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# The Ising Model in two dimensions, studies of phase transitions in magnetic systems using Monte Carlo methods and Metropolis algorithm.

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November 18, 2019

A method using Monte Carlo calculations and the Metropolis algorithm was applied to the solution of the Ising model for a two dimensional lattice. The code developed was compared to the analytical solution for a 2x2 lattice giving a convergent behaviour for increasing number of Monte Carlo cycles. A case of lattice size 20x20 gave an estimate for the time it takes for a state to reach its thermal equilibrium state. By applying the method to three larger lattice sizes the value for the critical temperature, $T_C$, in the thermodynamic limit is found to be 2.248 giving a relative error of $\approx 1\%$ from the known analytical value calculated by Lars Onsager[3].

## Introduction and theory:

For millennia people have tried to understand magnetism. Today we have theories that aim to explain this phenomena, one of which is the Ising model, which is one way to model ferromagnetism in statistical physics. The model is named after the physicist Ernst Ising and was put forth in 1920. He solved the one dimensional Ising model analytically himself but the two dimensional model was not solved analytically until later in the year 1944 by Lars Onsager. An analytical solution has not been obtained beyond two dimensions.[4] The original intention of the Ising model was the application of magnetism but has it been used in applications ranging from social physics to neuroscience.

Here we will look at a two dimensional lattice of spins which take values $\pm 1$. First the theory needed to implement the solution of the two dimensional Ising model is put forth. As the analytical solution for a 2x2 lattice is relatively easily obtained this case is analysed and compared to the outcome from the Monte Carlo calculations. Finally the method is applied to larger lattices for an estimate of the critical temperature, $T_C$, associated with phase transitions in the thermodynamic limit.

### A. Ising Model

The Ising model is[1],

$$E = -J \sum_{<kl>}^{N} s_k s_l - B \sum_{k}^{N} s_k \qquad (1)$$

Where $B$ is an external field, $E$ represents the energy and $J$ is a coupling constant relating the strength of the spin-spin interaction. It also

represent whether the material is ferromagnetic og anti-ferromagnetic, with $1 \leq J$ being ferromagnetic and for $J < 1$ the material is anti-ferromagnetic. The spins are dimensionless, thus $J$ has unit of energy. The sum formulation $< kl >$ mean we only sum over the nearest neighbours.
For this article all calculations are done with zero external field, $B = 0$, meaning we can write a simpler expression for the Ising model,

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{2}$$

In statistical physics the partition function, $Z$, contains all ingredients to carry out interesting calculations and analysis.
The partition function is,

$$Z = \sum_{i}^{M} e^{-\beta E_i} \tag{3}$$

where the sum is over all possible microstates. $E_i$ represent the energy for a certain microstate and $\beta = 1/k_b T$ with $k_b$ being the Boltzmann constant and $T$ temperature. In this article natural units are used for the Boltzmann constant, $k_B = 1$.
When we know the partition function one can find the probability of being in a certain microstate at temperature $T$

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{4}$$

Here are four interesting quantities focused on in this article derived from the partition function[1]. The expectation value of energy is,

$$< E(T) >= -\frac{\partial ln(Z)}{\partial \beta} \tag{5}$$

From the expectation value of energy we can extract the heat capacity

$$C_V = \frac{\partial < E(T) >}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial < E >}{\partial \beta} \tag{6}$$

The mean magnetic moment is defined as

$$< M(T) >= \sum_i M_i P_i = \frac{1}{Z} \sum_i M_i e^{-\beta E_i} \tag{7}$$

We can also use the absolute value of mean magnetic moment, referred to as mean magnetization,

$$< |M(T)| >= \sum_i |M_i| P_i = \frac{1}{Z} \sum_i |M_i| e^{-\beta E_i} \tag{8}$$

The variance of the mean magnetization is given by,

$$\begin{aligned} \sigma_M^2 &=< M(T)^2 > - < |M(T)| >^2 \\ &= \frac{1}{Z} \sum_i M_i^2 e^{-\beta E_i} - \left( \frac{1}{Z} \sum_i |M_i| e^{-\beta E_i} \right)^2 \end{aligned} \tag{9}$$

from which we obtain the susceptibility, $\chi$

$$\chi = \frac{1}{k_B T} \sigma_M^2 \tag{10}$$

These four quantities are to be measured.

## B. Analytic solution for 2x2 case and the Ising model

For a 2x2 case the analytic solution is easily obtained. The following possible number of microstates are in total $2^4 = 16$. These are represented in table 1.

*Table 1: All possible state for 2x2 lattice using the Ising model. The degeneracy is stated along with the energy and magnetization.*

| No. spins up | Degeneracy | Energy [J] | Magnetization |
|---|---|---|---|
| 4 | 1 | -8 | 4 |
| 3 | 4 | 0 | 2 |
| 2 | 4 | 0 | 0 |
| 2 | 2 | 8 | 0 |
| 1 | 4 | 0 | -2 |
| 0 | 1 | -8 | -4 |

As we now know all possible microstates and their respective energies we can calculate the partition function from equation 3.

$$\begin{aligned} Z &= 2e^{-\beta(-8)} + 12e^{-\beta 0} + 2e^{-\beta 8} \\ &= 2e^{8\beta} + 12 + 2e^{-8\beta} \end{aligned} \tag{11}$$

and the resulting average energy from equation 5,

$$\begin{aligned} < E > &= -\frac{\partial ln Z}{\partial \beta} = -\frac{16(e^{8\beta} - e^{-8\beta})}{2e^{8\beta} + 12 + 2e^{-8\beta}} \\ &= -\frac{8sinh(8\beta)}{cosh(8\beta) + 3} \end{aligned} \tag{12}$$

From this result and equation 6 we get the heat capacity,

$$\begin{aligned} C_V &= -\frac{1}{k_B T^2}\frac{\partial < E >}{\partial \beta} \\ &= -\frac{1}{k_B T^2}\frac{\partial}{\partial \beta}\left( - \frac{8sinh(8\beta)}{cosh(8\beta) + 3}\right) \\ &= \frac{1}{k_B T^2}\frac{64(1 + 3cosh(8\beta))}{(cosh(8\beta) + 3)^2} \end{aligned} \tag{13}$$

We then turn to the mean magnetization from equation 8.

$$\begin{aligned} < |M| > &= \frac{1}{Z}\left(\sum_i |M_i| e^{-\beta E_i}\right) \\ &= \frac{8e^{8\beta} + 16}{2e^{8\beta} + 12 + 2e^{-8\beta}} \end{aligned} \tag{14}$$

And finally the susceptibility from equation 10. First we obtain,

$$\begin{aligned} \frac{1}{Z}\sum_i M_i^2 e^{-\beta E_i} &= \frac{1}{Z}(16e^{8\beta} + 16 + 16 + 16e^{8\beta}) \\ &= \frac{32}{Z}(1 + e^{8\beta}) \end{aligned}$$

then the susceptibility is

$$\begin{aligned} &\chi = \frac{1}{k_B T^2}\sigma_M^2 = \\ &\frac{1}{k_B T^2}\left(\frac{32}{Z}(1 + e^{8\beta}) - \frac{1}{Z^2}(8e^{8\beta} + 16)^2\right) \\ &= \frac{1}{k_B T^2}\left(\frac{32}{Z}(1 + e^{8\beta}) - \frac{64}{Z^2}(2 + e^{8\beta})^2\right) \end{aligned} \tag{15}$$

## C. Monte Carlo and Metropolis algorithm

As the lattice size increases calculating the partition function becomes a difficult task and in the thermodynamic limit near impossible, or atleast very time consuming. This is bad new as the partition function contains all interesting parameters. This is where Monte Carlo, referred to as MC, calculations and Metropolis algorithm step in and give us the tools needed for the problem.

To set up the solution and algorithm we need to briefly mention Markov processes and how that plays into the Metropolis algorithm. A Markov process is a random walk with a selected probability for making a certain move. This move has no knowledge of the history of the system and is therefore independent of states that came before the present one. This Markov process is used repeatedly in Monte Carlo simulations to generate new states. A Markov process is very important because eventually it will reach the most likely state. This has important consequence for the case of the two dimensional Ising model considered here as this means the system will eventually reach thermodynamic equilibrium. Two other important properties of a Markov process are the one of detailed balance and ergodicity. Ergodicity means that if the state is allowed to evolve long enough it can be found in every possible state in a finite amount of time[1].

For a Markov process we have a transition probability for going from state i to state j represented with a matrix $W(i \to j)$ for a discrete distribution. This means if we have PDF at time, $t = 0$, represented with $w_i(t = 0)$ the PDF at a later time, $t = \epsilon$, is related to the one at $t = 0$ with,

$$w_i(t = \epsilon) = \sum_j W(i \to j) w(t = 0) \tag{16}$$

The time development of the initial PDF can be represented by the action of the matrix $W(i \to j)$

sequentially. For naturally occurring phenomena the transition probability is generally unknown. Thus, it has to be modelled and that is the role of the Metropolis algorithm. This is done by taking the transition probability as a product of two probabilities which are; $A(j \to i)$: the probability for accepting the proposed move from the state j to the state i and $T(j \to i)$ is the probability for making the transition to the state i being in the state j, in other words

$$W(j \to i) = T(j \to i)A(j \to i) \tag{17}$$

This in addition with the requirement of detailed balanced at equilibrium is, which states the following, is crucial.

$$\frac{W(j \to i)}{W(i \to j)} = \frac{w_i}{w_j} \tag{18}$$

and by using equation 17 becomes,

$$\frac{A_{(j \to i)}}{A_{(i \to j)}} = \frac{w_i}{w_j}\frac{T_{(i \to j)}}{T_{(j \to i)}} \tag{19}$$

Now comes the assumption of what is often called the brute force Metropolis, which is that $T_{(j \to i)} = T_{(i \to j)}$. Then using the Boltzmann distribution which is the PDF in this case we obtain,

$$\frac{A_{(j \to i)}}{A_{(i \to j)}} = \frac{\frac{e^{-\beta E_i}}{Z}}{\frac{e^{-\beta E_j}}{Z}} = e^{-\beta(E_i - E_j)} \tag{20}$$

giving the final recipe for how to accept or decline new proposed states, that is the acceptance probability[1],

$$A(j \to j) = \begin{cases} 1 & \text{if } E_i < E_j \\ exp(-\beta(E_i - E_j)) & \text{else} \end{cases} \tag{21}$$

In short the method can be setup in the following pseudo-code.

---

- Initialize lattice of size LxL using a random number generator
- Loop over number of Monte Carlo Cycles
- Loop over number of spins in the lattice
(Done for each MC cycle)
- Randomly select location in the lattice
- Flip the spin at that site
- Calculate the change in energy, $\Delta E$, by flipping that spin
-Metropolis part:
If $\Delta E \leq 0$ accept the new configuration
If $\Delta E > 0$ generate random number, $r$.
-If $r \leq e^{-\beta \Delta E}$
Accept the configuration else decline it
Update relevant parameters:
(Energy,Energy$^2$,Magnetization,Magnetization$^2$)
- End loop over spins
- End MC loop
- Make the relevant analysis

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## D. Phase Transition

For Ising class of models the behaviour of various parameters around the critical temperature, $T_C$, can be characterized by power laws[2]. For mean magnetization this is,

$$< M(T) > \sim (T - T_C)^{\beta} \tag{22}$$

for the heat capacity,

$$C_V(T) \sim |T_C - T|^{\alpha} \tag{23}$$

and the susceptibility,

$$\chi(T) \sim |T_C - T|^{\gamma} \tag{24}$$

with exponents $\beta = 1/8$, $\alpha = 0$ and $\gamma = 7/4$.
The correlation between spins increases as the temperature gets closer to $T_C$, meaning the correlation length, $\xi$, increases. This divergent behaviour can also be characterized by a power law,

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{25}$$

By finite scaling relations the critical temperature scales as

$$T_C(L) - T_C(L=\infty) = aL^{-1/\nu} \tag{26}$$

where $a$ is a constant. The exact results were calculate by Lars Onsager[3] to be $kT_C/J \approx 2.269$, with $\nu = 1$.

### E. Parallelization, code and data

Each measurement for a certain temperature using MC and Metropolis algorithm is independent of any other measurement. This makes it straightforward to implement so called embarrassing parallelization. The naming has nothing to do with the problem being embarrassing, rather it used as a term for tasks or problems which require little effort to run in parallel. In the implementation of this article this sort of parallelization was used. The full implementation, code and data can be found on: `https://github.com/bjornaki/CompPhysics/tree/master/Project4`.

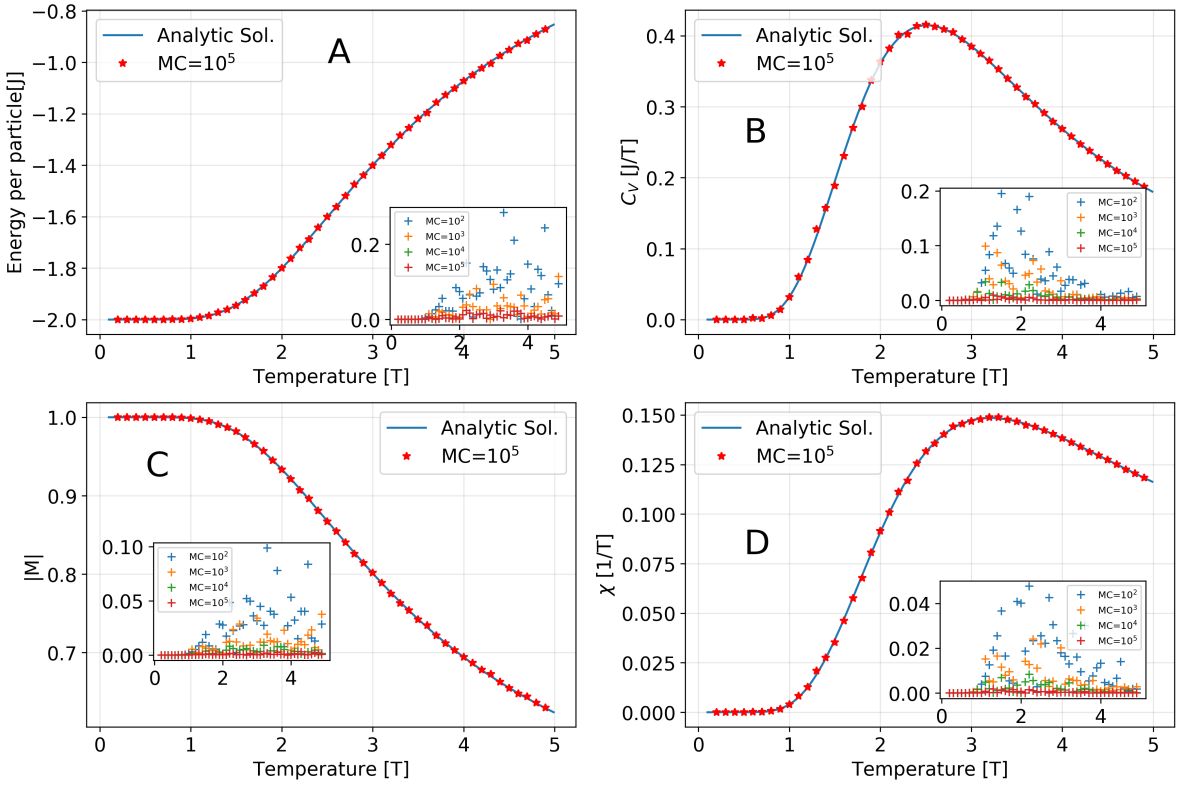


Figure 1: Comparison of analytical solution and MC calculation for a 2x2 case. The insets show the absolute error for four different values of MC cycles. **A**. Average energy per spin. **B**. Heat Capacity. **C**. Mean magnetization . **D**. Susceptibility.

## Results

### A. Monte Carlo and analytical values for a 2x2 Lattice

At first a comparison for a simple 2x2 case is made, giving the ability to compare the analytical values against the results from MC calculations. In figure 1 the average energy per particle can be seen as function of temperature as well as the absolute error in the inset for four different values of MC cycles. The MC measurement

value falls close to the analytical for $10^4$ MC cycles and when the number of cycles is increased to $10^5$ the absolute error of the analytical value and MC calculation is nominal meaning the behaviour is convergent. The same can be seen for the heat capacity, mean magnetization and the susceptibility.

## B. Lattice with 20x20 spins

We now extend our calculations to a bigger lattice to get an estimate for how many MC cycles are needed to reach the equilibrium state and how the system behaves for two different values of temperature, in this case a lattice of size 20x20, in total 400 spins. When a state is initialized it can either be done randomly or ordered. Measurements were made to look at how the initial state affects the time it takes for the lattice to reach its equilibrium state. In this case for temperature $T = 1.0$ and $T = 2.4$. The measurements of desired quantities are carried out after the lattice has reached its equilibrium state. In figure 2 one can see energy as function of MC cycles. For low temperatures the state reaches its equilibrium quicker for an ordered initial state. For the higher temperature it has less effect on the equilibrium time whether the state is initialized ordered or randomly. This behaviour is also visible when mean magnetization is plotted as a function of MC cycles. Worth noting is that if the system is initialized randomly it might reach a metastable state before eventually settling to its equilibrium state as is seen in figure 2.

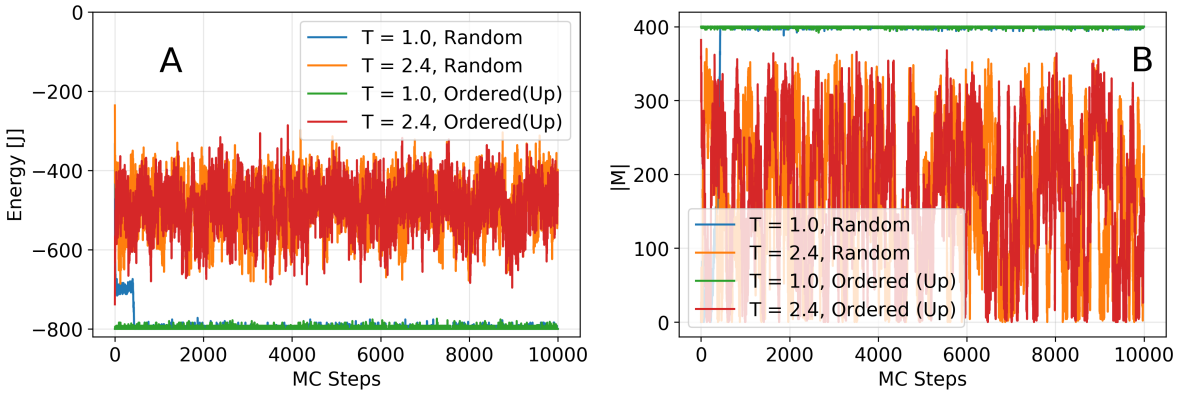


Figure 2: Measurements for two different initial state as a function of MC cycles, ordered and random, at two different values of temperature, $T = 1$ and $T = 2.4$. Lattice size is 20x20. **A**. Total energy of the lattice. **B**. Mean magnetization of the lattice.

As the temperature is increased more proposed configurations of the system are accepted. Figure 3 shows how number of accepted configurations behaves as a function of MC Cycles. In figure 3 it can also be seen for the lower temperature that the system spends most of its time in the ground state compared to a much broader distribution when $T = 2.4$. For higher temperature the spread is substantially higher, which directly translates to the heat capacity with equation 6. It is evident from these two measurements that for the higher temperature measurement the lattice has higher heat capacity, meaning the system can be found in more number of states resulting in a bigger spread in the PDF.

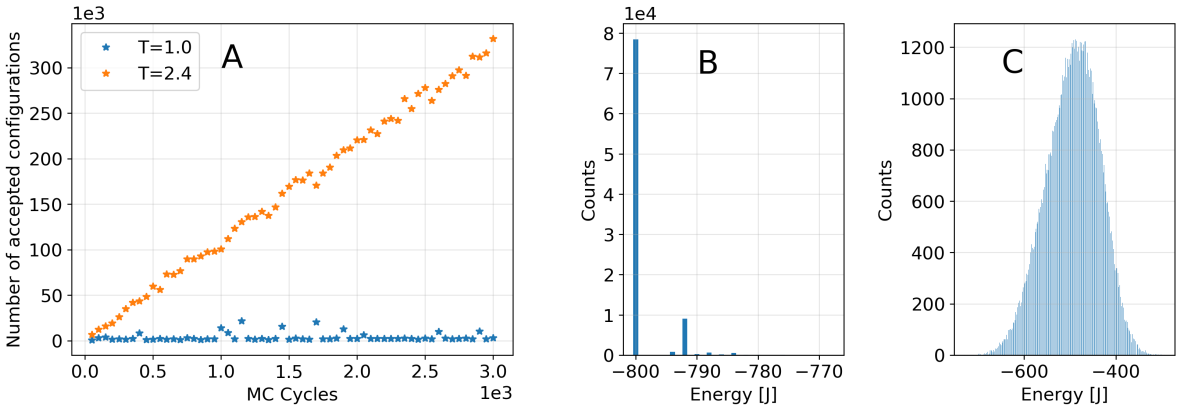


Figure 3: Behaviour for a 20x20 lattice at two different temperatures. **A.** Number of accepted configurations as a function of MC Cycles for $T = 1$ and $T = 2.4$. **B**. Probability distribution of energy for 20x20 lattice with $T = 1.0$. **C**. Probability distrisbution $T = 2.4$. Both probability distributions contain $9 \cdot 10^4$ MC cycles.

## C. Timing

*Table 2: Timing for 24 values of temperature both with and without parallelization. Number of MC Cycles was* $2 \cdot 10^4$.

| Lattice size | Parallel | Time [s] |
|---|---|---|
| 30x30 | Yes | 658 |
| 30x30 | No | 830 |

The nature of Monte Carlo and Metropolis algorithm make it easily embarrassingly parallelizable due to the fact many measurements are taken for different temperature, each of which is independent of the other. To show the gain of parallelizing the code measurements were taken for a lattice of size 30x30 with 24 different values of temperature. These runs were timed and results can be seen in table 2. The system used for calculations has a two core processor and each temperature has $2 \cdot 10^4$ MC cycles. The speed increase is not double but becomes more apparent as the lattice size is increased.

## D. Phase Transitions:

We now do measurements for four different lattice sizes, $L \in [4, 8, 16, 40]$, as a function of temperature. As the lattice size is increased a phase transition becomes apparent around $T = 2.3$. To get a better estimate of the transition temperature measurements with smaller temperature steps and bigger lattice sizes were made. Table 2 shows the three lattice sizes measured as well as the evaluated $T_C$ for each case. To evaluate the $T_C$ the maximum value in heat capacity is taken to be at $T_C$. The maximums for the three different lattice sizes can be seen in figure 4.

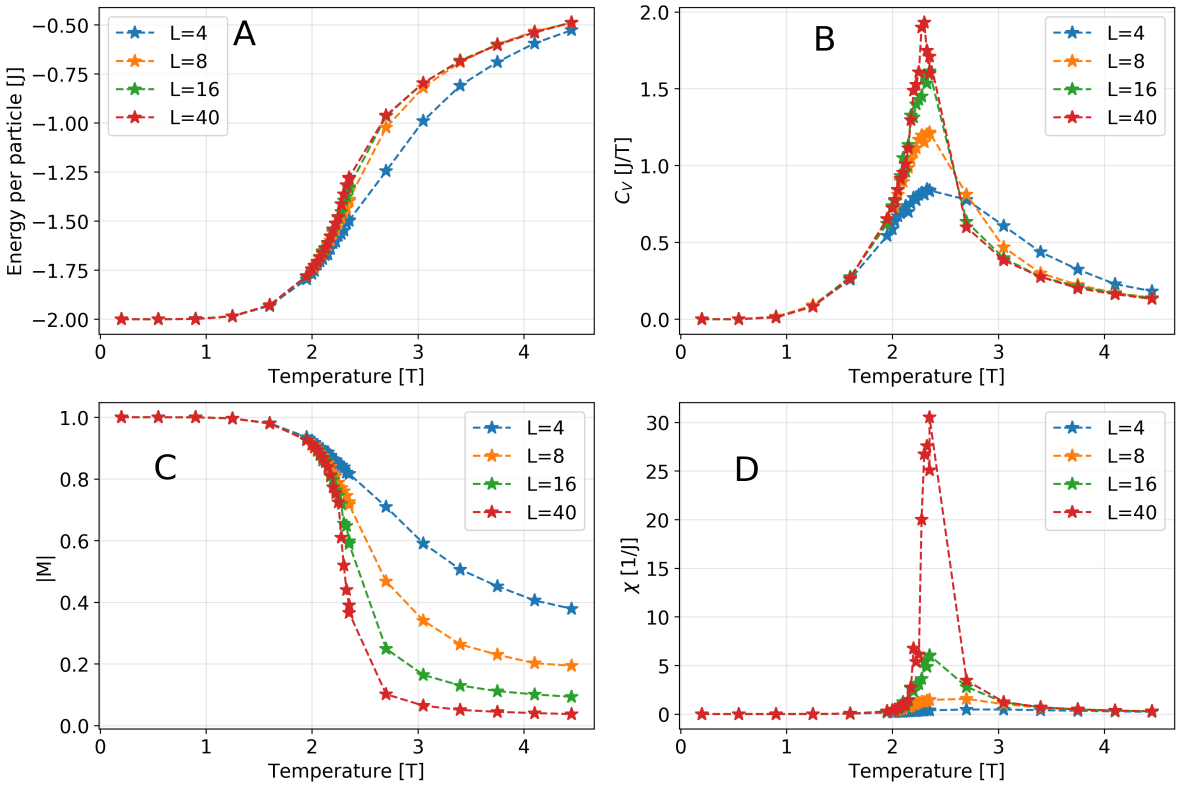


Figure 4: Measurements for four different lattice sizes. A phase transition becomes more apparent as the lattice size is increased. **A**. Energy per particle. **B**. Heat capacity.**C**. Mean magnetization per particle. **D**. Susceptibility per particle.

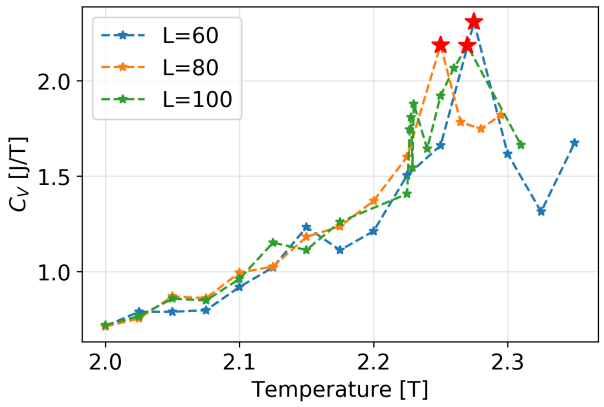


Figure 5: Locating $T_C$ for three different lattice sizes using the maximum in heat capacity, marked with red stars.

To evaluate $T_C$ in the thermodynamic limit we do a linear fit in accordance with equation 26 and get a value for the critical temperature,

$$T_C(L = \infty) = 2.248 \tag{27}$$

meaning a relative error against analytical value[3] of

$$RelativeError(T_C) = \frac{|T_C^{(analytical)} - T_C^{(measured)}|}{T_C^{(analytical)}} = 0.0091 \tag{28}$$

*Table 3: Transition temperature, $T_C$, for three different lattice sizes.*

| Lattice size | $T_C$ |
|---|---|
| 60x60 | 2.275 |
| 80x80 | 2.250 |
| 100x100 | 2.27 |

## Discussion

### A. Monte Carlo and analytical values for a 2x2 Lattice

Having an analytical solution for a problem gives the possibility of comparing the solution against the algorithm developed. Here we looked the case of 2x2 lattice where the partition function is easily obtainable. For the MC simulation we see that the as the number of MC cycles is increased the solution converges to that of the analytical one for each of the four parameters measure; energy, heat capacity, mean magnetization and susceptibility. This results motivates the investigation of larger case lattice.

### B. Lattice with 20x20 spins

Having established the analytical solution and MC simulation for a 2x2 case we extended our machinery to a lattice of size 20x20. At first energy and mean magnetization per particle were plotted as a function of MC steps to roughly establish when the most likely state is reached, in other words when the system has reached its thermodynamic equilibrium. In figure 2 these measurements are seen for two different temperature and an initial state when the system is ordered or random. For the lower temperature this has the effect that the random initial state takes longer to settle. For the higher temperature the effect of starting our in either random or non-random initial state is not as pronounced. At low temperature, $T < 1$, the system is found to reach its equilibrium state after around $10^3$ MC cycles.

As the temperature is increased a greater number of moves to new configurations are accepted and the system can occupy a larger number of macro states, that is states with same energy, as is apparent in figure 3. This translates to a greater variance in the PDF or in other words the heat capacity as can be seen from equation 6.

### D. Phase Transitions

To try and evaluate the critical temperature from power laws and equation 26 measurements for three larger lattice sizes were made. Each measurement was run in parallel and taken after a system has reached its equilibrium state, around $10^3 - 10^4$ MC cycles. From these measurements a linear fit was used to estimate the critical temperature, $T_C = 2.248$, which has a relative error of 0.0091 from the known analytical value. Possible sources of error might be that the resolution in the MC simulations is not high enough. For each lattice size a finite number of measurements are made and each of these is very time consuming. This can result in the $T_C$ for each lattice size being estimated incorrectly carrying an error to the extraction to an infinite lattice. Another source of error is the generation of random numbers. As the random number generator(RNG) is not a true RNG there is correlation between numbers, but in the analysis for this article this is not treated. The third reason might that the system hasn't reached its thermal equilibrium when the measurement is started.

## Conclusions and next steps

The Ising model for 2 dimensional lattice has now been analysed using Monte Carlo calculations and the Metropolis algorithm. For comparison a 2x2 case was investigated both analytically and using MC simulations. This gives the motivation to apply the algorithm developed to a bigger lattice which would otherwise be very time consuming to solve. By looking at a case of lattice size 20x20 the equilibrium time was estimated and the behaviour of the probability distribution function quantified, giving a larger variance for the higher energy case, resulting in a bigger heat capacity.

By applying the algorithm to a bigger and bigger lattice a phase transition becomes apparent. With three fine scale runs and relatively large

lattice sizes the transition temperature was estimated to be $T_C(L = \infty) = 2.248$. The errors have not been properly quantified but three possible sources of errors are: Not enough resolution in temperature steps, correlation between random number generated by RNG and the measurements including states of the system when it has not reached its thermodynamic equilibrium. These MC calculations are time consuming and benefited from being run in parallel. Further work would be to trying to get a better estimate for the $T_C$ by running the simulations on a more powerful computer as well as better quantify the errors associated with these calculations. Using the MC calculations and the Metropolis algorithm gives result close to the analytical one in two dimensions, thus, the next step would be to expand this method for the Ising model in three dimensions.

## References


[1] Morten Hjorth-Jensen. Computational Physics, Lecture Notes Fall 2015.

[2] Morten Hjorth-Jensen. Project 4, Studies of phase transition in magnetic systems. `https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2019/Project4/pdf/Project4.pdf`, 2019.

[3] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65(3-4):117–149, Feb 1944.

[4] Steven H. Simon. *The Oxford Solid State Basics*. Oxford University Press, 2013.