambda_2^N \tag{8}$$

This formulation of Z encapsulates the sum over all possible configurations of the spins, weighted by their Boltzmann factor $e^{-\beta H}$. The eigenvalues, functions of the temperature β, coupling constant J, and external magnetic field h, determine the system's behavior.

In the thermodynamic limit, where N tends to infinity, the partition function is dominated by the largest eigenvalue, as the contribution from the smaller eigenvalue becomes negligible. This results in the final expression for the partition function:

$$Z \approx \lambda_{\max}^N \tag{9}$$

where $\lambda_{\max}$ is the larger of two eigenvalues λ_1 and λ_2. According to the Perron-Frobenius theorem [14], $\lambda_{\max}$ is positive and real, affirming that the partition function Z is positive and real, a necessary condition for a physical system. This validates that the 1D Ising Model is not merely a mathematical abstraction but represents a physically realizable system.

In the special case of $h = 0$, the eigenvalues simplify to:

$$\lambda_1 = 2\cosh(\beta J), \quad \lambda_2 = 2\sinh(\beta J) \tag{10}$$

These eigenvalues, especially under special conditions like $h = 0$, can be computed analytically, providing valuable insights into the thermodynamic properties of the system. This exact solution is a fundamental result in statistical mechanics, demonstrating the efficacy of the transfer matrix method in solving one-dimensional models.

3.2.3 Thermodynamic Properties of the 1D Ising Model

As discuessed in equation 9, the partition function is given by the largest eigenvalue $\lambda_{\max}$ in the thermodynamic limit. Therefore, for h = 0, the partition function is given by:

$$Z = \lambda_{\max}^N = (2\cosh(\beta J))^N \tag{11}$$

The free energy F is given by:

$$F = -k_B T \ln(Z) = -k_B T N \ln(2\cosh(\beta J)) \tag{12}$$

The internal energy U is given by:

$$U = -\frac{\partial}{\partial \beta} \ln(Z) = -\frac{\partial}{\partial \beta} N \ln(2\cosh(\beta J)) = -JN\tanh(\beta J) \tag{13}$$

The magnetization M is given by:

$$M = -\frac{\partial}{\partial h} \ln(Z) = -\frac{\partial}{\partial h} N \ln(2\cosh(\beta J)) = 0 \tag{14}$$

The heat capacity C is given by:

$$C = -\beta^2 \frac{\partial^2}{\partial \beta^2} \ln(Z) = -\beta^2 \frac{\partial^2}{\partial \beta^2} N \ln(2\cosh(\beta J)) = k_B \beta^2 N \text{sech}^2(\beta J) \tag{15}$$

The susceptibility χ is given by:

$$\chi = \beta \frac{\partial^2}{\partial h^2} \ln(Z) = \beta \frac{\partial^2}{\partial h^2} N \ln(2\cosh(\beta J)) = 0 \tag{16}$$

These thermodynamic properties are fundamental to understanding the behavior of the Ising Model. The heat capacity and susceptibility are both zero, indicating that the system is stable and does not undergo a phase transition. This is consistent with the physical behavior of the Ising Model, as the 1D Ising Model does not exhibit a phase transition.

3.3 Monte Carlo Simulations

Monte Carlo methods belongs to a category of computational algorithms that utilize repeated random sampling to derive numerical outcomes. These methods are extensively employed across various fields such as physics [15], chemistry, [16] and finance [17]. In this thesis, Monte Carlo methods are specifically applied to simulate the Ising model.

The Ising model is characterized as a stochastic system [18], meaning its behavior is inherently probabilistic rather than deterministic. In such a system, the state at any given moment is subject to random variation, making precise prediction unfeasible. This contrasts with deterministic systems, where, provided the initial conditions and the governing rules are known, the future state of the system can be accurately forecasted.

In the context of the Ising model, stochasticity arises primarily from thermal fluctuations. These fluctuations spontaneously induce spin reversals, leading to unpredictable variations in the system's energy state. Consequently, the evolution of the system's state over time remains indeterminable.

Given these characteristics, the Monte Carlo method emerges as an apt approach for simulating systems like the Ising model, where randomness plays a pivotal role in their evolution.

For this thesis, the goal of the Monte Carlo simulation is to estimate the expectation values:

$$\langle \mathcal{O} \rangle \equiv \sum_{\text{states } \sigma} \mathcal{O}(\sigma) e^{-\beta \mathcal{H}(\sigma)} / \mathcal{Z} \tag{17}$$

where $\mathcal{O}$ is an observable of the system defined by its Hamiltonian $\mathcal{H}$ and with canonical partition function $\mathcal{Z}$ as:

$$\mathcal{Z} = \sum_{\text{states } \sigma} e^{-\beta \mathcal{H}(\sigma)} = \sum_{E} \Omega(E) e^{-\beta E} \tag{18}$$

where $\Omega(E)$ is the density of states at energy E.

3.3.1 Importance Sampling and Markov Chain Monte Carlo Methods

Importance sampling is a Monte Carlo technique that enhances the efficiency of simulations by reducing the variance of estimated expectation values. This technique involves drawing samples not randomly but in accordance with a specified equilibrium distribution. In many physical systems, this equilibrium distribution is defined by the canonical ensemble's Boltzmann weight, expressed as

$$\mathcal{P}_i^{eq} \equiv \mathcal{P}^{eq}(\sigma_i) = \frac{e^{-\beta H(\sigma_i)}}{Z} \tag{19}$$

although the principle of importance sampling is not restricted to this particular form.

In the context of Markov Chain Monte Carlo (MCMC) methods, a Markov chain is established to select a microstate σ_i according to the given equilibrium distribution. A Markov chain is characterized by its transition probabilities $W_{ij} \equiv W(\sigma_i \to \sigma_j)$, which dictate the likelihood of a system evolving from one microstate σ_i to another σ_j. This evolution is subject to the condition that the probability depends only on the current state σ_i and not on the entire history of the system's trajectory, rendering the process almost local in time.

For MCMC algorithms to accurately reflect the equilibrium distribution, the transition probability W_{ij} must satisfy three conditions:

1. $W_{ij} \geq 0 \qquad \forall i, j$ (positivity),
2. $\sum_j W_{ij} = 1 \qquad \forall i$ (normalization),
3. $\sum_i W_{ij} \mathcal{P}_i^{eq} = \mathcal{P}_j^{eq} \qquad \forall j$ (balance condition).

The balance condition ensures that the equilibrium distribution is a fixed point of the transition matrix W, maintaining the desired distribution across the Markov chain. A commonly used strategy to satisfy this condition is the detailed balance, which states that $W_{ij} P_i^{eq} = W_{ji} P_j^{eq}$. This condition, when combined with normalization, ensures the general balance condition.

After an initial equilibration period, expectation values in the system can be estimated as the arithmetic mean over the Markov chain. This means calculating the average of a quantity $\mathcal{O}$ over different states of the system, represented as follows:

$$\langle \mathcal{O} \rangle = \sum_{\sigma} \mathcal{O}(\sigma) \mathcal{P}^{eq}(\sigma) \approx \overline{\mathcal{O}} \equiv \frac{1}{N} \sum_{k=1}^{N} \mathcal{O}(\sigma(k)) \tag{20}$$

where $\sigma(k)$ denotes the state of the system at step k in the Markov chain. This approach provides an unbiased estimator $\overline{\mathcal{O}}$ for the expectation value $\langle\mathcal{O}\rangle$, thus effectively capturing the equilibrium behavior of the system.

3.3.2 Local Update Algorithms

The Markov chain conditions outlined above are general and can be satisfied by a variety of algorithms. In the context of the Ising model, the Metropolis algorithm is a widely used local update algorithm that satisfies the conditions and is therefore suitable for Monte Carlo simulations.

Local update algorithms are characterized by their ability to update the system by changing only a small portion of the lattice. This is in contrast to global update algorithms, which require the entire lattice to be updated at each step. Local update algorithms are more efficient than global update algorithms, as they require less computational resources to simulate the system.

The selection of a local update algorithm is not arbitrary. The algorithm must satisfy the detailed balance condition, which is a necessary condition for achieving the equilibrium distribution. The Metropolis algorithm is one such algorithm that satisfies this condition. The probability of a potential transition from state σ_i to σ_j is given by the so called selection probability f_{ij}, which is defined as:

$$f_{ij} = f(\sigma_i \to \sigma_j), \qquad f_{ii} \geq 0, \qquad \sum_j f_{ij} = 1 \tag{21}$$

The proposed transition is then accepted with the probability w_{ij}, defined as:

$$w_{ij} = w(\sigma_i \to \sigma_j) = \min\left(1, \frac{f_{ji}\mathcal{P}_i^{eq}}{f_{ij}\mathcal{P}_j^{eq}}\right) \tag{22}$$

where $\mathcal{P}_i^{eq}$ is the equilibrium probability of the state. Otherwise, the system remains in the same state which may also happen when $f_i \neq 0$.

This implies that the transition probability W_{ij} is given by:

$$W_{ij} = \begin{cases} f_{ij}w_{ij} & j \neq i \\ f_{ii} + \sum_{j\neq i} f_{ij}w_{ij} & j = i \end{cases} \tag{23}$$

As $f_{ij} \geq 0$ and $0 \leq w_{ij} \leq 1$, it follows that $W_{ij} \geq 0$ and $\sum_j W_{ij} = 1$, satisfying the Markov chain conditions.

The update prescription is still general, as the probability $\mathcal{P}^{ij}$ can be chosen arbitrarily. Moreover, the selection probability f_{ij} can be chosen to be symmetric, i.e. $f_{ij} = f_{ji}$, which is the case for our simulations and it has not been specified how to choose the trail state σ_j. After simplification, the Boltzmann weight from the importance sampling is obtained which results in:

$$\frac{\mathcal{P}_j^{eq}}{\mathcal{P}_i^{eq}} = e^{-\beta\Delta E} \tag{24}$$

where $\Delta E = E_j - E_i$ is the energy difference between the two states.

3.3.3 Metropolis Algorithm

The Metropolis Algorithm was first introduced by Nicholas Metropolis [19] in 1953, revolutionizing the simulation of stochastic systems. It has since found extensive applications in diverse fields, including physics, chemistry, and biology, with a notable impact on the study of the Ising model.

This algorithm falls under the category of Markov chain Monte Carlo (MC MC) methods. It generates a Markov chain, ensuring that its stationary distribution aligns with the target probability distribution. In the Ising model, this entails creating a sequence of spin configurations, each derived from its predecessor, converging towards the Boltzmann distribution: the equilibrium probability distribution for the model.

The Metropolis algorithm operates on a rejection-based principle. It involves the following steps:

1. Initialize the system with a random spin configuration.
2. Randomly select a spin within the lattice.
3. Compute the energy change, ΔE, resulting from the inversion of the selected spin.
4. Accept the new configuration if $\Delta E < 0$.
5. For $\Delta E > 0$, accept the new configuration with a probability of $e^{-\beta \Delta E}$.
6. Iterate steps 2-5 until a predetermined number of iterations is achieved.

The Metropolis algorithm's simplicity and efficacy make it an ideal tool for simulating the Ising model. Its versatility allows for adaptations to different scenarios, such as varying the temperature in the Ising model simulations by adjusting the acceptance probability in the algorithm.

Based on above steps, the acceptance probability is given by:

$$w_{ij} = \min\left(1, \frac{f_{ji}\mathcal{P}^{eq}i}{fij\mathcal{P}_j^{eq}}\right) = \min\left(1, e^{-\beta \Delta E}\right) = \begin{cases} 1 & \text{if } \Delta E \leq 0, \\ e^{-\beta \Delta E} & \text{if } \Delta E > 0. \end{cases} \tag{25}$$

If the energy difference is negative, the new state is always accepted. If the energy difference is positive, the new state is accepted with a probability defined in the equation above. This is illustrated in Figure 1. This ensures the proper treatment of entropic contributions in thermal equilibrium. The free energy, $F = U - TS$ has to be minimized and not the internal energy U.

For the Ising model with only two possible spin states, a spin flip is the only possible local update. This means that the selection probability f_{ij} is symmetric, i.e. $f_{ij} = f_{ji}$. The selection probability is also independent of the

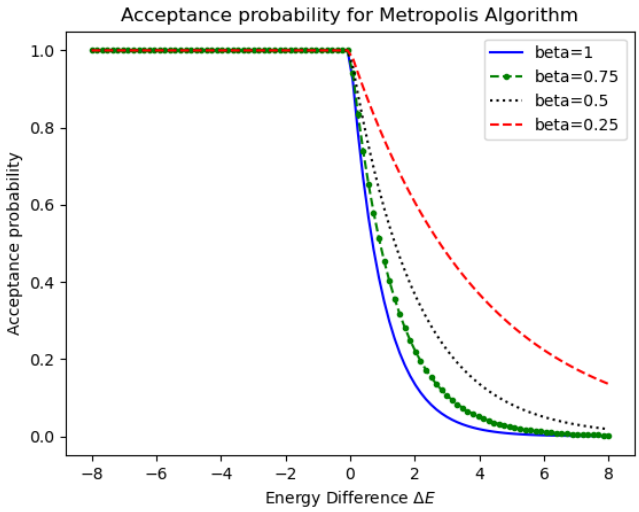

Figure 1: The Metropolis algorithm for the Ising model.

state σ_i and σ_j, i.e. $f_{ij} = f_{ji} = f_i$. This implies that the transition probability W_{ij} is given by:

$$W_{ij} = \begin{cases} f_{ij} w_{ij} & j \neq i \\ f_{ii} + \sum_{j \neq i} f_{ij} w_{ij} & j = i \end{cases} \tag{26}$$

The update prescription is still general, as the probability $\mathcal{P}^{ij}$ can be chosen arbitrarily. Moreover, the selection probability f_{ij} can be chosen to be symmetric, i.e. $f_{ij} = f_{ji}$, which is the case for our simulations. To decide whether the proposed transition is accepted or not, we draw a random number r from a uniform distribution between 0 and 1. If $r \leq w_{ij}$, the transition is accepted, otherwise it is rejected and we continue with next step in the Markov chain.

3.4 Temporal Correlation

When data is generated by using a Markov chain method, it is temporally correlated which can be seen in the autocorrelation function given by equation [20]:

$$A(k) = \frac{\langle \mathcal{O}_i \mathcal{O}_{i+k} \rangle - \langle \mathcal{O}_i \rangle \langle \mathcal{O}_i \rangle}{\langle \mathcal{O}_i^2 \rangle - \langle \mathcal{O}_i \rangle \langle \mathcal{O}_i \rangle} \tag{27}$$

where $\mathcal{O}_i$ is the observable at time i for example the energy or magnetization. The autocorrelation function is a measure of how correlated the data is at a given time step. If the data is uncorrelated the autocorrelation function will be zero for all k. For large time steps k the autocorrelation function $A(k)$ will decay exponentially as:

$$A(k) \xrightarrow{k\to\infty} A(0)e^{-k/\tau_{\mathcal{O},exp}} \tag{28}$$

where $\tau_{\mathcal{O},exp}$ is the exponential autocorrelation time. The autocorrelation function also contains some other modes because of which $A(k)$ does not decay exponentially for all k.

The influence of the autocorrelation time is particularly important for phase transitions. Near the critical point, the autocorrelation time $\tau_{\mathcal{O},exp}$ scales in infinite volume limit as [20]:

$$\tau_{\mathcal{O},exp} \sim \xi^z \tag{29}$$

where z is the dynamical critical exponent greater than 0. ξ is the spacial correlation length which diverges at the critical point as $\xi \sim |T - T_c|^{-\nu} \to \infty$ when $T \to T_c$. This implies that the autocorrelation time diverges at the critical point as $\tau_{\mathcal{O},exp} \sim |T-T_c|^{-\nu z}$. This effect is very large at local dynamics ($z \approx 2$). This leads to a phenomenon called critical slowing down [21; 22] resulting in a large increase in the simulation time required to generate uncorrelated data. The issue of critical slowing down can be avoided by using cluster algorithms [23].

3.4.1 Estimators

Estimators are used to estimate the expectation value of an observable $\mathcal{O}$ from a set of N measurements $\mathcal{O}_k$ of the observable $\mathcal{O}$ as:

$$\langle\mathcal{O}\rangle = \sum_{\sigma} \mathcal{O}(\sigma)P^{eq}(\sigma) \approx \overline{\mathcal{O}} = \frac{1}{N}\sum_{k=1}^{N} \mathcal{O}_k \tag{30}$$

where σ is the microstate of the system and $P^{eq}(\sigma)$ is the equilibrium probability distribution of the microstates. The estimator $\overline{\mathcal{O}}$ is an unbiased estimator of the expectation value of the observable $\mathcal{O}$. In case of Markov chain Monte Carlo simulations, the observable $\mathcal{O}$ is a quantity like energy or magnetization which is measured at each time step k of the simulation with N as the total number of measurement sweeps. The estimator $\overline{\mathcal{O}}$ is only valid after a sufficiently long thermalization period necessary to reach the equilibrium state after starting from a random initial state.

It is important to differentiate between the estimator $\overline{\mathcal{O}}$ and the expectation value $\langle\mathcal{O}\rangle$. The expectation value $\langle\mathcal{O}\rangle$ is the true value of the observable which is often unknown. The estimator $\overline{\mathcal{O}}$ is an approximation of the former. In contrast to the expectation value $\langle\mathcal{O}\rangle$ being a constant, the estimator $\overline{\mathcal{O}}$ is a random variable which fluctuates around the expectation value $\langle\mathcal{O}\rangle$ for finite values of N.

From a single simulation, we can only obtain a single value of the estimator $\overline{\mathcal{O}}$. It might seem that we need to run multiple simulations to obtain statistical error of the estimator. However, it is possible to obtain the statistical error of

the estimator $\overline{\mathcal{O}}$ from a single simulation. We can express the variance of the estimator $\overline{\mathcal{O}}$ as:

$$\sigma^2_{\mathcal{O}} = \langle \overline{\mathcal{O}}^2 \rangle - \langle \overline{\mathcal{O}} \rangle^2 \tag{31}$$

$$= \frac{1}{N^2} \sum_{k=1}^{N} \langle \mathcal{O}_k^2 \rangle - \langle \mathcal{O}_k \rangle^2 + \frac{1}{N^2} \sum_{k \neq l}^{N} (\langle \mathcal{O}_k \mathcal{O}_l \rangle - \langle \mathcal{O}_k \rangle \langle \mathcal{O}_l \rangle) \tag{32}$$

where we have collected the diagonal and off-diagonal terms separately. The off-diagonal terms encode the temporal correlation between the measurement k and l and hence vanishes for uncorrelated data. At equilibrium, the diagonal terms are independent of time "k" and hence $\sigma^2_{\mathcal{O}_k} = \sigma^2_{\mathcal{O}}$. This simplifies the expression 32 to:

$$\sigma^2_{\overline{\mathcal{O}}} = \sigma^2_{\mathcal{O}} / N \tag{33}$$

The distribution of $\mathcal{O}_k$ is often Gaussian by the central limit theorem atleast for weakly correlated data in asymptotic limit of $N \to \infty$. The variance of the mean $\sigma^2_{\overline{\mathcal{O}}}$ is the squared width of this Gaussian distribution which is also called the statistical error of the estimator $\overline{\mathcal{O}}$. This means that 68% of the measurements $\mathcal{O}_k$ will lie within one standard deviation $\sigma_{\mathcal{O}}$ from the mean $\overline{\mathcal{O}}$.

For strongly correlated data, the off-diagonal terms in equation 32 are non-zero and the distribution of $\mathcal{O}_k$ is not Gaussian. Using the symmetry $k \leftrightarrow l$ in equation 32 we can rewrite the summation $\sum_{k \neq l}^{N}$ as $2 \sum_{k=1}^{N} \sum_{l=k+1}^{N}$. By reodering the terms and using time translation invariance of the correlation function $A(k)$ we can obtain:

$$\sigma^2_{\overline{\mathcal{O}}} = \frac{1}{N} \left[\sigma^2_{\mathcal{O}} + 2 \sum_{k=1}^{N} (\langle \mathcal{O}_k \mathcal{O}_{k+1} \rangle - \langle \mathcal{O}_k \rangle \langle \mathcal{O}_{k+1} \rangle) \left(1 - \frac{k}{N} \right) \right] \tag{34}$$

Factoring out $\sigma^2_{\mathcal{O}}$, we obtain:

$$\sigma^2_{\overline{\mathcal{O}}} = \frac{\sigma^2_{\mathcal{O}}}{N} 2 \tau_{\mathcal{O},exp} \tag{35}$$

where $\tau_{\mathcal{O},exp}$ is the integrated autocorrelation time defined as:

$$\tau_{\mathcal{O},exp} = \frac{1}{2} + \sum_{k=1}^{N} \frac{\langle \mathcal{O}_k \mathcal{O}_{k+1} \rangle - \langle \mathcal{O}_k \rangle \langle \mathcal{O}_{k+1} \rangle}{\sigma^2_{\mathcal{O}}} \left(1 - \frac{k}{N} \right) \tag{36}$$

$$= \frac{1}{2} + \sum_{k=1}^{N} A(k) \left(1 - \frac{k}{N} \right) \tag{37}$$

where $A(k)$ is the normalized autocorrelation function such that $A(0) = 1$. For a proper simulation, we must choose N such that $N >> \tau_{\mathcal{O},exp}$ so that

$A(k)$ is already exponentially small before the correction term $\left(1 - \frac{k}{N}\right)$ becomes significant.

Equation 35 implies that due to temporal correlations in the data, the statistical error of the estimator $\epsilon = \sqrt{\sigma^2_{\overline{\mathcal{O}}}}$ is increased by a factor of $\sqrt{2\tau_{\mathcal{O},exp}}$. This can be rephrased as the effective number of measurements N_{eff} being reduced by a factor of $\sqrt{N_{\text{eff}}}$ as compared to uncorrelated data. The term $\sqrt{N_{\text{eff}}}$ is called the effective sample size and is given by $\sqrt{N_{\text{eff}}} = N/2\tau_{\mathcal{O},exp}$. This implies that we obtain uncorrelated data approximately every $2\tau_{\mathcal{O},exp}$ time steps.

3.4.2 Bias in the Estimator

As discussed above, the effective number of measurements N_{eff} is reduced by a factor of $\sqrt{2\tau_{\mathcal{O},exp}}$ due to temporal correlations in the data. Some quantites like specific heat C are underestimed if effective statistics becomes too small. The standard estimator for variance is given by:

$$\hat{\sigma^2_{e_i}} = \overline{\mathrm{e}^2} - \overline{\mathrm{e}}^2 = \frac{1}{N}\sum_{k=1}^{N}(e_k - \overline{e})^2 \tag{38}$$

where e_k is the energy at time step k and $\overline{e}$ is the mean energy. To obtain the expectation value of the variance, we can subtract and add $\langle\overline{e}\rangle^2$ as:

$$\langle\hat{\sigma_{e_i}}^2\rangle = \langle\overline{\mathrm{e}^2}\rangle - \langle\overline{\mathrm{e}}\rangle^2 - (\langle\overline{\mathrm{e}}^2\rangle - \langle\overline{\mathrm{e}}\rangle^2) \tag{39}$$

The first two terms give $\sigma^2_{e_i}$ and the last terms gives $\sigma^2_{\overline{e}_i} = \sigma^2_{e_i} 2\tau_{\mathrm{e,\ int}}/N$. This results as follows:

$$\langle\hat{\sigma_{e_i}}^2\rangle = \sigma^2_{e_i}\left(1 - \frac{2\tau_{\mathrm{e,\ int}}}{N}\right) = \sigma^2_{e_i}\left(1 - \frac{1}{N_{\text{eff}}}\right) \tag{40}$$

The estimator $\hat{\sigma_{e_i}}^2$ is biased and underestimates the true variance $\sigma^2_{e_i}$ by a factor of $1/N_{\text{eff}}$. This type of estimator is called a weakly biased estimator.

Hence, we observe that for large autocorrelation times or small effective statistics, the bias in the estimator $\hat{\sigma_{e_i}}^2$ becomes large. Therefore, special care must be taken to ensure that the effective statistics are large enough to obtain unbiased results especially in case of local update algorithms.

3.5 Spatial Correlation

4 Methodology

For the purpose of this thesis, we needed to create a dataset of consisting the spatial correlation between the spins of a 1D Ising model. To simulate the Ising model, we used Monte Carlo simulations [15; 16]. The simulations were implemented in Python 3.10.9 [24] using the NumPy library [25]. To proform the Monte Carlo simulations, we used the Metropolis algorithm [19] with periodic boundary conditions [15].

From the Monte Carlo simulations, we obtained a dataset of the spin configurations, their corresponding energy and magnetization at each Monte Carlo step. The data obtained was temporally correlated (Section : 3.4), and we needed to remove this correlation. To do this, we calculated the autocorrelation function of magnetization. Using these correlation values, we calculated the integrated autocorrelation time [26]. Finally, we used the integrated autocorrelation time to decorrelate the data by first discarding the first $20\tau_{int}$ Monte Carlo steps, and then only keeping every $4\tau_{int} - th$ step [27]. The decorrelated data was then used to calculate the spatial correlation functions (Section : 3.5) which is the main focus of this thesis.

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