THE ISING MODEL IN TWO DIMENSIONS

FYS3150: COMPUTATIONAL PHYSICS

SEBASTIAN G. WINTHER-LARSEN
GITHUB.COM/GREGWINTHER

Abstract. Ising model in 2D. Metropolis algorithm etc. Shit goes down.

Contents

Date: November 6, 2016.

1. Introduction

2. Theory

The model we will employ in this study of phase transitions at finite temperature for magnetic systems is the Ising model, named after Ernst Ising who solved a one-dimensional variant of the model[1]. The two-dimensional square lattice model, employed herein, was given an analytic description much later by Lars Onsager[2].

2.1. The general Ising model.

Let Λ be a set of lattice positions, each with adjacent positions, forming a d-dimensional lattice. For each lattice site, $k \in \Lambda$, there is a discrete variable $\sigma_k \in \{+1, -1\}$, representing the spin of the site, $\uparrow$ and $\downarrow$, respectively. A spin configuration σ is a specific spin configuration of the lattice.

For two adjacent sites, $i, j \in \Lambda$, one has an interaction J_{ij}. A site $j \in \Lambda$ will also have an external magnetic field h_j interacting with it. The energy of a specific system is given by the following Hamiltonian

$$E = H(\sigma) = -\sum_{\langle ik \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j \sigma_j, \tag{1}$$

where the first sum is over pairs of adjacent spins. The notation $\langle ij \rangle$ indicates that sites i and j are nearest neighbours. In the second sum, μ is the magnetic moment.

The probability of a certain configurations is given by the Boltzmann distribution

$$P_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta} \tag{2}$$

where Z_β is the partition function acting as a normalisation constant, and $\beta = (k_B T)^{-1}$. This would mean that by increasing the temperature T, finding the system in one particular configuration decreases. It must be so, because with a relatively higher temperature, one would expect previously unfavourable configuration to become more feasible.

There are two important expected values that are important in order to characterise a magnetic system. The *mean energy* of the system is

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_\beta(\sigma) = \frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i}, \tag{3}$$

and the *mean magnetisation* is

$$\langle \mathcal{M} \rangle = \sum_{i=1}^{M} \mathcal{M}_i P_\beta(\sigma) = \frac{1}{Z}\sum_{i=1}^{M} \mathcal{M}_i e^{\beta E_i}, \tag{4}$$

where $\mathcal{M}_i = \sum_{j\in\Lambda} \sigma_j$ for all configurations σ, and M denotes the number of possible configurations. Another quantity of interest is *magnetic susceptibility* χ which tells us how much an extensive parameter changes when an intensive parameter increases. It is given by

$$\chi = \frac{1}{k_B T}(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2). \tag{5}$$

The *heat capacity*, at constant volume, is given by

$$C_V = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{6}$$

The minus sign on each term of the Hamiltonian $H(\sigma)$ in equation 1 is conventional. By this sign convention, the Ising model can be classified according to the sign of the interaction. If, for all pairs i, j:

- $J_{ij} > 0$, the interaction is ferromagnetic,
- $J_{ij} < 0$, the interaction is anti-ferromagnetic,

- $J_{ij} = 0$, the spins are non-interacting.

In a ferromagnetic Ising model, spins desire to be aligned: the configurations in which adjacent spins are of the same sign have higher probability. In an anti-ferromagnetic model, adjacent spins tend to have opposite signs.

2.2. **Simplified ferromagnetic Ising model.** The general Ising model, as described above, will not be used in this study, but a much simpler version of it. Firstly, we will examine a system with no external magnetic field, as was originally solved analytically by Onsager[2]. Because the second sum in the Hamiltonian in equation 1 is zero, and we are left with

$$E = H(\sigma) = -\sum_{\langle ik \rangle} J_{ij}\sigma_i\sigma_j. \tag{7}$$

Secondly, we assume that the coupling constant J_{ij}, that describe the interaction of a spin with its neighbour, to be constant. That is $J_{ij} = J \forall i, j \in \Lambda$ and equation 7 is simplified further to

$$E = H(\sigma) = -J\sum_{\langle ik \rangle} \sigma_i\sigma_j \tag{8}$$

In this study, we will assume that we have a ferromagnetic ordering, id est $J > 0$. This means that neighbouring spins are aligned, because it would lead to lower energy. It is easy to see why it must be so, as $\sigma_i\sigma_j = 1$ whenever spin i and j have the same sign.

2.3. **Example:** 2×2 **Ising model.** It would be beneficial to test the waters of the ocean of the vast ocean that is the Ising model, by a two-dimensional model with lattice dimension $L = 2$ and periodic boundary conditions. This model has $s = 2^4 = 16$. different configurations σ. The energy of a given configuration would be

$$E_i = -J\sum_{\langle kl \rangle}^{4} \sigma_k\sigma_l.$$

Figure 1 shows an arbitrary configuration of a 2×2 spin lattice. The energy for this configuration is

$$E_i = -J((+1)(-1) + (+1)(-1) + (+1)(-1) + (+1)(-1)) = 8J$$

which happens to be the highest energy possible for the system. When all spins are parallel we see that $E_i = -8J$ which is the lowest energy possible. If only one spin would differ from the others, the energy would be $E_i = 0$ and so on. Of the 16 possible configurations, several will have degeneracies $(\Omega(E_i))$, which corresponds to the number of configurations with the same energy. Moreover, the magnetisation of a particular configuration is simply the sum of the spins and is easy to calculate. All the possible configurations of this system can be found in table 1.

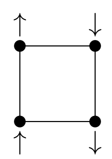

FIGURE 1. Sample 2×2 spin lattice.

Now to compute the physical quantities as discussed above, expected value for energy $\langle E \rangle$, expected value for magnetisation $\langle \mathcal{M} \rangle$, expected value for specific heat

TABLE 1. All possible configurations of a 2×2 Ising model

No of $\uparrow$	$\Omega(E_i)$	E_i	$\mathcal{M}_i$
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

$\langle C_V \rangle$, and susceptibility χ. For the 2×2 Ising model these quantities have closed form expressions. The partition function for the system is given by

$$Z = \sum_{i=1}^{1} 6e^{-\beta E_i} = e^{\beta 8J} + 12 + 2e^{-\beta 8J} + e^{\beta 8J} = 4\cosh(\beta 8J) + 12 \tag{9}$$

The expected energy is

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \ln(4\cosh(\beta J) + 12) = -8J \frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3}. \tag{10}$$

The mean magnetisation for this system is easiest to compute with equation 4, merely adding all possible states and dividing by the partition function.

$$\langle \mathcal{M} \rangle = \frac{1}{Z}(-4e^{8\beta J} - 8e^0 + 8e^0 + 8e^{8\beta J}) = 0 \tag{11}$$

the expected absolute magnetisation, on the other hand, becomes

$$\langle |\mathcal{M}| \rangle = \frac{1}{Z}(4e^{8\beta J} + 8e^0 + 8e^0 + 4e^{8\beta J}) = \frac{4 + 2e^{8\beta J}}{\cosh(8\beta J) + 3}. \tag{12}$$

The expected value for specific heat is

$$\langle C_V \rangle = \frac{1}{k_b T^2} \frac{\partial^2}{\partial \beta^2} \tag{13}$$

inserting equation 10 gives

$$\begin{aligned}
\langle C_V \rangle &= -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta} \left(-8J \frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3} \right) \\
&= \frac{1}{k_B T^2} \left(\frac{64J^2 \cosh(8\beta J)}{\cosh(8\beta J) + 3} - \frac{64J^2 \sinh^2(8\beta J)}{(\cosh(8\beta J) + 3)^2} \right) \\
&= \frac{1}{k_B T^2} \frac{64J^2}{\cosh(8\beta J) + 3} \left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3} \right)
\end{aligned}$$

The susceptibility χ of a thermodynamic system is easy to compute if one knows what the variance of magnetisation, $\sigma^2_{\mathcal{M}}$), is. Rewriting equation 5 gives

$$\chi = \frac{1}{k_B T} \sigma^2_{\mathcal{M}}. \tag{14}$$

Using equations 11 and 12 one can deduce that the variance of the magnetisation must be

$$\sigma^2_{\mathcal{M}} = \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 = \frac{32}{Z}(e^{8\beta J} + 1) - 0 = \frac{8(e^{8\beta J} + 1)}{\cosh(8\beta J) + 3}. \tag{15}$$

Inserting 15 into 14 yields the susceptibility for the system

$$\chi = \frac{8(e^{8\beta J} + 1)}{k_B T(\cosh(8\beta T) + 3)} \tag{16}$$

Bear in mind that $\beta = \frac{1}{k_B T}$, and that all the quantities computed are functions of T. The results computed here can be used as comparison for numerical computations.

3. Algorithm

4. Results

5. Discussion

6. Conclusion

References

[1] Ising, E., Beitrag zur Theorie des Ferromagnetismus, *Z. Phys.,* 31, pp. 253-258 (1925).

[2] Onsager, L., Crystal statistics. I. A two-dimensional model with an order-disorder transition, *Physical Review,* Series II, 65 (3-4), pp. 117-149 (1944).