

UNIVERSITY OF BONN

PHYSICS760: COMPUTATIONAL PHYSICS

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# Ising Model

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# Contents

## 1 Introduction

### 1.1 Ising Model

The Ising model is a lattice representation of magnetic dipole moments of atomic spins,  $\sigma_i$ . The hamiltonian,  $\mathcal{H}$  for a specific configuration of spins is given by;

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \mu H \sum_i \sigma_i \quad (1)$$

Where  $\langle i, j \rangle$  denotes that the summation is over pairs of neighboring spins.  $J$  is the interaction constant discussed below, while  $H$  is an external magnetic field and  $\mu$  the magnetic moment. The value of the spins, which are confined to the lattice sites are restricted to be either up or down, i.e,  $\sigma$  takes values of  $\pm 1$ . The system favors a state of minimum energy, hence the sign of  $J$  dictates the nature of the material such that  $J > 0$  indicates a **ferromagnetic** material while for an **antiferromagnetic**, an anti-parallel alignment of spins is favored, hence  $J < 0$ .

The net alignment of unpaired electron spins of atoms in a material determine the nature of the material. For a paramagnetic material, in the presence of an applied external magnetic field,  $H$ , the spins align parallel to  $H$ , resulting in attraction. In a diamagnetic material, the net alignment of the unpaired spins is such that the net dipole moment opposes  $H_{ext}$ , resulting in repulsion. In a ferromagnet, ordering exists in regions known as domains which in the absence of  $H_{ext}$  are randomly oriented in the material. In the presence of an external magnetic field, the domain boundaries are shifted such that domains parallel to  $H_{ext}$  grow, while the rest shrink, resulting in a net magnetization; retained even in the absence of the external field. At a certain temperature known as the critical temperature,  $T_c$ , a ferromagnet goes through a second order phase transition<sup>1</sup> due to thermal motions, such that the domains are randomly distributed and the material exhibits paramagnetic behavior.

The two dimensional Ising Model is among the simplest lattice models and is used to study systems undergoing a phase transitions; it was initially formulated to show that a ferromagnet loses its magnetization above a certain

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<sup>1</sup>The second order derivatives of the free energy are discontinuous at  $T_c$

critical temperature,  $T_c$ . Here a phase transition is described for a system in thermal equilibrium that undergoes a change between an ordered state to a disordered state at  $T_c$  which can be described by an order parameter[?]. In the case of a ferromagnet, the defined order parameter is the spontaneous magnetization,  $M$ ;

$$M = M_o \epsilon^\beta \quad (2)$$

with  $\epsilon = |1 - T/T_c|$  and  $\beta$  the critical exponent. The order parameter is a property of the system which is non-zero in the ordered phase but identically zero in the disordered phase.

While a one dimensional lattice Ising Model shows no phase transition, Onsager solved the two dimensional Ising model analytically using the transfer matrix method, in the absence of a magnetic field. In this study, we solve the Ising Model numerically using computational methods. we use computational methods to study the Ising Model. Ising Model brief introduction. (2 dimensional) Why do we use computational methods. Moreover the Ising Model has been used to study other problems such as phase separation in binary alloys and crystal growth.

## 1.2 Computational Methods

The Ising model is a canonical ensemble, with a partition function for a particular spin configuration  $x$  is given by;

$$\mathcal{Z} = \sum_x \exp(-\mathcal{H}/(K_B T))$$

And the probability of the system to be in a certain state at a time  $t$  is given by

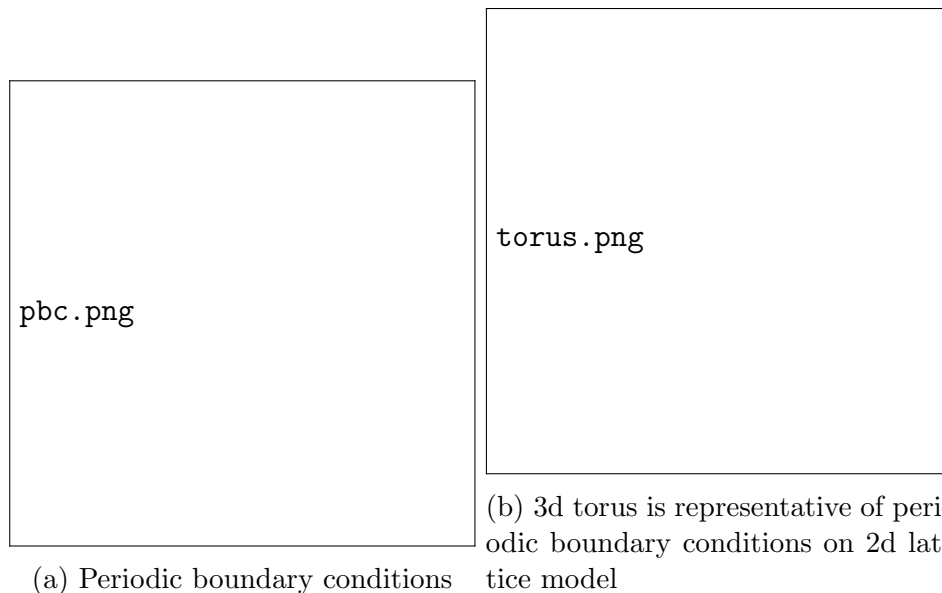
$$P_x(t) = \frac{1}{\mathcal{Z}} e^{-\frac{\mathcal{H}}{k_b T}} \quad (3)$$

For a system with large  $N$ , few of the states are realized hence it is not efficient to sample states uniformly, rather we apply an importance sampling; importance sampling Monte Carlo methods, which involves repeated random sampling to obtain numerical results, where states are chosen that have a large weight in  $\mathcal{Z}$ .

### 1.2.1 Periodic Boundary Conditions

Since the simulations are carried out on a finite lattice with boundaries, a way around this is to ‘eliminate’ the boundaries by applying periodic boundary

conditions. This is done such that the spins on the first row interact or ‘see’ the spins of the last row, and the same with the columns of the lattice such that the 2d lattice is folded into a 3d torus; this is shown in figure ??.



The results of this configuration differ from those of an infinite lattice since the correlation length is limited to  $L/2$  [?]

### 1.3 Finite size scaling

The finite size of the lattice limits the determination of a second order phase transition (point of divergence). While the use of periodic boundary conditions minimizes this effect, the problem is resolved by extrapolating the theoretical value given the limited resource of a finite lattice[?]. We define the critical exponents of the Ising Model showing their dependence on lattice size;

$$M = \tag{4}$$

$$23 \tag{5}$$

$$(6)$$

Thus by plotting ln-ln graphs, the critical exponents (with the exception of  $\alpha$ ) can be obtained from the slopes. Finally, the fourth order cumulant [?] is used to determine  $T_c$  defined by equation ??

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2} \quad (7)$$

## 1.4 Metropolis Algorithm

The probability of the system being in state  $n$  at time  $t$  is given by;

$$\frac{\partial P_n(t)}{\partial t} = - \sum_{n \neq m} [P_n(t)W_{n \rightarrow m} - P_m(t)W_{m \rightarrow n}]$$

Where  $W_{n \rightarrow m}$  is the transition rate for  $n \rightarrow m$ . The probability of the  $n$ th state is given by equation ?. The value of the denominator,  $Z$  is not known and hence a Markov chain<sup>2</sup> of states is generated, such that the denominator cancels out and the transition rate depends only on the energy difference,  $\Delta E$  between the two states;

$$W_{n \rightarrow m} = \begin{cases} \tau^{-1} e^{(-\Delta E/k_B T)} & \Delta E > 0 \\ \tau^{-1} & \Delta E < 0 \end{cases}$$

$\tau^{-1}$  is the time taken for a spin flip and is set to one. The metropolis algorithm can be summarized as;

1. The lattice is initialized with a random spin configuration<sup>3</sup>  $s = (s_1, s_2, \dots, s_N)$  and temperature  $T$
2. For each Monte Carlo<sup>4</sup> sweep performed through the lattice;
  - (a) The change in energy  $\Delta E$  is calculated resulting from a new configuration  $s' = (s_1, s_2, \dots, s_i \dots s_N)$  generated by flipping the spin at lattice site  $i$ .
  - (b) If  $\Delta E < 0$ , then the spin flip is accepted else; a random number  $r$  is generated such that  $0 < r < 1$  and the new configuration,  $s'$  is accepted if  $r < \exp(-\Delta E/k_B T)$ .

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<sup>2</sup>Markov chain

<sup>3</sup>A random configuration has the benefit of using less computing time compared to a homogeneous configuration

<sup>4</sup>Every lattice in the system is considered once

3. The required observables Magnetization,  $M$ , specific heat,  $C_v$ , and energy  $E$  are stored.

Since we want to observe a phase transition, the algorithm is implemented within a temperature loop; for each temperature step, the average magnetization  $\langle M \rangle$ , specific heat  $C$  and susceptibility  $\chi$  defined below were stored. Results depend on temperature, lattice size. The observables used are defined as;

$$\langle M \rangle = \frac{1}{N} \sum_{i=1}^N s_i \quad C = \frac{\partial E}{\partial T} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_b T^2} \quad \chi = \frac{\partial M}{\partial T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_b T}$$

QUESTION: HOW DO WE ACTUALLY DETERMINE THE CRITICAL TEMPERATURE?? EQUILIBRATION Since initial conditions are random, it may take a while for the system to equilibrate; for this reason, the averages are only calculated and

## 1.5 Heat Bath

The heat bath algorithm is a modified metropolis and is most applicable in cases where the Metropolis algorithm has a low acceptance rate such as in lattice gauge models. A spin flip  $-s_i$  at lattice site  $i$  is determined by considering all its possible states in the heat bath of its neighbors, which are considered fixed. The transition probability is given by;

$$W_{n \rightarrow m} = \frac{\exp(-\beta k_b T s'_i h_0)}{\exp(\beta k_b T h_0) + \exp(-\beta k_b T h_0)} = \frac{\exp(-\beta \Delta E)}{\exp(-\beta \Delta E) + 1} \quad (8)$$

With  $\beta = \frac{1}{k_b T}$  and  $h_0 = \sum_{j \in \langle i, j \rangle} s_j$ ,  $\Delta E = (s'_i - s_i) h_0$  WHAT IS THE ACTUAL ALGORITHM?

In this case the acceptance for a trial spin configuration,  $s'$  is not determined by  $\Delta E$  but is accepted if for a given random number,  $r$ ;

$$r < \exp(-E'/k_B T)$$

Where  $E'$  is the energy of the trial state. The difference in the two algorithms is seen when  $\Delta E = 0$ ; in the metropolis algorithm, the spin flip is always accepted, while in the heat bath method, the flip is only accepted half of the time. A comparison in the efficiencies of the two methods is done in this study. Spin configuration is generated from a previous state using a transition probability depending on the energy difference,  $\Delta E$  between the final and initial states.

## 1.6 Wolff Algorithm

This algorithm involves flipping a cluster of spins rather than a single spin of the lattice; known as a cluster algorithm. Reason for this is that Critical slowing down is observed close to  $T_c$  attributed to large spatial correlations [?]. A solution to this is to apply non-local/collective updates to the system, hence the use of clusters. A cluster is formed by selecting an initial site and creating bonds between pairs of spins in the same state with probability,

$$p = 1 - e^{-K\delta_{s_i s_j}} \quad (9)$$

With  $K = J/k_b T$ . Th This process is continued until no new bonds are created and the entire cluster of similar spins is then flipped. Another site is selected and the process repeated. Another initial is site is selected and the process repeated. The probability in equation ?? is derived from the q-state Potts model [?] with partition function  $Z = \sum_{s_i} e^{-K \sum_{i,j} \delta_{s_i s_j} - 1}$  and the sum is over all states of  $s_i = 1, 2, \dots, q$ . In this model, a bond is formed between nearest neighbors only if they are in the same state.

## 1.7 Finite size scaling results

# 2 Results

## 2.1 Comparison to Onsager's Results

# 3 Theoretical Background

Magnetism(ferro, para), Critical Temp.. Heat capacity, Magnetisation, Susceptibility - Critical exponents. Onsager's solution.

# 4 Computational methods

Monte Carlo Boundary conditions Metropolis and Heat Bath Wolf Algorithm  
Finite size scaling (since finite lattice does not exhibit phase transitions.)

## 5 Results

Comparison of lattice size (with both heat bath and metropolis). Mention  $T_c$ , critical exponents etc. Onsager's results (with both heat bath and metropolis) Finite size scaling Wolf algorithm? Cluster algorithm? N dimensions?

## 6 Conclusion

## References

- [1] David P. Landau and Kurt Binder *A guide to Monte Carlo Simulations in Statistical Physics*
- [2] Jacques Kotze *Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet*
- [3] Wolfhard Janke *Monte Carlo Methods in Classical Statistical Physics* Institut für Theoretische Physik and Centre for Theoretical Sciences, Universität Leipzig