Numerically estimating the two-point correlation function in spin systems

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1 Introduction

2 Ising Model

The Ising model or Lenz-Ising model, named after the german physicists Ernst Ising and Wilhelm Lenz, is a mathematical model for ferromagnetism in statistical mechanics. It consists of discrete variables known as spins, which 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.

The model consists of discrete variables, which represent the magnetic dipole moments of atomic "spins". These spins, which can be in one of two states (+1 or -1), are arranged in a lattice. 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. While the system naturally tends towards a state of lowest energy, thermal fluctuations can disrupt this tendency, leading to various structural phases. 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, 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, marking a significant advancement in statistical mechanics.

2.1 Mathematical Formulation of the 1D Ising Model

The Ising Model, a theoretical construct, represents 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.

2.1.1 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.

2.1.2 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 $\{\sigma_i\}$. The Boltzmann factor $e^{-\beta H}$ is a measure of the probability of a state occurring, with lower energy states being more probable. The partition function is a central concept in statistical mechanics, as it allows us to calculate the thermodynamic properties of a system.

2.1.3 Exact Solution of the 1D Ising Model

The 1D Ising Model can be solved exactly, as demonstrated by Ernst Ising in his 1924 thesis. This solution employs the transfer matrix method, where the partition function is formulated as a product of matrices. The partition function for the 1D Ising Model is defined as:

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

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 the 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 the two eigenvalues λ_1 and λ_2. According to the Perron-Frobenius theorem, $\lambda_{\max}$ 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 Motivation

3.1 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.
- *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, which we alluded to earlier.
- *Richness of Features*: Besides these, the Ising model harbors other rich features that deepen our understanding of phase transitions in various systems.

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 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 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. This principle posits that 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.

3.2 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 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.

- *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.