Monte Carlo Approach for simulation in Physics

**Abstract:**

The Monte Carlo method has long been recognised as a powerful technique for performing certain calculations, generally those too complicated for a more classical approach. Since the use of high-speed computers became widespread in the 1950s, a great deal of theoretical investigation has been undertaken and practical experience has been gained in the Monte Carlo approach. Monte Carlo methods are being essential as computational tools in physics, enabling the simulation of a wide range of systems, from simple spin models to complex theories of fundamental forces and spacetime. This report provides an overview of the Monte Carlo approach, beginning with basic algorithms like Metropolis-Hastings applied to models such as the Zn​ lattice and spin glasses, which is widely used to study phase transitions and critical behaviour in statistical mechanics. As simulations extend to more complex systems, including lattice field theories, advanced techniques like cluster algorithms, replica exchange, and Hybrid Monte Carlo become necessary to efficiently explore the vast and intricate configuration spaces of these models.

We highlight how these advanced algorithms have expanded the applicability of Monte Carlo methods, allowing physicists to investigate fundamental interactions, particle behaviour, and even aspects of quantum gravity. By examining this progression from simpler models to more abstract applications, the report illustrates the flexibility and growing importance of Monte Carlo simulations in modern physics.

# History and Introduction to Monte Carlo Methods and Simulation

Monte Carlo (MC) approach to analysis was developed in the 1940's, it is a computer based analytical method which employs statistical sampling techniques for obtaining a probabilistic approximation to the solution of a mathematical equation or model. MC simulation was developed as part of the atomic program. Scientist at the Los Alamos National Laboratory originally used it to model the random diffusion of neutrons. The scientist who developed this simulation technique gave it the name “Monte Carlo” after the city in Monaco and its many casinos. MC simulation are used in a wide array of applications, including physics, finance, and system reliability.[2]

The above definition should be supplemented by a somewhat narrower but more enlightening definition as given by Halton [1]: the MC method is defined as representing the solution of a problem as a parameter of a hypothetical population, and using a random sequence of numbers to construct a sample of the population, from which statistical estimates of the parameter can be obtained.

Let us express the solution of the problem as a result F, which may be a real number, a set of numbers, a yes/no decision, etc. The MC estimate of F will be a function of, among other things, the random numbers used in the calculation. The introduction of randomness into an otherwise well-defined problem produces solutions with rather special properties which, as we shall see, are sometimes surprisingly good. MC simulation is a versatile tool to analyse and evaluate complex measurements using a model of a system, and to experiment with the model towards drawing inferences of the system’s behaviour.

Historically, the first large-scale calculations to make use of the MC method were studies of neutron scattering and absorption, random processes for which it is quite natural to employ random numbers. Such calculations, a subset of MC calculations, are known as direct simulation, since the ‘hypothetical population’ of the narrower definition above corresponds directly to the real population being studied. However, as those involved were well aware, the numerical results obtained were perfectly ‘deterministic’ and, in principle, obtainable by classical computational techniques (in fact, integration). Whether or not the MC method can be applied to a given problem does not depend on the stochastic nature of the system being studied, but only on our ability to formulate the problem in such a way that random numbers may be used to obtain the solution. This can be seen by inverting the neutron scattering problem and considering first the classical solution in terms of a complicated multidimensional integral. ’The value of this integral is quite non-random, but happens also to be the solution of a problem involving random processes. The MC method may be applied wherever it is possible to establish equivalence between the desired result and the expected behaviour of a stochastic system. The problem to be solved may already be of a probabilistic or statistical nature, in which case its MC formulation will usually be a straightforward simulation, or it may be of a deterministic or analytic nature, in which case an appropriate MC formulation may require some imagination and may appear contrived or artificial. In any case, the suitability of the method chosen will depend on its mathematical properties and not on its superficial resemblance to the problem to be solved.

MC methods play a crucial role in computational physics, physical chemistry, and a range of applied fields, with applications spanning from intricate quantum chromodynamics computations to the design of heat shields, aerodynamic structures, and modelling radiation transport for dosimetry calculations [3, 4, 5]. In statistical physics, Monte Carlo molecular modelling serves as an alternative to molecular dynamics simulations, and these methods are essential for computing statistical field theories in both particle and polymer systems [6, 7]. Quantum Monte Carlo techniques provide solutions to the many-body problem in quantum systems [8, 9]. Within radiation materials science, the binary collision approximation, commonly used for simulating ion implantation, typically relies on Monte Carlo methods to identify subsequent collision partners [10]. In experimental particle physics, these methods are instrumental in detector design, understanding detector responses, and aligning theoretical models with experimental data. In astrophysics, Monte Carlo techniques are applied in areas as diverse as modelling galaxy evolution [11] and simulating microwave radiation transmission across uneven planetary surfaces [12]. Additionally, MC approaches are foundational to ensemble models, which are integral to modern weather forecasting.

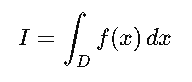
# Background

## The Mathematical Basics of Monte Carlo Method [13]

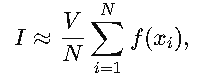
The Monte Carlo method is a versatile computational technique that uses random sampling to approximate solutions for complex, high-dimensional problems, especially when classical methods are insufficient. Originating from early applications in neutron scattering simulations, Monte Carlo methods have become fundamental in areas like statistical physics and complex system modeling​

### Estimating Integrals with Monte Carlo

One principal use of Monte Carlo is to estimate integrals. For a function f(x)f(x)f(x) over a domain D, the integral



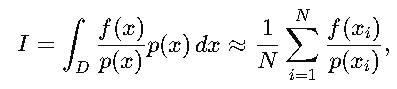
can be approximated by taking N random samples xi from a uniform distribution over D and computing the average:



where V is the volume of D. The Monte Carlo estimate converges to the true integral as N→∞, an outcome backed by the law of large numbers.

### Importance Sampling

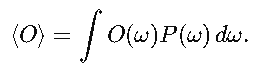
To improve efficiency, especially when some regions contribute more to I than others, **importance sampling** is used. This technique samples more frequently from regions where f(x) is larger. By selecting a probability density p(x) tailored to the shape of f(x), we can rewrite I as:



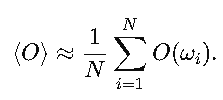
where samples xi​ are drawn according to p(x). This approach reduces variance, increasing the accuracy of the approximation​.

### Monte Carlo for Expectation Values

Monte Carlo is commonly used to approximate expectation values in physical systems. Given a system with states ω distributed according to P(ω), the expectation of an observable O(ω) is:



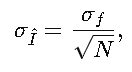
This can be approximated by generating N samples from P(ω) and calculating the average:



This estimation is foundational for Monte Carlo applications in physics, including simulations in statistical mechanics​.

### Statistical Error and Convergence

Monte Carlo estimates have statistical errors due to random sampling. For an estimator I^ of I, the standard error σI^​ is:



where σf is the standard deviation of f(x) over D. This error decreases with N, making Monte Carlo particularly useful for high-dimensional problems where deterministic methods are inefficient​.

## Markov Chain Monte Carlo method

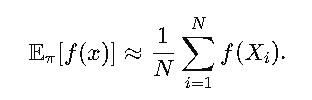
Markov Chain Monte Carlo (MCMC) is a collection of algorithms used for generating samples from a complex probability distribution π(x) by constructing a Markov chain with the desired distribution as its stationary distribution. In practical terms, MCMC methods generate a sequence of dependent random variables {X\_t}\_{t=0}^{∞} in such a way that, as t→∞, the distribution of X\_t​ approaches π(x). This sequence of samples can then be used to approximate expectations and other statistical properties of the target distribution, which may be difficult to compute directly in high-dimensional spaces.

In MCMC, the samples are generated as a **Markov chain**, a sequence where each state depends only on the immediate prior state, a property known as the **Markov property**. This memoryless characteristic can be described as:



The evolution of the chain is governed by a **transition kernel** P(x′∣x), which specifies the probability of transitioning from state x to state x′. This kernel is chosen to ensure that the chain has the target distribution π(x) as its stationary distribution, which the chain will converge to under certain conditions.

Once the Markov chain has reached equilibrium, samples from the chain can be used to approximate expectations of functions f(x)f(x)f(x) with respect to π(x). If X1, X2, …, XN are samples from the chain, the expectation Eπ[f(x)] can be approximated as:



By the **law of large numbers**, this sample average converges to the true expectation Eπ[f(x)] as N→∞, assuming the chain has reached its stationary distribution and samples are sufficiently independent. In practice, MCMC chains often exhibit **autocorrelation**, which means successive samples may be correlated. To account for this, techniques such as **thinning** (selecting every k-th sample) or **block averaging** are used to reduce the impact of correlation on estimates. [15]

One of the strengths of MCMC methods is their applicability to high-dimensional and complex distributions, where direct sampling is challenging. However, the efficiency of MCMC depends on the **mixing rate** of the chain, or how quickly it explores the configuration space. Slow mixing, often caused by poor choices of the transition kernel, can lead to biased estimates, as the chain may not fully represent π(x) within the time frame of the simulation. Advanced MCMC techniques, such as the Metropolis-Hastings algorithm and Gibbs sampling, address these issues by carefully tuning the acceptance criteria and proposal distributions to enhance mixing and ensure accurate convergence to the target distribution.

In the sequel we will see the Metropolis-Hastings algorithm, a particular form of a MCMC methods.

## A MCMC method: Metropolis-Hasting Algorithm

### Historical Background

The development of the Metropolis-Hastings algorithm began in the 1940s, during the Manhattan Project at the Los Alamos Laboratory, where scientists faced challenges in modeling complex physical systems, particularly in nuclear physics. Nicholas Metropolis, along with colleagues such as Stanislaw Ulam and John von Neumann, pioneered the MC method to simulate the random behavior of particles, an approach that laid the groundwork for what would become known as the Metropolis algorithm.

The foundational 1953 paper by Metropolis and co-authors, including Marshall and Arianna Rosenbluth and Edward and Augusta Teller, introduced a systematic method for sampling from high-dimensional probability distributions. Their approach relied on a probabilistic rule to accept or reject new configurations based on changes in energy, forming a Markov chain that converged to the target distribution. This technique, initially aimed at solving problems in statistical mechanics, enabled the practical computation of configurations for complex systems by iteratively sampling states weighted by their likelihood​.

The Metropolis algorithm was later generalized by W. K. Hastings in 1970, who introduced flexibility by allowing asymmetric proposal distributions. This extension broadened the algorithm's applicability, marking the inception of the "Metropolis-Hastings" algorithm as it is known today. Despite its power, the algorithm initially saw limited use outside of physics; it gained widespread attention among statisticians only in the 1990s as computing power increased, making such simulations more accessible​. [14]

### Mathematical basis

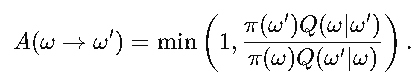
The Metropolis-Hastings algorithm, one of the foundational methods in MC simulations, based on Markov Chain Monte Carlo (MCMC) technique, is designed to sample from a target probability distribution π(ω) on a configuration space E={ω} by constructing a Markov chain that converges to this distribution. In practical terms, the algorithm enables efficient sampling from complex, high-dimensional distributions, particularly where direct sampling is impractical. The Metropolis-Hastings approach achieves this by iteratively generating a sequence of states {X\_t} that, as t→∞, approximates the target distribution.

**Initial Setup and Proposal Mechanism**

To begin, the algorithm requires an initial state X\_0∈E and a **proposal distribution** Q(ω′∣ω) that governs the generation of candidate states ω′ given the current state ω. This proposal distribution, which need not be symmetric, is chosen to enable the exploration of the configuration space effectively, balancing moves that explore new areas with those that improve the fit to π(ω). The flexibility of Q allows the algorithm to adapt to a wide range of distributions by tuning the proposal to the specifics of the problem at hand.

**Acceptance Probability and Transition Process**

Once a candidate state ω′ is proposed, the algorithm evaluates whether to accept this new state based on an **acceptance probability** A(ω→ω′). The acceptance probability is given by



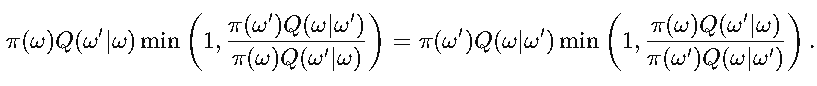
This formula incorporates the ratio of the target probabilities π(ω′)/π(ω) as well as the proposal probabilities Q(ω∣ω′) and Q(ω′∣ω), ensuring that moves to states with higher probability in π\piπ are favored while still allowing occasional moves to less probable states. This characteristic enables the algorithm to traverse energy landscapes by occasionally "jumping" out of local minima, fostering convergence toward the equilibrium distribution. If A(ω→ω′)=1, the algorithm unconditionally accepts the proposed state ω′; otherwise, it accepts ω′ with probability A(ω→ω′). Practically, this step is implemented by generating a uniform random number u∈[0,1] and accepting the move if u≤A(ω→ω′). If accepted, the chain transitions to the new state Xt+1=ω′; otherwise, it remains at Xt+1=ω.

**Detailed Balance Condition and Stationarity**

The Markov chain created by the Metropolis-Hastings algorithm converges to the target distribution π(ω) by satisfying the **detailed balance condition**, a property that ensures the equilibrium behavior of the chain. Formally, detailed balance requires that for any two states ω and ω′,



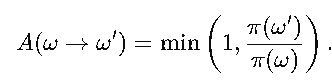
where P(ω→ω′) is the transition probability from ω to ω′, defined as P(ω→ω′)=Q(ω′∣ω)A(ω→ω′). Substituting the acceptance probability, detailed balance becomes:



This balance ensures that the probability flux between any pair of states is symmetrical, enabling the Markov chain to achieve and maintain the stationary distribution π(ω). Thus, as the number of iterations grows, the distribution of states in the chain increasingly approximates π(ω).

**Symmetric Proposal Distributions and the Metropolis Criterion**

A common simplification in the Metropolis-Hastings algorithm occurs when the proposal distribution Q(ω′∣ω) is symmetric, i.e., Q(ω′∣ω)=Q(ω∣ω′). In this case, the acceptance probability reduces to:



For systems in statistical physics, where π(ω) often represents a Boltzmann distribution, π(ω)∝e−E(ω)/kBT, this further simplifies to

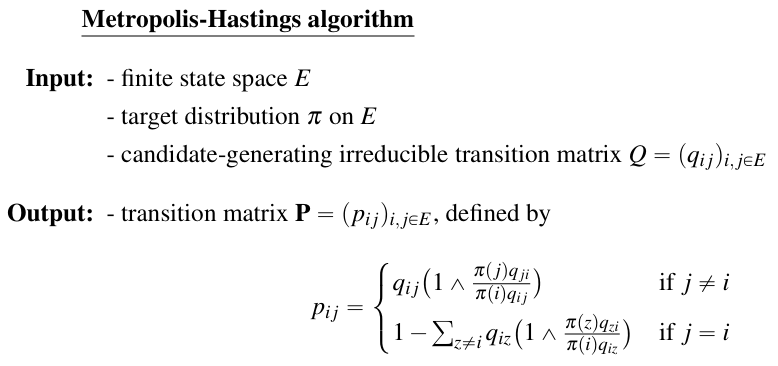


where E(ω) is the energy associated with configuration ω, and T represents temperature. This form, known as the **Metropolis criterion**, favors transitions to lower-energy states, though it occasionally allows transitions to higher-energy states, facilitating exploration.

**Ergodicity and Convergence to the Target Distribution**

The convergence of the Metropolis-Hastings algorithm to the target distribution π(ω) relies on the ergodicity of the Markov chain, meaning that it is possible to reach any state ω′ from any other state ω over time. This condition, along with detailed balance, guarantees that the Markov chain will sample from π(ω) as t→∞. Thus, under ergodic and balanced conditions, the algorithm provides a rigorous basis for approximating complex distributions through iterative sampling, making it invaluable across fields that require probabilistic modeling of high-dimensional systems​. [15]

To summarize



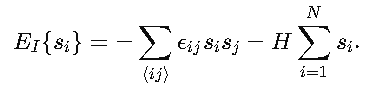
# Applications in simulation: Case Study of Z\_n Model

In this section, we examine two case studies: the Z\_{n}, which generalizes the Ising model to n-state spins and provides a platform for studying discrete phase transitions, and spin glasses, a class of disordered magnetic systems with complex energy landscapes.

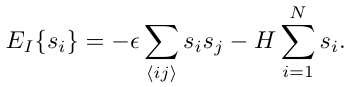
## Ising Model and extension to Z\_{n} model

The Ising model (or Lenz–Ising model), is a [mathematical model](https://en.wikipedia.org/wiki/Mathematical_models_in_physics) of [ferromagnetism](https://en.wikipedia.org/wiki/Ferromagnetism) in [statistical mechanics](https://en.wikipedia.org/wiki/Statistical_mechanics). The model consists of [discrete variables](https://en.wikipedia.org/wiki/Discrete_variables) that represent [magnetic dipole moments of atomic "spins"](https://en.wikipedia.org/wiki/Nuclear_magnetic_moment) that can be in one of two states (+1 or −1).

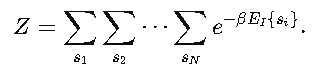
We consider a d-dimensional periodic lattice with n points in every direction so that there are N=n^d points in total in this lattice. In every point (lattice site) we put a spin variable s\_i(i = 1,…,N) which can take either the value +1 or −1. A configuration of this system of N spins is therefore specified by a set of numbers {s\_i}. In the Ising model, the energy of this system of N spins in the configuration {s\_i} is given by:



he parameter H is the external magnetic field. The symbol ⟨ij⟩ stands for nearest neighbour spins. The sum over ⟨ij⟩ extends over γN/2 terms where γ is the number of nearest neighbours. In 2, 3, 4 dimensions γ=4,6,8. The parameter ϵ\_ij is the interaction energy between the spins i and j. For isotropic interactions ϵ\_ij=ϵ. For ϵ>0, we obtain ferromagnetism while for ϵ<0 we obtain antiferromagnetism. We consider only ϵ>0. The energy becomes with these simplifications given by:



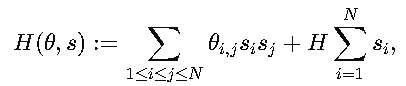
The partition function is given by



There are 2^N terms in the sum and β=1/kT.

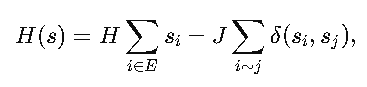
In d=2, we have N=n^2 spins in the square lattice. The configuration {s\_i} can be viewed as an n×n matrix. We impose periodic boundary condition as follows. We consider an (n+1)×(n+1) matrix where the (n+1)th row is identified with the first row and the (n+1)th column is identified with the first column. The square lattice is therefore a torus. [16]

In the Sherrington-Kirkpatrick model, introduced in 1975 [17], the Hamiltonian function is given by:

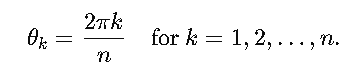


where θ\_i,j​ are assumed to be i.i.d. centered Gaussian random variables. This introduces disorder to the model, allowing for interactions between any pair of spins with random strengths, reflecting the complex energy landscape typical of spin glass systems. More general disordered models can be defined in terms of random mappings Θ:(i,j)∈{1,…,N}2↦θi,j, where the θ\_i,j​ values determine the nature of interaction between spin pairs.

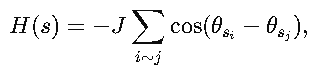
Another way to extend the Ising model is to replace the spin state {−1,+1} with a finite set of colours C:={c1,…,cn}, for some n≥1. In this situation, the energy of a configuration s∈S:=C^E is described by the Hamiltonian:



where H is the external field, J is the interaction strength, and δ(s\_i, s\_j) is the Kronecker delta function, which equals 1 if s\_i=s\_j and 0 otherwise. This model, originally introduced by Renfrey Potts in his 1951 PhD thesis, generalizes the Ising model by allowing each site to adopt one of n possible states. A more physical variant, known as the planar Potts model or clock model, was suggested by Cyril Domb. In this model, the spins are replaced by angles defined as



The energy of a configuration s∈S:={1,…,n}^E is given by the Hamiltonian:

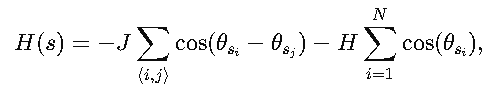


where the cosine term captures the angular interaction between neighbouring spins on a lattice. The four-state clock model is sometimes termed the Ashkin-Teller model was introduced by in 1943 by Julius Ashkin and Edward Teller in [18]. This model, which generalizes the Z\_n model, allows for studying systems with n-fold rotational symmetry, providing insights into phase transitions and symmetry breaking behaviours in discrete systems with cyclic symmetry.

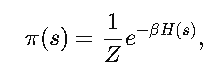
## Simulations of Z\_model via Metropolis-Hasting algorithm

To simulate the Zn​ model, we apply the Metropolis-Hastings algorithm, that generates samples from a desired probability distribution by constructing a Markov chain with the target distribution as its stationary distribution. In this case, the target distribution is the Boltzmann distribution for the Zn model, which assigns probabilities to configurations based on their energies. This approach allows us to study equilibrium properties of the​ model, particularly as the system undergoes phase transitions.

In the Zn​ model, each lattice spin s\_i​ can take one of n discrete states, represented as phases θsi=2πk/n​ where k=0,1,…,n−1. This setup imparts n-fold rotational symmetry to the model. The Hamiltonian H(s) for a configuration s={si}:



The Boltzmann (Gibbs) distribution, which is the target distribution for the Markov chain, assigns a probability to each configuration s as: [15, 17]



The partition function Z normalizes the distribution, summing over all configurations s. Directly computing Z is generally infeasible for large systems, as it involves summing over an exponentially large number of configurations. Therefore, we use the Metropolis-Hastings algorithm to sample from π(s) without explicitly calculating Z.

### Steps of the Metropolis-Hastings Algorithm for the Zn​ Model

The Metropolis-Hastings algorithm generates a sequence of configurations (states) by proposing small modifications to the current configuration and accepting or rejecting these modifications based on a probabilistic criterion. The goal is to construct a Markov chain that converges to the equilibrium distribution π(s)\pi(s)π(s).

**Step 1: Initialization**

We begin with an initial configuration s^(0) where each spin s\_i is assigned one of the n possible states. This initial configuration can be randomly generated or set to a predefined state, such as all spins aligned in one direction. The energy H(s^(0)) of this configuration is computed using the Hamiltonian.

**Step 2: Proposal Step**

In each iteration t of the algorithm, we randomly select a single spin si and propose a new state si′ for this spin. The proposed state si′ is drawn uniformly from the n possible states. The proposal distribution Q(si′∣si) is symmetric, so the probability of proposing s\_i′ from s\_i​ is the same as proposing s\_i​ from s\_i′​, i.e., Q(s\_i′∣s\_i)=Q(s\_i∣s\_i′).

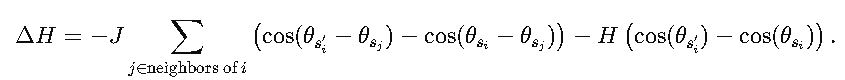
The new configuration s′ is identical to s except for the change at site i, where s\_i is updated to s\_i’. We denote the proposed configuration as s′={s1,s2,…,si−1,si′,si+1,…,sN}.

**Step 3: Energy Difference Calculation**

To determine whether to accept the proposed move, we calculate the energy difference ΔH\Delta HΔH between the proposed configuration s′ and the current configuration s:



Since only one spin si is modified, this energy difference can be efficiently calculated by considering only the interactions involving si and its neighbours, rather than recalculating the entire Hamiltonian. The energy change ΔH is given by:



**Step 4: Acceptance Criterion**

The Metropolis-Hastings algorithm accepts the proposed state s′ with probability:



This acceptance probability ensures that the Markov chain satisfies **detailed balance**, a key property that guarantees convergence to the equilibrium distribution π(s)\pi(s)π(s). Detailed balance requires that, at equilibrium, the probability flux from s to s′ equals the flux from s′ to s, i.e.,



Given that Q(si′∣si)=Q(si∣si′) due to the symmetry of the proposal distribution, the acceptance probability is sufficient to satisfy detailed balance.

To implement this step, a uniform random number uuu is generated from the interval [0,1]. If u≤P(accept), the proposal is accepted, and we set s^(t+1)=s′. Otherwise, the proposal is rejected, and the configuration remains unchanged: s^(t+1)=s^(t).

**Step 5: Iteration and Convergence**

Steps 2 to 4 are repeated over many iterations, constructing a sequence of configurations s^(0),s^(1),…,s^(T) that approximates samples from the equilibrium distribution π(s) after a sufficient number of steps. This sequence of configurations forms a Markov chain that, given enough time, converges to the target distribution.

**Equilibration and Sampling**

After an initial **equilibration phase**—during which the chain reaches a steady state—samples are collected periodically to calculate thermodynamic observables such as magnetization M, susceptibility χ, and specific heat C. These observables help characterize the system’s behaviour, particularly near phase transitions.

## Observation and Results

### 3.3 Observations and Results

In this section, we present the theoretical background for key observables in the \( \mathbb{Z}\_n \) model, particularly those related to critical phenomena, phase transitions, and correlations. These concepts are essential for understanding the behavior of the system near critical points, where phase transitions occur. By simulating the \( \mathbb{Z}\_n \) model using the Metropolis-Hastings algorithm, we can numerically compute these observables and analyze the results to gain insights into the physical properties of the system.

#### 3.3.1 Critical Exponents

Critical exponents describe the behavior of physical quantities near a phase transition and are a hallmark of universality in statistical physics. For the \( \mathbb{Z}\_n \) model, the critical exponents characterize how observables such as magnetization \( M \), susceptibility \( \chi \), correlation length \( \xi \), and specific heat \( C \) diverge or vanish as the system approaches the critical temperature \( T\_c \). The key critical exponents include:

- \*\*Magnetization exponent \( \beta \)\*\*: Near \( T\_c \), the magnetization \( M \) behaves as

\[

M \propto (T\_c - T)^{\beta}

\]

for \( T < T\_c \).

- \*\*Susceptibility exponent \( \gamma \)\*\*: The susceptibility \( \chi \) diverges as

\[

\chi \propto |T - T\_c|^{-\gamma}.

\]

- \*\*Correlation length exponent \( \nu \)\*\*: The correlation length \( \xi \), which measures the range over which spins are correlated, diverges near \( T\_c \) as

\[

\xi \propto |T - T\_c|^{-\nu}.

\]

- \*\*Specific heat exponent \( \alpha \)\*\*: The specific heat \( C \) behaves as

\[

C \propto |T - T\_c|^{-\alpha}.

\]

The values of these exponents depend on the dimensionality of the system and the symmetry of the model (characterized by \( n \)). In many cases, they follow universal behavior that is independent of microscopic details, placing the system in a specific universality class. The \( \mathbb{Z}\_n \) model, for varying \( n \), belongs to different universality classes, ranging from Ising-like behavior (\( n = 2 \)) to more complex classes for larger \( n \).

\*// Insert computed critical exponents for the simulated \( \mathbb{Z}\_n \) model here, comparing with theoretical predictions or known universality classes.\*

#### 3.3.2 Correlation Functions

The \*\*correlation function\*\* \( G(r) \) measures the extent to which spins separated by a distance \( r \) are correlated. In the \( \mathbb{Z}\_n \) model, the correlation function for spins \( s\_i \) and \( s\_j \) separated by \( r = |i - j| \) is defined as:

\[

G(r) = \langle s\_i s\_j \rangle - \langle s\_i \rangle \langle s\_j \rangle,

\]

where \( \langle \cdot \rangle \) denotes an ensemble average. At temperatures far from \( T\_c \), \( G(r) \) decays rapidly, indicating short-range order. Near \( T\_c \), \( G(r) \) decays more slowly, with a characteristic length scale given by the correlation length \( \xi \).

As \( T \to T\_c \), the correlation length \( \xi \) diverges, and the decay of \( G(r) \) follows a power law:

\[

G(r) \sim \frac{e^{-r/\xi}}{r^{d-2+\eta}},

\]

where \( \eta \) is another critical exponent, and \( d \) is the dimensionality of the system.

\*// Insert plots of correlation functions for different temperatures, showing how \( G(r) \) changes as the system approaches \( T\_c \).\*

#### 3.3.3 Renormalization and Scaling Theory

Renormalization group (RG) theory provides a powerful framework for understanding phase transitions and critical phenomena. It describes how systems behave under changes in scale and explains why different physical systems can exhibit similar behavior near critical points. In the context of the \( \mathbb{Z}\_n \) model, RG theory can be used to determine the scaling behavior of observables near \( T\_c \).

Scaling theory postulates that near a phase transition, physical quantities follow universal scaling forms. For instance, the free energy \( f(T, h) \) in the presence of an external field \( h \) can be written as:

\[

f(T, h) = b^{-d} f(b^{y\_T} (T - T\_c), b^{y\_h} h),

\]

where \( b \) is a rescaling factor, and \( y\_T \) and \( y\_h \) are scaling exponents associated with temperature and external field, respectively. By iteratively rescaling the system, we can analyze how observables behave under scale transformations, leading to predictions for the critical exponents.

\*// Insert discussion or theoretical application of renormalization concepts for the observed critical behavior in the \( \mathbb{Z}\_n \) model.\*

#### 3.3.4 Phase Transitions: Primary and Secondary Transitions

The \( \mathbb{Z}\_n \) model can exhibit different types of phase transitions depending on the value of \( n \) and the temperature \( T \).

- \*\*Primary Phase Transition\*\*: This is the transition between ordered and disordered phases. For \( T < T\_c \), the spins are aligned in one of the \( n \) preferred directions, breaking symmetry and resulting in a long-range order. For \( T > T\_c \), thermal fluctuations destroy this order, leading to a disordered phase. This transition is often continuous (second-order) for smaller values of \( n \) (e.g., \( n = 2, 3, 4 \)), where critical behavior is governed by the universality class of the system.

- \*\*Secondary Phase Transition\*\*: In certain cases, particularly for larger \( n \), the \( \mathbb{Z}\_n \) model can undergo additional transitions within the ordered phase. These secondary transitions reflect changes in the internal ordering structure of the spins without fully breaking symmetry. Such transitions are often associated with changes in the nature of the spin configurations, such as transitions between distinct ordered phases (e.g., from a partially ordered to a fully ordered phase).

\*// Insert plots or computed results that show the behavior of order parameters (like magnetization) as a function of temperature, indicating the primary and secondary phase transitions.\*

#### 3.3.5 Specific Heat and Susceptibility

The \*\*specific heat\*\* \( C \) and \*\*susceptibility\*\* \( \chi \) are key observables in studying phase transitions. Peaks in \( C \) and \( \chi \) typically occur near \( T\_c \), reflecting the system’s enhanced response to temperature and external field fluctuations, respectively.

- \*\*Specific Heat \( C \)\*\*: This measures the response of the system’s energy to changes in temperature and is given by:

\[

C = \frac{\langle H^2 \rangle - \langle H \rangle^2}{k\_B T^2}.

\]

Near \( T\_c \), the specific heat often shows a peak, with its height and sharpness depending on the dimensionality and symmetry of the system. In continuous phase transitions, \( C \) typically diverges as \( T \to T\_c \) following a power law with exponent \( \alpha \).

- \*\*Susceptibility \( \chi \)\*\*: The susceptibility measures the response of the magnetization to an external magnetic field \( H \) and is defined as:

\[

\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k\_B T}.

\]

It diverges as \( T \to T\_c \), indicating long-range correlations and large fluctuations in magnetization near the critical point.

\*// Insert computed specific heat and susceptibility plots, highlighting peaks at \( T\_c \) to illustrate critical behavior.\*

#### Summary of Results

In summary, the simulation of the \( \mathbb{Z}\_n \) model provides insights into critical phenomena and phase transitions by allowing us to compute and analyze observables such as critical exponents, correlation functions, and susceptibility. By examining these quantities near the critical temperature, we can observe and characterize both primary and secondary phase transitions, study scaling behavior, and explore the model’s universality class.

\*// Insert a concluding table or summary of numerical results for observables and critical exponents, comparing with theoretical values and known results.\*

# Conclusion

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