THE ISING MODEL IN TWO DIMENSIONS

FYS3150: COMPUTATIONAL PHYSICS

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

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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.

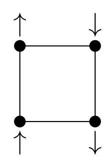

FIGURE 1. Sample 2×2 spin lattice.

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

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

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).