On the magnetic phases of the 2 dimentional Ising model

Gunnar Thorsen Liahjell

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Abstract

The Ising model and the metropolis algorithm are used to aproximate a critical temperature for phase transitions in ferromagnetic materials. Good results were reached for a 2 by 2 lattice with only 100 000 monte carlo cycles. By running 10 million cycles on lattices of sices 40,60,80 and 100 a critical temperature of 2.2704 was extracted where the analytical is 2.262

Introduction

The Ising model named after Ernest Ising, who first solvedthe one dimensional case, was first proposed to model the interaction of between magnetic moments in Ferromagnetic materials. Later it has been used in fields spanning from political sciences to neuroscience [1][6]. In this paper it wil be used for its original purpose by doing calculations on a 2-dimensional lattice of spins. The 2-dimensional problem was analytically solved by Norwegian-american Lars Onsager in 1944. He found the critical temperature for a magnetic phase transition to be 2.262, and this is what this paper is concerned with replicating numerically. To solve this the metropolis algorithm will be implemented and run over large numbers of temeratures. This is CPU-heavy calculations and parralelization will be implemented alongside with use of numbas jit[2] to severley decrease computing time.

Theory and Methods

Ferromagnetic materials and the Ising model

In most materials the the magnetic dipole moment of atomic spins have random orientation and sum up to a macroscopic net magnetic moment of zero. In ferromagnetic materials (such as for instance iron, nickel and cobalt) however these spins interact in a way such that beneath a certain critical temperature, the Curie temperature, the material exhibits a phase transition from zero magnetic moment and randomly configured spins, to spontaneous alignment of the spins, resulting in a net magnetic moment $>$ zero.

The 2D Ising model captures this phase transition as showed by Lars Onsager[3], who solved the system with no external magnetic field analytically in 1944, found proof for a phase transition and found the critical temperature to be 2.296 in units of $\frac{T}{k_b}$. Here the system is modeled by representing the spins as ones and minus ones on a lattice where energy of a configuration i of the lattice is given by

$$E_i = -J \sum_{<kj>}^{N} s_k s_j - B \sum_{k}^{N} s_k$$

N being the total number of spins in the lattice, $s = \pm 1$, J is a coupling constant,$< kj >$ indicates a sum over nearest neighbors, and B is an external magnetic field. In this project B will be 0.

The corresponding magnetic moment is then simply given by

$$M_i = \sum_j^N s_j$$

Being that positive and negative magnetic moments are equally likely, and that the interesting property is whether or not the system has net magnetic moment, the absolute value of M will be used.

The probability of finding the system with a given energy E_i is given by the Boltzmann distribution:

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}$$

Where $\beta = \frac{1}{kT}$, k being the Boltzmann constant and T being the temperature. Z is the partition function defined as

$$Z = \sum_i^W e^{-\beta E_i}$$

summing over all the W micro states of the system.

From here we can see that the expectation value for the energy and magnetic moment is

$$\langle E \rangle = \sum_{i=1}^W E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^W E_i e^{-\beta E_i}$$

and

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^W |M|_i e^{-\beta E_i}$$

With variances

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum_{i=1}^W E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^W E_i e^{-\beta E_i} \right)^2$$

and

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2 = \frac{1}{Z} \sum_{i=1}^W M_i^2 e^{-\beta M_i} - \left(\frac{1}{Z} \sum_{i=1}^W M_i e^{-\beta M_i} \right)^2$$

which in turn gives the expressions for Specific heat capacity and magnetic susceptibility, as they are defined by

$$C_v = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) = \frac{\sigma_E^2}{k_B T^2}$$

and

$$\chi = \frac{1}{k_B T} (\langle M^2 \rangle - \langle M \rangle^2) = \frac{\sigma_M^2}{k_B T}$$

([1],p 426)

Markov Chains

A Markov chain or a Markov process is a series of states where the probability of a given state solely depends on the previous state[5]. In this paper the states will be the spin configurations of the lattice and the probabilities will be the transition probabilities

The Metropolis algorithm

The Metropolis algorithm is a Markov-Chain-Monte-Carlo method, combining the random walk of a markov chain with the "brute-force" sampling of Monte Carlo methods.

The beauty of the metropolis algorithm is that you don't need to calculate the partition function, which becomes very demanding at high values of L, as the transition probability is given by

$$P_T = \frac{\frac{e^{(-\beta E_1)}}{Z}}{\frac{e^{(-\beta E_2)}}{Z}} = e^{(-\beta \Delta E)}$$

The algorithm follows the basic structure ([1],p 435):

1. Initialize the lattice with a spin-configuration and an accompanying energy.
2. Flip a random spin
3. Compute ΔE
4. If $\Delta E \leq 0$ the new configuration is accepted and step 5 and 6 are skipped
5. If $\Delta E > 0$ calculate the Boltzmann probability $w = e^{-(\beta \Delta E)}$
6. Compare w to a random number r. If $r \leq w$, the new configuration is accepted, if not the previous is kept.
7. Update the expectation values in question.
8. Repeat 2-7 as many times as wanted. One repetition constitutes a Monte-Carlo cycle

In this project steps 2-6 will be done L^2 times each MC-cycle, that is before step 7. With this approach one can think of each cycle as a time-step, in addition it lowers the correlation between consecutive states.

When only flipping one spin at the time, the energy delta is limited to 5 different values. these can be precalculated for increased efficiency.

Implementation

All programs can be found on https://github.com/gunnartl/fys-stk4155/tree/master/project4 The programs are written in python and sped up using numbas jit[2], and explicit parallel loops [4].

Testing

To test the algorithms a 2×2 lattice with periodic boundary conditions will be used, with only 4 spins it has $2^4 = 16$ micro states which makes the partition function rather manageable and the results can be calculated analytically.

No. spins up	Multiplicity	E	M
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

Table 1: Macro states of the 2×2 system and their corresponding multiplicity, energy (in units of the coupling constant J) and magnetic moment

Putting the information from into the expression for the partition function yields

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 12e^{0\beta J} + 2e^{-8\beta J} + 2e^{8\beta J} = 12 + 4cosh(8\beta J)$$

Leaving the rest of the expectation values easy to compute
Energy

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{16} E_i e^{-\beta E_i} = \frac{2(8e^{-\beta 8J}) + 2(-8e^{\beta 8J})}{12 + 4cosh(8\beta J)} = \frac{32(\frac{e^{-\beta 8J} - e^{\beta 8J}}{2})}{4(3 + cosh(8\beta J))} = -\frac{8Jsinh(\beta 8J)}{3 + cosh(8\beta J)}$$

magnetic moment

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{16} M_i e^{-\beta E_i} = \frac{(4e^{8\beta J} + 8e^0 - 8e^0 - 4e^{8\beta J})}{12 + 4cosh(8\beta J)} = 0$$

absolute magnetic moment

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{16} |M_i| e^{-\beta E_i} = \frac{(4e^{8\beta J} + 8e^0 + 8e^0 + 4e^{8\beta J})}{12 + 4cosh(8\beta J)} = \frac{4 + 2e^{8\beta J}}{\cosh(8\beta J) + 3}$$

magnetic susceptibility

$$\chi = \frac{\sigma_M^2}{kT} = \frac{1}{kT}[\langle M^2 \rangle - \langle M \rangle^2] = \frac{1}{kTZ} \sum_{i=1}^{W} M_i^2 e^{-\beta E_i} - 0 = \frac{32e^{8\beta J} + 32}{kTZ} = \frac{8(e^{8\beta J} + 1)}{kT(\cosh(8\beta J) + 3)}$$

and Specific heat witch can also be expressed as

$$C_v = \frac{1}{kT^2} \frac{\partial^2 \ln(Z)}{\partial \beta^2} = \frac{1}{kT^2} \frac{\partial}{\partial \beta} \left(- \frac{8J \sinh(8\beta J)}{\cosh(8\beta J) + 3} \right) =$$

$$\frac{1}{kT^2} \frac{64J^2(-\sinh^2(8\beta J) + \cosh^2(8\beta J) + 3\cosh(8\beta J)}{(\cosh(8\beta J) + 3)^2}$$

Results

$MC-cycles$	$\langle E \rangle$	$\langle M \rangle$	C_v	χ
10^2	-1.9400	9.900e-01	7.856e-01	9.840e-02
10^3	-1.9980	1	4.798e-02	0.000e-00
10^4	-1.9928	9.976e-01	6.059e-02	3.312e+00
10^5	-1.9952	9.984e-01	3.815e-02	3.987e+00
10^6	-1.9962	9.988e-01	2.975e-02	3.990e+00
10^7	-1.9960	9.987-01	3.210e-02	3.993e+00
Analytic:	-1.9960	0.9987	0.0321	3.9933

Table 2: Development in various parameters for a 2×2 lattice as the Monte Carlo cycles increase compared to the analytic solutions All parameters are per spin

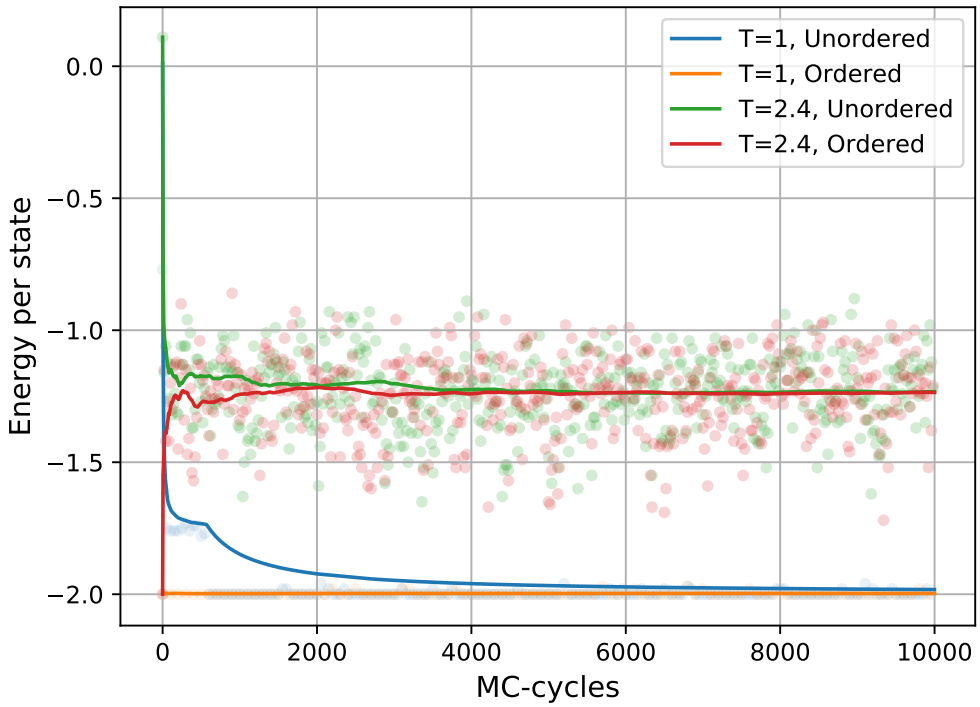

Figure 1: Energy in a 20×20 lattice as a function of monte carlo cycles. The dots are the the values in the given monte carlo cycle, and the lines are the running means from the start.

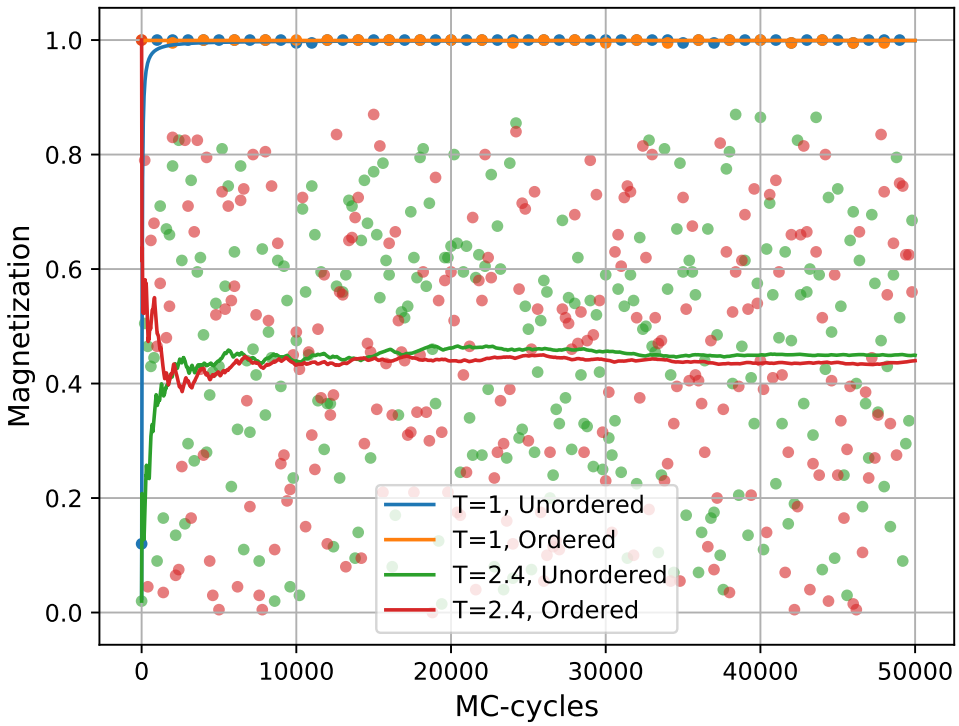

Figure 2: The magnetic moment per spin of a 20×20 lattice. Dots are values at the end of a cycle and lines are the running mean

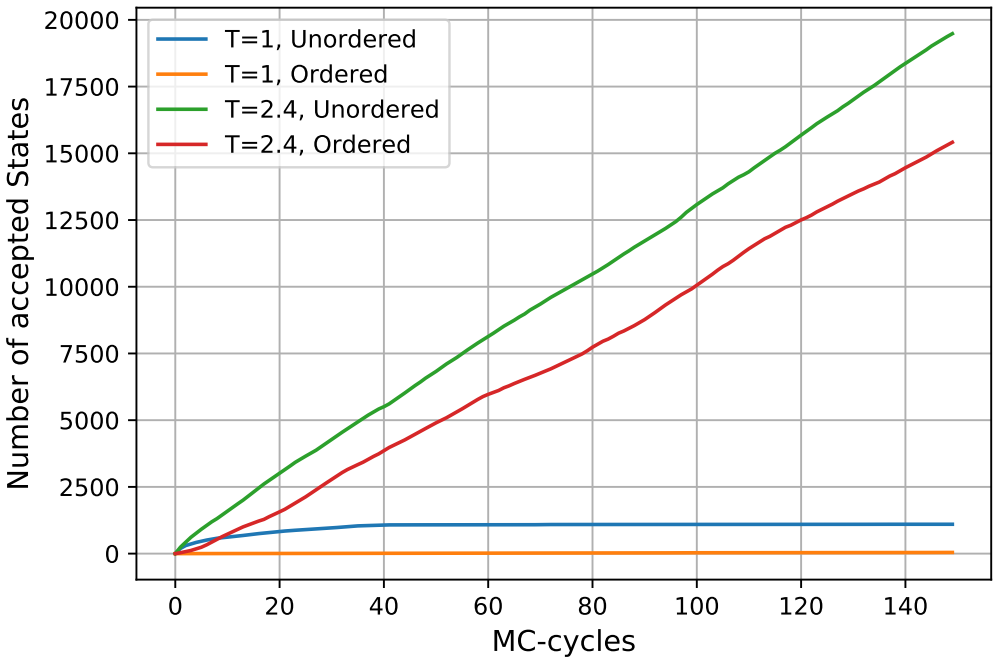

Figure 3: Number of accepted states for a 20×20 lattice with temperatures 1 and 2.4, with both random and ordered starting configurations for both temperatures.

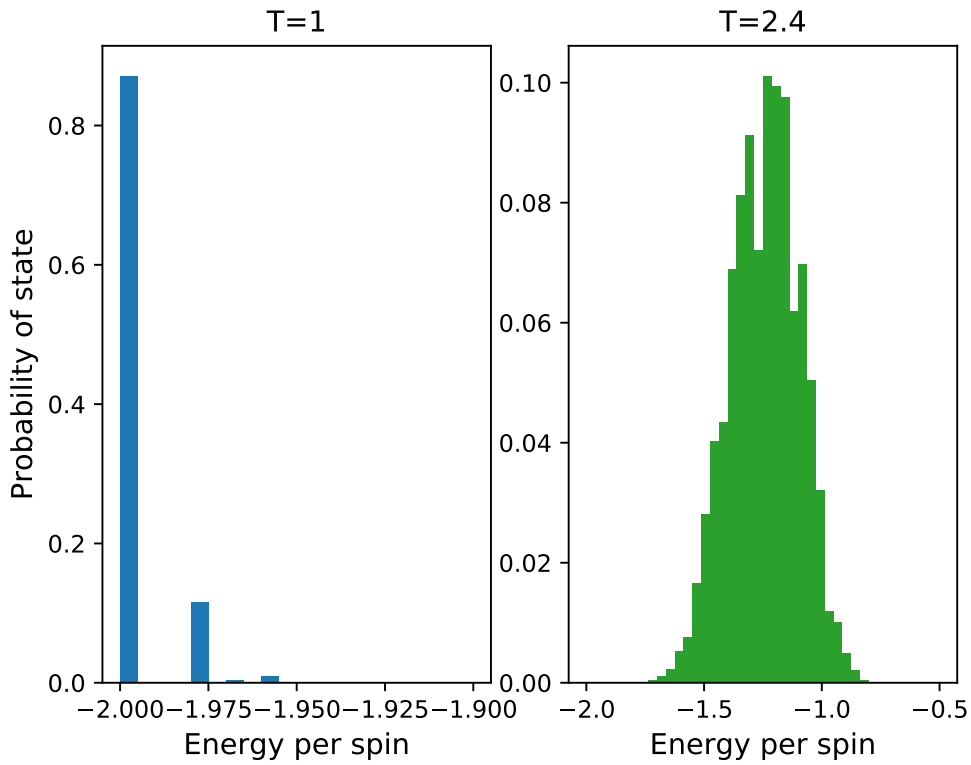

Figure 4: The probabilities for different energy states in a 20×20 lattice with temperatures 1 and 2.4

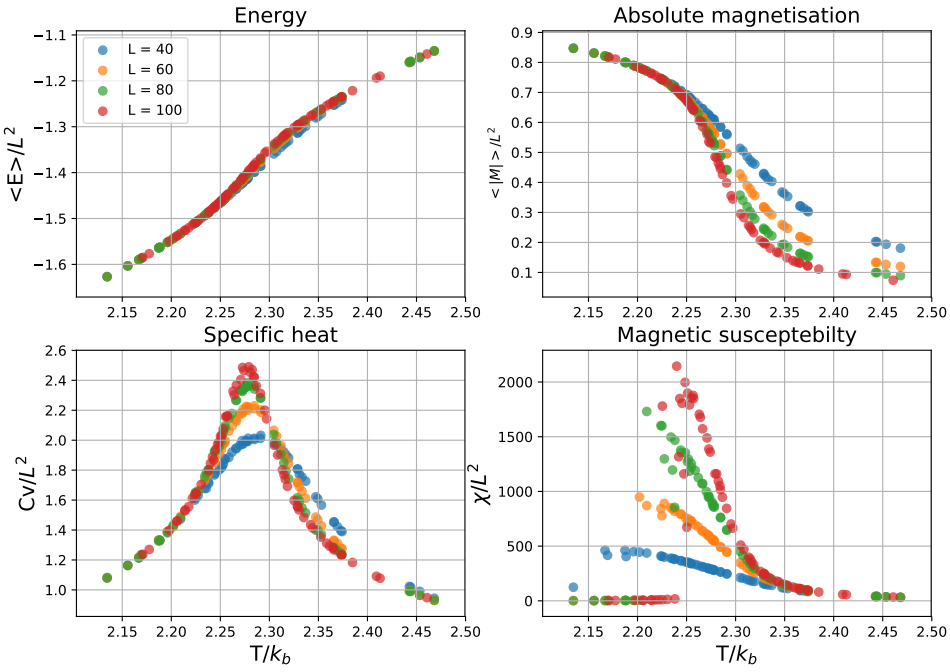

Figure 5: The development of energy, magnetic moment, heat capacity and magnetic susceptibility of four different system in temperatures around the critical point. All values are normalized by the size of the lattice for comparison.

Discussion

2×2 lattice

Table 2 shows how the parameters of a 2×2 lattice move toward the analytic results as the Monte Carlo cycles increase. One can see that the energy and magnetism converge faster than the specific heat and suceptebility. This is probably because they are functions of the variance, and need more time to stabelize. At 10 million monte carlo cycles there is good agreement between analytoc and numerical results.

20×20 lattice

Figure 1 shows a 20×20 lattice going toward energetic equilibruim for four different starting points. $T = 1$ ordered phase is already where it should be, and doesnt move much, and the unordered state moves toward it rather fast. $T = 2.4$ both ordered and unordered jumps around more, but the running mean has flattendt out at around 10000 MC-cycles.

Figure 2 shows alot of the same as figure 1, but shows that the magnetization jumps even more around than the energy at $t = 2.4$ and that it takes longer to reach an equilibrium. As they are more spread out the running mean takes longer to flatten out, but it is rather flat after 10000MC-cycles aswell.

Figure 3 shows how many states pass the if-test in step 6 of the metropolis algorithm. One can se that the ordered state of $T = 1$ accepts very few states. This because it is already in its most energetically favourable state, and there is only a small chance for it to make a jump to a higher energy. The same temperature with a random starting configuration accepts states ata much hogher rate, until it hit equilibrium at around 40 and flattens out. Both the ordered and unordered states of $T = 2.4$ accepts roughly the same amounts. These both needs to move away from the starting point to reach equilibria, and when found the jump around a lot more as seen in figures 1 and 2, so the accepted states keep rising equally fast for the entire simulation.

Figure 4 shows histograms for the probabilities of different energy states, calculated by counting the times they occur and deviding by cycles. The system is alowed 10000 cycles to equilibrate before the counting starts. T=1 has almost all states in the lowest possible while T = 2.4 spreds out over a higher temperature. here it resembles a normal distribution or a possion distribution, around the mean value.

Phase transition

Figure 5 are made with 10 million monte carlo cycles, letting it reach an equilibrium in 50000 cycles before updating the expectation values. There are 64 points along the temperature axis, made by two normal-distributions, one with a high standard deviation to get the desired width, and one with a smaller standard deviation to get even more points around the critical temperature, is this is the interesting area. All lattice sizes shows signs of the phase transition, the energy makes a slight jump, the heat capacity peaks, the suceptebility makes a jump, and most obvious, the magnetic moment goes to zero.

Using how the Critical temperature scales :

$$T_C(L) - T_C(L = \infty) = \frac{a}{L}$$

and putting in values for the critical temperatures and the lattice size from the top point, for lattice sizes 100 and 80 and then solving the equations results in a critical temperature of 2.2705.

Parallelization

Some runs with and with out use of numbas atomatic paralellization resulted in a speed up of 2.15. That is in adition to jits speedup of, on this task, around 250.

Conclusions

Even for relativley small lattice sizes and rather modest amounts of Monte Carlo cycles the Metropolis algorithm produces good results with a critical temperature of 2.2705 compared to Onsagers 2.269.

References

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