

2D ISING MODEL

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Abstract

This report provides the basic physics of the Ising model for the exam of "Software and Computing for Nuclear and Subnuclear Physics".

1 Introduction

The Ising model is a mathematical model developed to describe magnetism in materials. In particular, this model provides a description of the phase transition from ferromagnetism to paramagnetism when the temperature exceeds a certain critical value. The Ising model considers a lattice of particles, each characterized by a binary variable known as spin, which can take values of either +1 or -1. These spins interact with their nearest neighbors, leading to the emergence of collective magnetic properties. Ferromagnetic materials are characterized by the alignment of all spins, whereas paramagnetic materials exhibit disordered spins due to thermal fluctuations. An example of such system is represented in Fig.(1) .

2 Ising model

The Ising model is defined on a lattice, where each site i on the lattice is associated with a spin variable s_i . These spins interact with their nearest neighbors, leading to an energy associated with each configuration of spins. The Hamiltonian, or energy function, of the system is given by:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - \mu B \sum_i s_i \quad (1)$$

The coupling constant J is positive, the ferromagnetic interaction favors the alignment of the spins. The minus sign in front of the expression is necessary because the favored configurations are those that minimise the energy: two aligned spins will have, in case of null external magnetic field B , $E = -J$, on the contrary two opposite spins will have $E = J$. Since the energy is an integer multiple of J , we decide to use it as unit, we thus take it as equal to 1. What makes this system so interesting to study is the fact that an analytical solution

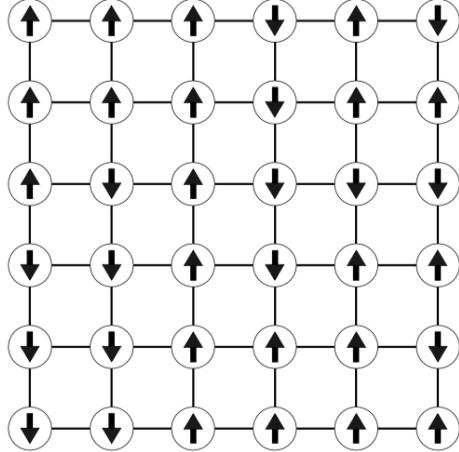


Figure 1: Representation of the Ising model on a bi-dimensional square lattice.

exists, making a comparison possible, thus it is a strong test to understand whether the numerical code presented in the repository is accurate. This is in general a very important feature for Monte-Carlo based simulations, when a new analysis is developed it is important to test on known solutions or experimental data, if the tests are successful further analyses can be performed. In the Ising model we can associate at each microscopical configuration s a macroscopical quantity, two possible macroscopical quantities are the magnetization and the energy. They are defined as:

$$m(s) = \frac{M(s)}{N} = \frac{1}{N} \sum_{i=1}^N s_i \quad e(s) = \frac{E(s)}{N} = -\frac{1}{N} \sum_{(i,j)} s_i s_j \quad (2)$$

Naturally each system tends to relax towards minimum energy configurations when the temperature is low enough, when the temperature is high the thermal agitation allows the configurations at higher energies. To study the properties of the model at temperature T we can use the canonical ensemble in each spin configuration has a weight equal to the Gibbs-Boltzmann measure:

$$P_{GB}(s) = \frac{\exp(-E(s)/T)}{Z} \quad (3)$$

where Z is the partition function known as $Z = \sum_s \exp(-E(s)/T)$. From 3 we see that in the limit where $T \rightarrow \infty$ all the configurations share the same probability, in the limit where $T \rightarrow 0$ the probability distribution favors the two minimum energy configurations. For what follows it is useful to define the ensemble average of the canonical ensemble as:

$$\langle A \rangle_T = \frac{\sum_s A(s) \exp(-E(s)/T)}{\sum_s \exp(-E(s)/T)} = \sum_s A(s) P_{GB}(s) \quad (4)$$

where the sum is extended to the 2^N configurations of the system. In the bi-dimensional Ising model the average absolute value, in the thermodynamic limit $N \rightarrow \infty$, has the following expression:

$$\langle |m| \rangle_T = m_0(T) \equiv \left(1 - \left(\sinh \frac{2}{T} \right)^{-4} \right)^{1/8} \quad (5)$$

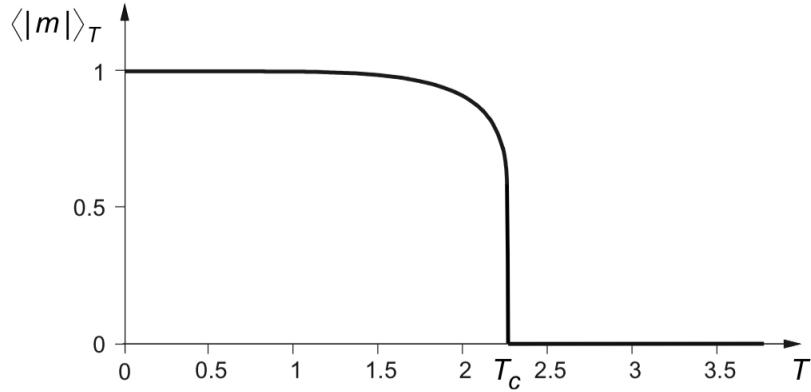


Figure 2: Average magnetization as a function of the temperature.

At the critical temperature $T_C = \frac{2}{\log(1+\sqrt{2})} \simeq 2.269$ the model experiences a phase transition switching from the paramagnetic phase, where $T > T_C$, in which the average magnetization is null, to the ferromagnetic phase where the average magnetization is provided by the above expression 5, as shown in Fig.(4). The exact solution of the Ising model requires the calculation of the canonical averages of the type 4, making necessary a number of operations proportional to 2^N , exponential in N. Fortunately an alternative route exists: the application of Monte Carlo method.

3 Monte Carlo method and the Ising model

Consider a discrete integral of the form:

$$\sum_C A(C)P(C), \quad \sum_C P(C) = 1, \quad P(C) \geq 0 \quad \forall C \quad (6)$$

$P(C)$ is a very dense probability distribution in an extremely small region of the integration domain, $A(C)$ is a function that is slowly varying in that domain. The sum is of course extended over a large number of configurations, in the application to the Ising model it is exponential in the number of variables as

seen in the previous section. Monte Carlo method provide a way to compute this sum in an efficient way. To understand it properly the concepts of Markov Chains and the Metropolis algorithm are necessary.

3.1 Markov Chains

Consider a discrete and limited set of configurations or states and consider a dynamical process on this set that evolves discretely. If the evolution is such that the probability that the system is in a configuration $C(t+1)$ at the discrete time $t+1$ only depends only on the preceding configuration $C(t)$ the system forms a *Markov Chain*. The essential feature is that the evolution does not depend on the overall history of the system, the Markov Chain is memory-less. A Markov Chain is defined by a set of states and by the transition probabilities w_{ij} from a generic state i and a generic state j . In general the probability of being in a state i at the discrete time $t+1$ can be written as:

$$p_i(t+1) = \sum_j p_j(t) w_{ij} \quad (7)$$

where $p_j(t)$ is the probability of being at time t in the state j and w_{ij} is the probability of evolving from state j to state i . Clearly for the axioms of probability we need:

$$\sum_i p_i(t) = 1 \quad (8)$$

implying that:

$$\sum_j w_{ij} = 1 \quad (9)$$

Combining these equations we can rewrite 7 in the *master equation* form:

$$p_i(t+1) - p_i(t) = \sum_j p_j(t) w_{ji} - \sum_j p_i(t) w_{ij} \quad (10)$$

Once the probability distribution at the initial state is known, i.e. $p_i(0) \forall i$, with the master equation we are able to compute the probability of finding the dynamical process in each state of the Markov Chain for each time. The master equation can be written in a vector form as:

$$\vec{p}(t+1) = \vec{p}(t) \cdot \hat{w} \quad (11)$$

where the vector $\vec{p}(t) \equiv (p_1(t), \dots, p_N(t))$ contains the whole probability distribution at the time t and the elements of the matrix \hat{w} are the transition probabilities w_{ij} . In this notation it is straightforward to write the solution at time t from the initial condition:

$$\vec{p}(t) = \vec{p}(0) \cdot \hat{w}^t \quad (12)$$

where \hat{w}^t is the t -th power of the matrix \hat{w} . A Markov Chain is said to irreducible if for any pair of states, a sequence of non-zero probability transition allows to

move from one state to another. For long times the probability is concentrated only on the irreducible part of a Markov Chain. If the probability of recurrence of a state is non-zero in the long time limit the Markov Chain is said to be *ergodic*. If the Markov Chain is irreducible and ergodic it is possible to show that the following limit exists and does not depend on the initial condition:

$$\pi_i = \lim_{t \rightarrow \infty} p_i(t) \quad (13)$$

The vector $\vec{\pi}$ defines the asymptotic probability distribution that solves the master equation in the long time limit.:

$$\pi_i = \sum_j \pi_j w_{ji} \quad (14)$$

This equation shows that the asymptotic distribution is stationary, all the states visited by the dynamical process with a time-independent probability. Equation 14 can be rewritten as the *balance equation*:

$$0 = \pi_i - \sum_j \pi_j w_{ji} = \sum_j (\pi_i w_{ij} - \pi_j w_{ji}) \quad \forall i \quad (15)$$

The easiest way to solve this equation is to set:

$$\pi_i w_{ij} = \pi_j w_{ji} \quad (16)$$

Possible solutions are:

$$w_{ij} = 1, w_{ji} = \pi_i / \pi_j \quad (17)$$

and

$$w_{ij} = \pi_i / \pi_j, w_{ji} = 1 \quad (18)$$

3.2 Metropolis algorithm

The Metropolis algorithm allows the exploration of a large number of states at a fixed number of steps. For this purpose it is desirable to have a low probability of remaining in the same state. Let's see how this is possible thanks to the Metropolis algorithm, assuming the initial state i , the phases are:

- Propose a new state j with a symmetric probability $u_{ij} = u_{ji}$.
- Accept the new state j with a probability equal to $\min(1, \frac{\pi_j}{\pi_i})$, otherwise you reject it and remain in the initial state at time $t + 1$.

In other words the system changes if the new state has a larger probability compared to the previous one. Otherwise it moves only with a probability given by the ratio between the two probabilities, thus it's unlikely that it will move on states with low probability, unless it comes from an even more unlikely state. Let's see if these transition probabilities are in agreement with the detailed balance equation. From the definition of the algorithm we have:

$$w_{ij} = u_{ij} \min\left(1, \frac{\pi_j}{\pi_i}\right) \quad (19)$$

this is the probability that the j state is proposed times the probability that it is accepted. Inserting this solution in 15 we have:

$$\pi_i u_{ij} \min(1, \frac{\pi_j}{\pi_i}) = \pi_j u_{ji} \min(1, \frac{\pi_i}{\pi_j}) \quad (20)$$

From the symmetry of the matrix u we have that the identity is exact.

3.3 Back to the Ising model

As previously said the exact solution of the Ising model requires the computation of the thermodynamic averages over a large number of configurations, exponential in the number of sites in the lattice. To reduce the number of configurations to visit we can apply the Monte Carlo method and the Metropolis algorithm to explore only the regions that contribute mostly to the average, neglecting the states with low probability. We can apply the algorithm considering the Gibbs-Boltzmann measure as asymptotic distribution π_i of the Markov Chain. We apply now the algorithm and consider a new configuration that differs only by the spin of a single site, known as single spin flip. In this way any configuration can be changed in N different ways. For simplicity we consider a random site in the lattice. The steps to follow to study the Ising model are:

- Choose randomly a site of the lattice and flip the spin, we call s the initial configuration and s' the configuration after the single spin flip.
- Compute the energy difference $\Delta E = E(s') - E(s)$
- If $\Delta E \leq 0$ we accept the new configuration and the step is over
- Else we extract a random number r uniformly in the interval $[0, 1]$
 - If $r \leq \exp(-\Delta E/T)$ we accept the new configuration s'
 - If $r > \exp(-\Delta E/T)$ we discard the new configuration s'

At the end of the steps, enough to reach the equilibrium condition, the averages are computed. In the code `2D.cpp` the energy, magnetization and heat capacity are computed. The total energy is computed as follows, including also the contribution of an external magnetic field:

$$E = -J \sum_{i,j} \langle i,j \rangle s_{ij} s_{i'j'} - \mu B \sum_{i,j} s_{ij} \quad (21)$$

Total magnetization is defined as the sum of all the spins in the lattice sites:

$$M = \frac{1}{L^2} \left| \sum_{i,j} s_{ij} \right| \quad (22)$$

Heat capacity is instead defined as:

$$C_V = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \quad (23)$$

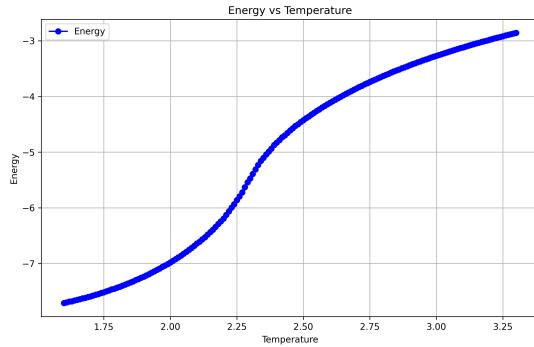


Figure 3: Energy as a function of temperature

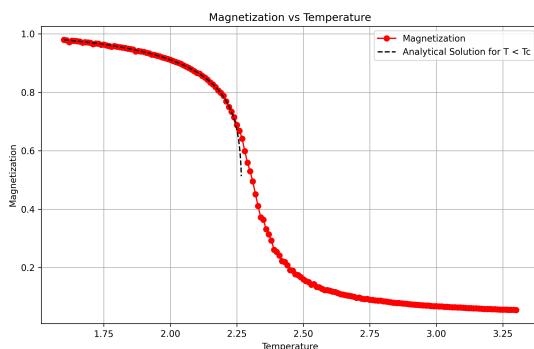


Figure 4: Magnetization as a function of temperature

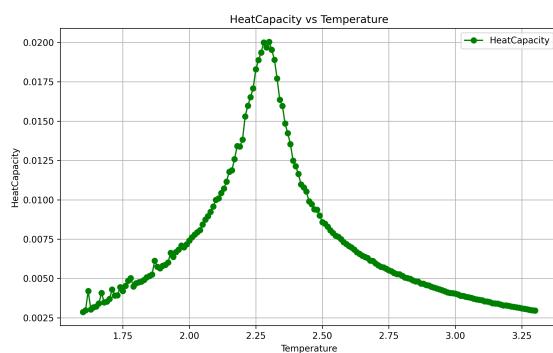


Figure 5: Specific heat as a function of temperature

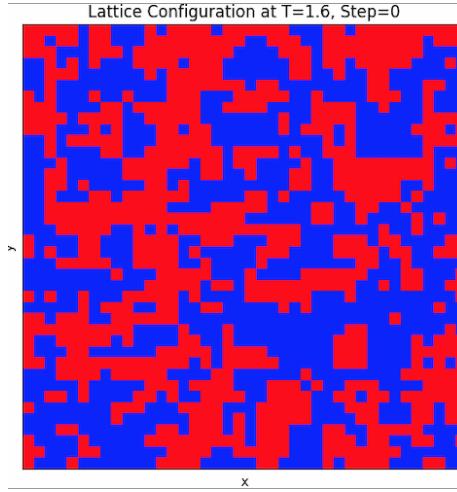


Figure 6: Initial random spin states configuration at $T=1.6$

The results obtained from the numerical simulation for a squared lattice 40×40 for a number of steps equal to 3×10^6 in absence of magnetic field are shown in Fig. 3, 4 and 5. The transition between the ferromagnetic phase and the paramagnetic phase is clearly visible both in the magnetization and in the specific heat plots, in fact where the specific heat reaches the maximum value is where the transition happens. It is easier to understand in terms of magnetization, in fact when the temperature of the material exceeds the critical temperature, the thermal energy becomes sufficiently high to break alignment of magnetic moments. At higher temperatures thermal agitation dominates the interactions and the magnetic moments start to orientate randomly. This leads to the loss of magnetization and the material becomes paramagnetic. This can be understood looking at the equilibrium configurations of the lattice at different temperatures, in particular at $T = 1.6 < T_C$, $T = 2.3 \simeq T_C$ and $T = 3.3 > T_C$. As visible from 6 the spins are randomly distributed. From fig.(7) you can see that the system is approaching the equilibrium. From fig.(8) you can see that the system, still in the ferromagnetic phase, has reached a state where almost all spins are aligned as expected. Considering now $T = 2.3$ you can see that, in fig.(9) and (10), the system evolves at the equilibrium to the formation of clusters of sites oriented in the same way, they are known in electromagnetism as domains. The last case regards the study of the system when the temperature exceeds the critical temperature. As you can see from fig.(11) and (12) there is no clear difference between the initial and the evolved state, giving an indication that the system is in the paramagnetic phase.

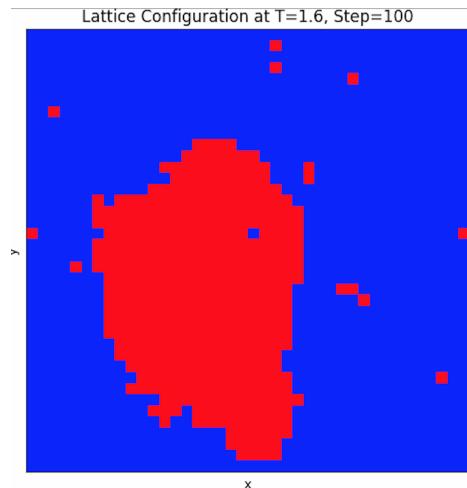


Figure 7: Spin states configuration at $T=1.6$ after 100 steps.

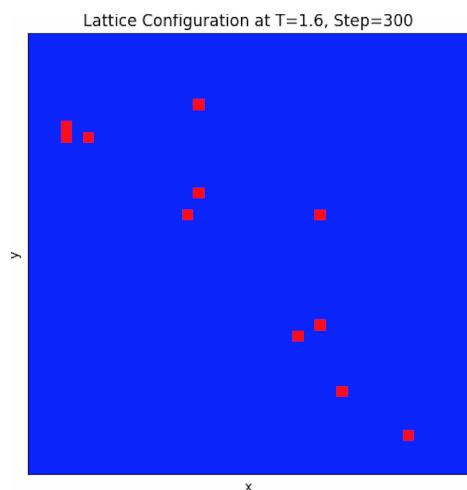


Figure 8: Spin states configuration at $T=1.6$ after 100 steps.

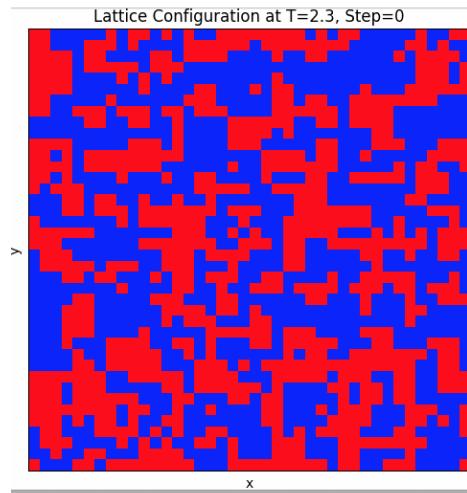


Figure 9: Initial random spin states configuration at $T=2.3$

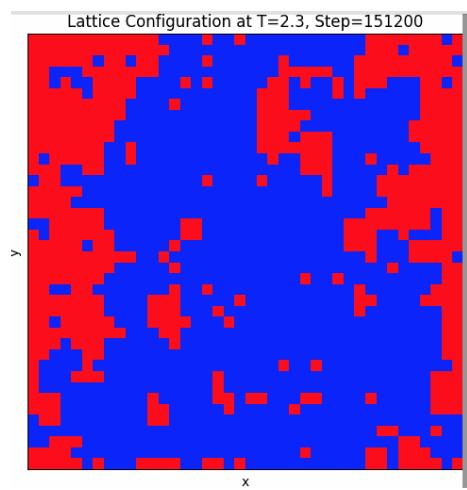


Figure 10: Spin states configuration at $T=1.6$ after 151200 steps.

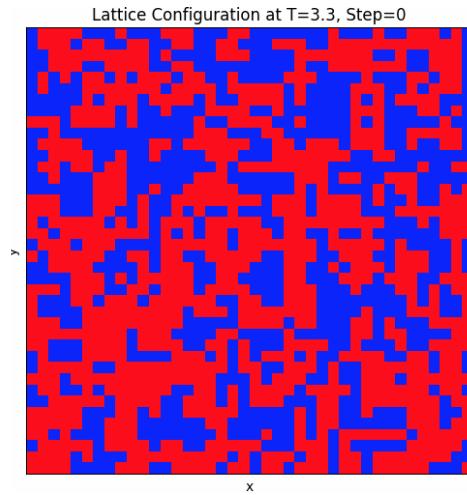


Figure 11: Initial random spin states configuration at T=3.3

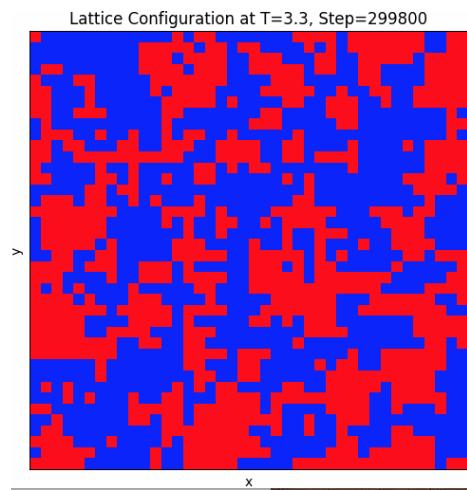


Figure 12: Spin states configuration at T=3.3 after 299800 steps.