Project 4: Simulating the Ising Model by the Applied Metropolis-Algorithm

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(Dated: November 20, 2018)

Within the field of condensed matter physics, magnetic phase transitions are aspects of common knowledge. However, there was such a time when these transitions were firstly demonstrated to exist. Namely by the late, Pierre Curie, who was responsible for further expanding the frontiers of atomic theory and material science.

This report introduces, with a dosage of historical events, the studies an atomic model of ferromagnetism, namely the Ising model; which will be simulated by the applied Metropolis algorithm (MCMC). Furthermore, the report is divided into three parts. Part I is concerned with Onsager's analytical solutions of the two-dimensional Ising model. The main findings of this part, were that for a computed sample of numerical results comprised of energy, magnetization, heat capacity and susceptibility. The agreement between the analytical and numerical values, became better approximated with a larger sample size. Secondly, the mean values of the computed maximum sample, resulted in numerical values which, when compared to the analytical values, agreed to the seventh decimal for energy and magnetization, while sixth decimal for heat capacity and susceptibility. The next part, part II, studies the equilibration of the system. It was found that by making the number of performed Monte Carlo iterations (cycles) analogous to time, that the equilibration time came to be approximately 10^4. Secondly, it was found that there were large difference in the probability of the most probable state, for lattices of different temperatures. Finally in part III, phase transitions were studied, where a simulated phase transition demonstrates that, by using large lattices of sizes $\{40, 60, 80, 100\}$, and by using the thermodynamic Helmholtz potential to argue that the simulation shows a phase transition. The Curie temperature, can be computed by fitting the results of heat capacity or susceptibility, by finite size scaling methods. It was found that there was an agreement, between the analytical and numerical Curie temperatures, to the order 10^{-3}.

I. INTRODUCTION

The physical phenomenon of magnetism was known in ancient times, dating back to a scientific discussion of the topic by Thales of Miletus in ancient Greece [4]. It was not, however, until the 19th century, that the relationship between electricity and magnetism, were beginning to be properly understood. Well after Maxwell's formalized electromagnetism and Boltzmann's kinetic theory of gases, and into the 20th century; numerical algorithms were being developed at Los Alamos, New Mexico in the 1950s. A paper published by Metropolis, Rosenbluth, Rosenbluth, Teller and Teller [5] presented a powerful algorithm, dubbed the Metropolis algorithm, for computing properties of a system comprised of interacting molecules, using Monte Carlo methodologies.

Figure 1: Nicholas Metropolis, a key founder of the metropolis algorithm. Image referance `https://upclosed.com/media/images/thumbs/N/nicholas-metropolis.jpg`

With the exponential increase in computing power from the time this paper was published, the applications of the algorithm has expanded greatly, extending it's applicability to various fields of mathematics.

In this report, the metropolis algorithm, or Markov Chain Monte Carlo (MCMC), will be applied to solve the Ising model. Which is a model for ferromagnetism in materials, that came at a historical midterm between thermodynamics/electromagnetism and quantum mechanics. It was during this midterm, that the time for studying materials, atoms and material phase transitions, was truly ripe. This also meant studying certain materials which had magnetic properties, and which could be externally magnetized, or were naturally magnetized. The specific variant of materials which the Ising model was written to describe, are ferromagnetic materials. Which are materials that have a tendency to be natural permanent magnets; they become increasingly magnetized with an applied external magnetic field. By the assumption that a material's microscopic state can be assumed to be a lattice of atoms with a lattice length L, and additionally restricting the electromagnetic dipole moment of the atoms to only take on one of two values, +1 or -1. One can model the macroscopic magnetic alignment of such a material and study the behaviour of the system under varying temperatures, using the second law of thermodynamics.

Modelling such a system (with potentially several moles of particles) is quite practically difficult; from a statistical mechanical view, one requires to be able to keep track of each individual particle's spin for all times. Thus

analytically, this presents as a large-dimensional integral. With numerical methods such as Gaussian quadrature, it is not numerically efficient. Since it would require a large amount of computations with polynomials, which in turn are used to solve for the inverses of potentially huge matrices. Thus, Monte Carlo methods are desirable when solving such large-dimensional integrals; the MCMC algorithm is then a prime candidate for simulating such a system.

The Ising model, is a mathematical model of ferromagnetism, under the field of statistical mechanics.

It is attributed to the physicist Ernest Ising, who solved it in one dimension, in 1924. Although it was his mentor, Wilhelm Lenz, who presented the actual model in 1920 [6].

Presenting as a statistical mechanical description of the conglomerate physics, in the modelled crystal lattices of materials, that show ferromagnetic properties. A model which is, in turn, founded on the phenomenon of magnetic dipole moment; an electromagnetic phenomenon.

One assumes, in the model, a lattice of any possible configuration of spins (up $\rightarrow$+1 or down $\rightarrow$ -1), but as time passes the system should tend towards equilibrium, if the second law of thermodynamics is to hold. With that being said, another result of thermodynamics, which is crucial to the Ising model, is one of the thermodynamic potentials. The lattice system is assumed enclosed by a thermal bath, keeping the temperature constant; in addition, the volume is also assumed constant due to the lattice crystalline structure. Which means that the thermodynamic potential which is minimized, is the Helmholtz potential. Knowing which potential to minimize means having the ability to quantify when the system is at thermodynamic equilibrium. In which, after several..., what will shall refer to as *sweeps of the lattice*; which means a double looped iteration over the entire lattice. The expectation values of the internal energy $\langle E \rangle$, magnetization $\langle \mathcal{M} \rangle$, heat capacity C_V and magnetic susceptibility χ can be computed. The heat capacity is defined as the amount of energy needed in order to raise the system temperature by a certain amount ΔT, and the magnetic susceptibility is the measure of a material's tendency, to be: increasingly magnetized ($\chi > 0$) or to repel other magnets ($\chi < 0$). The Ising model is concerned with paramagnetism which means $\chi > 0$.

Being able to predict quantities, such as the mentioned, were paramount in order to fully explain the magnetic properties of materials; which in turn allowed for development of technology using these materials. With that said, the Ising model's applications have since spread to a wide range of fields; from studies of social groups (elections) and economics [8] [7].

Considering magnetic phase transitions (which will simply be referred to as phase transitions). At some specific temperature, dubbed the Curie temperature, T_C after discovery by the physicist/chemist Pierre Curie, certain materials loose their ferromagnetic properties; examples of such materials are Iron or Nickel. This report will study such phase transitions using the Ising model.

For this rapport, there will be one main program written in C++, for the heavy computations; while various programs in python 2.7 will be written for creating plots and writing output from the extracted data.

The report is divided into three parts; part I deals with the analytical and numerical reproduction of Lars Onsager's result for the two dimensional lattice. In part II, the transition to thermal equilibrium will be studied with a larger dimensional lattice. Lastly, part III will revolve around the studies of the magnetic phase transitions of various even larger-dimensional lattices.

As of mentioning a few technicalities and practicalities. The quantities which will be studied in detail throughout the report are the expectation values of energy and the absolute value of magnetization. In addition to the heat capacity C_V and the magnetic susceptibility χ. However, the expectation value of the absolute value of magnetization and the magnetic susceptibility will be referred to, throughout the report, as the **magnetization** and **susceptibility**.

It is assumed that the reader is comfortably knowledgeable within undergraduate physical fields of: thermodynamics, electromagnetism, classical mechanics and scientific programming.

II. THEORY

A. The Ising Model

A system, in the Ising model, is a lattice of length L, in units of atoms. The area (in atoms) is thus dubbed $N = L^2$ and the number of possible spin configurations is dubbed $M = 2^N$. The system has the internal energy, E_i, for a certain state i; which is attributed to two factors: the magnetic interaction of neighbouring atoms in the lattice, and due the applied external magnetic field.

$$E_i = -J \sum_{\langle k,l \rangle}^{M} S_k S_l - B_{ext} \tag{1}$$

Where J is a constant which is a simplified approximation of the atom interactions in the lattice, some stemming from quantum mechanics.[10]

For the purpose of this report, it is assumed that there be no externally applied magnetic field. Thus, the general energy expression, for a system i, is given only by the first term in (1).

The notation $\langle k, l \rangle$, specifies that for a given atom, it's energy contribution is due to it's interaction with the nearest neighbours only. Which means that the atom, must be paired **once**, with all of (and only with) it's nearest neighbours in the lattice. The numerical implementation will be discussed in more detail in the numerical methods section.

The magnetization $\mathcal{M}_i$ of system i, is computed as the net sum of all spins in the system's lattice.

$$\mathcal{M}_i = \sum_{i=1}^{N} S_i \tag{2}$$

B. Statistical Mechanical Expressions

In the following , relevant formulas from statistical mechanics are presented.

1. Boltzmann Factor

Boltzmann's factor represents the probability of a state with energy E, relative to the probability of a state with zero energy.

$$e^{-E/k_B T} \tag{3}$$

Where k_B is the Boltzmann constant and T is the temperature of the system. It is common to define $\beta = 1/k_B T$.

2. Partition Function

For a canonical ensemble (statistical ensemble with constant temperature and volume), the partition function Z is given as the sum of all Boltzmann factors for the given system.

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{4}$$

The partition function connects to the probability distribution of the system, as being the normalization factor of the distribution.

3. The Probability Distribution

The probability of measuring a system in state i at equilibrium is given by

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{5}$$

where the probability distribution is assumed to be normalized $\sum_i P_i = 1$.

4. Expectation Values and the Variance

The expectation values represent the mean values of a sampled distribution of measurements, of the canonical ensemble. Lightly speaking it is what the mean value of energy, for instance, after a certain number of measurements of the system at equilibrium. Here are listed the expectation values of the: energy, magnetization and the variances σ_E^2, $\sigma_{\mathcal{M}}^2$ of the same.

$$\langle E^k \rangle = \sum_{i=1}^{M} E_i^k P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} E_i^k e^{-\beta E_i} \tag{6}$$

$$\langle \mathcal{M}^k \rangle = \sum_{i=1}^{M} \mathcal{M}_i^k P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i^k e^{-\beta E_i} \tag{7}$$

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{8}$$

$$\sigma_{\mathcal{M}}^2 = \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \tag{9}$$

5. Heat Capacity and Magnetic Susceptibility

$$C_V = \beta \frac{1}{T} \sigma_E^2 \qquad \chi = \beta \sigma_{\mathcal{M}}^2 \tag{10}$$

$$\tag{11}$$

C. Simplifying Computations with Scaling

By introduction of the dimensionless energy $\tilde{E} = \frac{E}{J}$, and the temperature $\tilde{T} = k_B T$ with units of energy, the Boltzmann factors simplify to

$$e^{-\tilde{E}/\tilde{T}} \tag{12}$$

Such that the any computation of the factors, for a given state i by (1), is done without considering the factor J.

D. Periodic Boundary Conditions PBCs

For a finite sized lattice, especially in lower dimensions, the boundaries of the lattice become important when computing the internal energy of the system. There is, however, also the choice of neglecting the boundaries, but as stated, it is a bad approximations for lower dimensional lattices. There are articles which solely discuss the significance of the periodic boundary conditions in the Ising model [9].

Let $\mathcal{L}$ be a $L \times L$ matrix representing the lattice. Then the matrix elements $\mathcal{L}_{ij}$ specifies the positions of the spin at row i and column j. If computing the energy contribution of a particular atom, which happens to be situated at a boundary position in the lattice, it's position is one of the following: $\mathcal{L}_{1j}$,$\mathcal{L}_{Lj}$, $\mathcal{L}_{i1}$ or $\mathcal{L}_{iL}$. Using PBCs then mean that the particular atom's nearest *non-existent* neighbor, is taken as the atom (with it's spin value) at the opposite end of the respective column or row in the lattice.

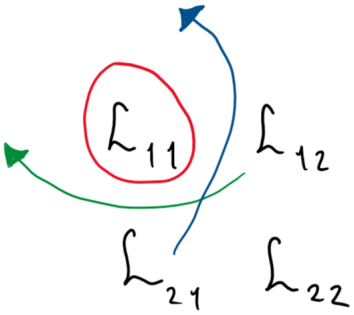


Figure 2: Periodic boundary conditions, illustrating by example how energy computations of $\mathcal{L}_{11}$ in a 2×2 lattice causes $\mathcal{L}_{12}$ and $\mathcal{L}_{21}$ to become the respective left and above nearest neighbour of $\mathcal{L}_{11}$.

However, as stated in section (II A) each pairing must only count once. Thus this seems to resort to a double counting of the neighbours. A solution to this is by diving the outcome of 2, or to realize the following.

By restricting each energy contribution from a position in the lattice to be computed only by two specific pairings, the left and above neighbour, the double counting is avoided. This yields the correct amount of pairings. Thus, since computational efficiency is desirable, the latter case results in less floating point operations (FLOPS) and would therefore be a better choice for computation. Which is what will be implemented for this simulation.

E. Onsager's Result

In the two-dimensional Ising model (2×2 lattice), there are $2^{N=2^{L=2}} = 16$ possible configurations of the atom spin orientations. Which means there are, theoretically, an equal number of energy and magnetization possibilities. A table of these possibilities can be made by initially letting all spins point down, meaning the number of spins pointing up $N_A = 0$. From this, flip one spin ($N_A+ = 1$), compute the energy and magnetization, then flip another spin ($N_A+ = 1$), and repeat the process 16 times. It is then quickly realized that there are several configurations, that give the same result, this equal number, which gives configurations with equal energy and magnetization, is what is known as the degeneracy Ω of the macrostate.

Table I: Table of $N_\uparrow$, energy E with corresponding degeneracy Ω and magnetization $\mathcal{M}$ for a 2×2 lattice.

$N_\uparrow$	Ω	E	$\mathcal{M}$
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

These lattice-specific values, can now be used to compute Onsager's results of the energy, magnetization, heat capacity and susceptibility.

Computing the partition function with (4); the sum of all Boltzmann factors for the system. The rows of table (I) will supply the specific multiplicity/degeneracy and energy. Also assuming that the temperature, equals to 1, for this case.

$$Z = \sum_{i=1}^{2} e^{8} + \sum_{i=1}^{12} e^{0} + \sum_{i=1}^{2} e^{-8} = 4\cosh 8 + 12 \tag{13}$$

Now applying the statistical mechanical expressions from section (II B) to compute the main results.

NB: the results are taken to be, per spin, which implies the following expressions are to be divided by the area of the lattice $N = 4$.

$$\langle E \rangle = \frac{\sum_{i=1}^{2}(-8)e^{8} + \sum_{i=1}^{12}(0)e^{0} + \sum_{i=1}^{2}(8)e^{-8}}{Z} \tag{14}$$

$$= \frac{-32\sinh 8}{Z}$$

the remaining values are computed similarly

$$\langle|\mathcal{M}|\rangle = \frac{8\left(e^8+2\right)}{Z} \tag{15}$$

$$C_V = \frac{256\cosh 8}{Z} - \left(\frac{32\sinh 8}{Z}\right)^2 \tag{16}$$

$$\chi = 32\frac{\left(e^8+1\right)}{Z} - 64\left(\frac{e^8+2}{Z}\right)^2 \tag{17}$$

Creating a table of the evaluated expressions: (14), (15), (16) and (17); divided by the lattice area.

Table II: Numerical values (per spin) of Onsager's result, rounded to ten decimals.

$\langle E\rangle$	-1.9959820859
$\langle\|\mathcal{M}\|\rangle$	0.9986607327
C_V	0.0320823319
χ	0.0040107395

The numerical and analytical comparison will turn out to require high accuracy, thus the high number of included decimals.

F. Thermodynamic Equilibrium

From the second law of thermodynamics, entropy increases in a non-equilibrated isolated system. Furthermore, as discussed in the introduction, the lattice system is assumed, to have a constant volume and temperature. Which means the minimized potential, at thermal equilibrium, is the Helmholtz free energy potential H.

$$F = \langle E\rangle - TS \tag{18}$$

where U is the internal energy of the system, and S is the entropy.

Consequentially as the lattice approaches thermal equilibrium, it will be at complete equilibrium in conjunction with the minima of the Helmholtz potential.

By using Boltzmann's definition of entropy, it can be shown that the: energy, magnetization, heat capacity and susceptibility, can be expressed as partial derivatives of the Helmholtz potential [3].

$$\langle E\rangle = \frac{\partial(\beta F)}{\partial\beta} \qquad C_V = -\frac{1}{k_B T^2}\frac{\partial^2(\beta F)}{\partial\beta^2}$$

similar proportionalities, with the first and second partial derivatives, also hold for the magnetization.

G. Curie Temperature and Finite Size Scaling

As mentioned in the introduction, Pierre Curie, demonstrated in the late 1800s that there existed various magnetic phase transitions in materials. The transition occurs at a certain temperature, for which the material becomes non-magnetized.

A useful relation, which will be applied as a curve fitting function in this report. Is the scaling of the Curie temperature for a certain lattice of length L, in conjunction with the Curie temperature at the thermodynamic limit ($L \to \infty$).

$$T_C(L) = aL^{-\nu} + T_C(L\to\infty) \tag{19}$$

Which, for a known lattice of $L = 2$, $\nu = 1$.

III. NUMERICAL METHOD

A. Metropolis Algorithm

The metropolis algorithm is a Markov Chain Monte Carlo (MCMC) method, which was presented in 1953 (by: Metropolis, Rosenbluth, Rosenbluth, Teller and Teller [5]), as a method for solving for various macrostates, in a complicated system of interacting molecules. The original algorithm, as presented in the paper, went as follows: move one of the molecules slightly, compute the change in energy in the system, if the energy is less than the previous state, accept it, otherwise accept the change with a probability of $\exp(\Delta\frac{E}{k_B T})$. In the following paragraph, the basic idea behind the original algorithm will be discussed; and analogies to the Ising model will be commented throughout the discussion in parentheses.

The basic idea was to pick a starting point for the simulation, perform a series of random walks through the probability distribution (flip a spin), and favour values (energies) with higher probabilities (second law of thermodynamics). Thus, for the readers who are more familiar with the mathematical formalism of random walks; let the walker favour higher probabilities.

A crucial consideration in the metropolis algorithm is take note of that fact that the walker only *favours* higher probabilities, which implies that even random walks which result in a lower probability may still be accepted. In this way the entire system (lattice) is potentially evaluated.

The specialized metropolis algorithm for the Ising model can then be presented as follows.

Algorithm 1 Metropolis Algorithm for the Ising Model

1: Initialize lattice $\mathcal{L}$
2: Initialize lattice energy E and magnetization $\mathcal{M}$
3: for sweep = 1,2,$\cdots$, N_{MC}

- Pick random lattice position $\mathcal{L}_{r_i r_j}$
- Flip spin of $\mathcal{L}_{r_i r_j}$ and evaluate ΔE

  IF: $\Delta E \leq 0 \rightarrow$ DO: Accept and compute expectation values

  ELSE:

  – Pick random number $\mathcal{R} \in (0, 1)$
  IF: $\mathcal{R} \leq \Delta E \rightarrow$ DO: Accept and compute expectation values
  ELSE: Do nothing

As seen, there are N_{MC} sweeps of the lattice. This is also a good point to begin realizing the scope of computational resources required. If the algorithm is to be run for a series of temperatures $T \in \{T_i, T_f\}$, there are: for each temperature, and each sweep, a (size of the lattice) number of operations required to evaluate and test the energy changes. Which again are to be done N_{MC} times, which in turn might be required to be run $(T_f - T_i)/h_T$ times, with h_T being the temperature step-size. So for a 100×100 lattice, with a million Monte Carlo cycles and, say, one hundred temperatures. It is theoretically possible that $100^2 \cdot 10^6 \cdot 10^2$ or a thousand billion operations, are required. From this point, both N_{MC} and #MC-cycles will refer to the same number, which is the number of Monte Carlo cycles.

B. The Markov Chain in MCMC

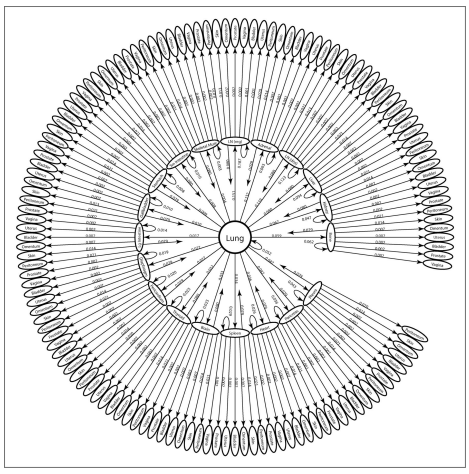


Figure 3: Example of a Markov chain diagram from a cancer research paper. Picture reference: `http://cancerres.aacrjournals.org/content/73/9/2760`

Since with each Monte Carlo cycle, on average makes the system tend towards a steady state, or equilibrium, and from the fact that any current state is only dependant on information from the previous state. The process is thus a Markov Chain. There is then a probability distribution (a stochastic matrix) which dictates how the system evolves from one state, to the next.

A key feature of the metropolis algorithm, is that it enables computations to be made for systems where the probability distribution is unknown. This is very much a computational convenience for the Ising model, since when performing computations for very large lattices $> (100 \times 100)$, the matrix containing the probability distribution would add even more computational operations to the already large stock.

This *bypass*, is seen in the Metropolis algorithm (1), as the IF-ELSE statements. As long as two principles are obeyed by the Markov chain: ergodicity and detailed balance, the algorithm holds. Ergodicity means for the Ising model's case that the entire lattice will be swept through, which is already discussed and satisfied. Detailed balance implies that the probability of **picking** any transition is equal. Thus preserving the Boltzmann statistics of the distribution. This is also upheld by using a high order random number generator.

C. Mersenne Twister

The Mersenne Twister is, by far, the most widely used pseudorandom number generators (PRNG). Which is mostly attributed to the fact that it's algorithm can generate $2^{19937} - 1$ various random numbers in a given interval. The extraordinarily high period guarantees, that the large computations required of the simulated Ising model will have a preserved statistical nature. As it should. With this, detailed balance is upheld for the purposes of this report.

In the following three subsections, the numerical stages of the report will be presented.

D. Part I: Onsager's result

To start with, several computations of the 2×2 lattice will be made, producing results for the desired expectation values. Each computation is run with 10^9 MC-cycles; the average of the result sample will then be taken and compared with the analytical results of Onsager.

Furthermore in order to quantify the stability and to demonstrate that numerical values truly do approach Onsager's result in the approximated limit of #MC-cycles. The mean of the resulted samples will be plotted as a function of increased terms from the sample to the mean.

E. Part II: Reaching Equilibrium

It is when the system is as close to as possible, or at thermal equilibrium, that the expectation values of the energy and magnetization will be computed. In this sense forming the probability distribution of the system. By making the number of Monte Carlo cycles analogous to time, the equilibration time for the system can be extracted by computations. Thus giving knowledge about when to compute the macrostates of the system.

For this part the lattice size is increased to $L = 20$, making the number of operations increased per Monte Carlo cycle. The matrix alone needed to store the lattice has an area of 20^2 meaning that an ideal (no breaks in the loop) full sweep requires 400 iterations.

The probability of the equilibrated state is also of interest, since it represents a maxima of the probability distribution as a result of the second law of thermodynamics. The probability distribution will be computed by counting the number of times a certain energy is *registered* by the Metropolis algorithm. Also the number of accepted spins will be computed as a function of #MC-cycles.

This part will study the mentioned for two temperatures; $T \in \{1, 2.4\}$. In addition to two different initial configurations (all up or all random).

F. Part III: Phase Transitions

The phenomenon of magnetic phase transitions will be demonstrated by simulation in this part.

The simulation will be run with a temperature span $T \in (2.2, 2.3)$; the lattice size will also be spanned $L \in \{40, 60, 80, 100\}$. The number of Monte Carlo cycles will be adjusted in accordance with computational efficiency. The goal of this section is to compare Onsager's analytical result of the Curie temperature.

$$k_B T_C / J = 2/\ln(1+\sqrt{2}) \approx 2.269 \tag{20}$$

To the computed numerical values. Which should become better and better approximated with the increase of the lattice length, i.e in the thermodynamic limit ($L \to \infty$). The main program *mcmcIsing.cpp* will be run for the span of lattices with an appropriate #MC-cycles. The energy, magnetization, heat capacity and susceptibility curves will then be fitted, by a polynomial of an appropriate degree using the least squares method. The maxima of these curves will serve as data points for our curve fitting with (19) in order to compute the Curie temperature in the thermodynamic limit. This will be compared to Onsager's result (16) for the 2×2 lattice.

IV. RESULTS

*Computations performed with an i7-4770 CPU 3.40GHz*2, 12GB RAM system and the programs are compiled with the -O3 optimization flag*

A result which is independent of parts I-III, is the computational runtime as a function of cycles, for increasing Ls. This serves as a useful pointer for available computational resources in the computational process.

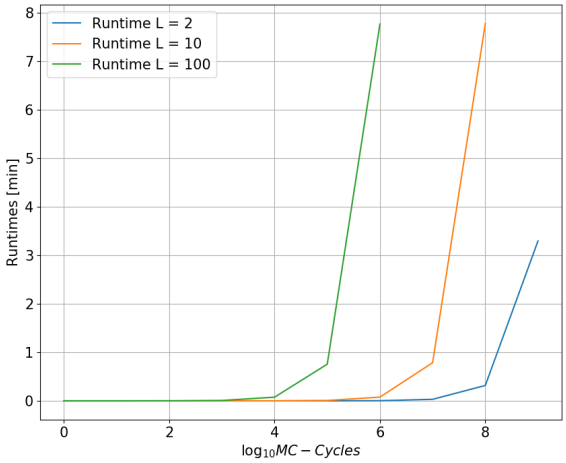


Figure 4: Runtime as a function of $\#MC$-cycles for increasing Ls.

A. Part I: Onsager's Results

The results for this part stems from output from *p4subbOnsager.py*.

Computing a sample of results, from 33 runs with 10^9 #MC-cycles and plotting the absolute error between the mean value of the results as function of increasing sample size to Onsager's results.

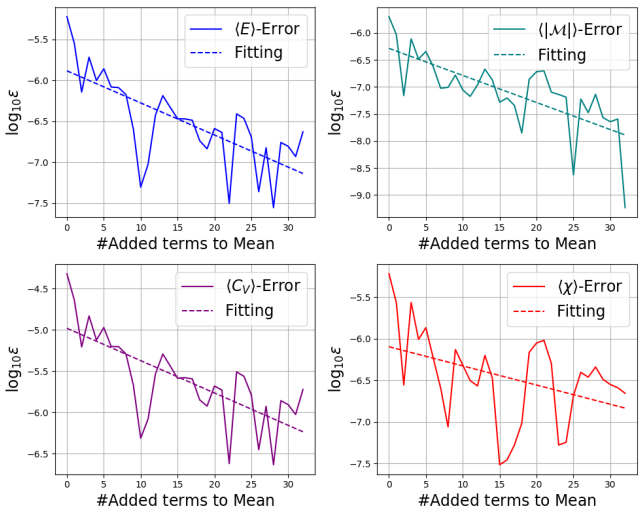


Figure 5: Error plot, comparing numerical values to Onsager's results.

Taking the mean of the whole sample and computing the standard error (the standard deviation divided by the square root of the sample size) yields the results. (The tables denote Onsager's values by $\mathcal{O}_i$, while the numerical values are denoted $\mathcal{N}_i$ where i is the respective value to be compared).

Table III: Comparisons of $\langle E \rangle$.

$\mathcal{O}_{\langle E \rangle}$	-1.9959820859
$\mathcal{N}_{\langle E \rangle}$	$-1.9959823212 \pm 7 \cdot 10^{-7}$

Table IV: Comparizon of $\langle |\mathcal{M}| \rangle$.

$\mathcal{O}_{\langle \lvert\mathcal{M}\rvert \rangle}$	0.9986607327
$\mathcal{N}_{\langle \lvert\mathcal{M}\rvert \rangle}$	$0.9986607333 \pm 3 \cdot 10^{-7}$

Table V: Comparizon of C_V.

$\mathcal{O}_{C_V}$	0.0320823319
$\mathcal{N}_{C_V}$	$0.0320804267 \pm 6 \cdot 10^{-6}$

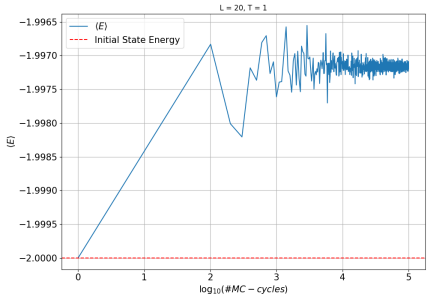
Table VI: Comparizon of χ.

$\mathcal{O}_{\chi}$	0.0040107395
$\mathcal{N}_{\chi}$	0.0040109596 ± 10^{-6}

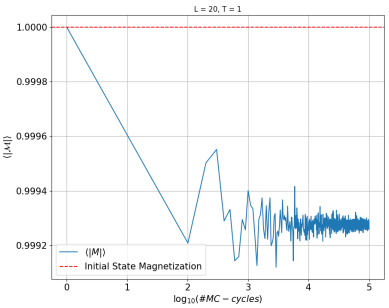
B. Part II: Reaching Equilibrium

The results for this part stems from output from *p4subc.py* for the (IV B) plots and *p4subd.py* for the probability distributions.

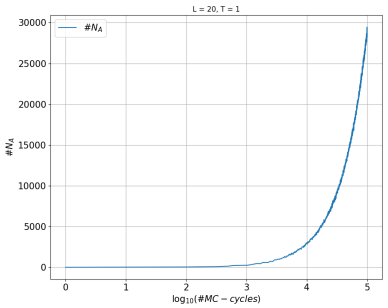
The resulting plots from 6*2 runs for $T \in \{1, 2.4\}$, with both a random and non-random (all up) initial configuration, are displayed on page 9. The number of accepted spins are dubbed N_A.



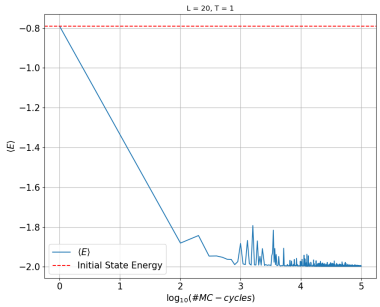
(a)T = 1, energy plot. Initial configuration: all up



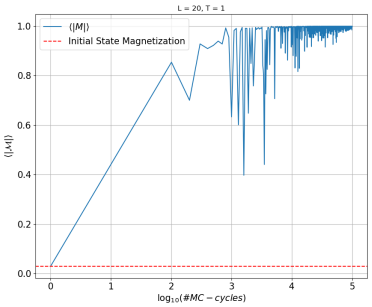
(b)T = 1, Magnetization plot. Initial configuration: all up



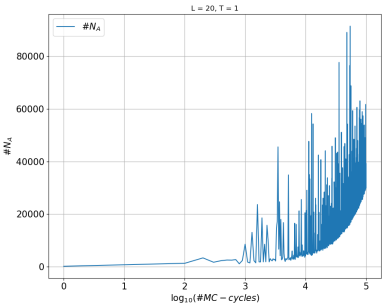
(c)T = 1, #Accepted spins plot. Initial configuration: all up



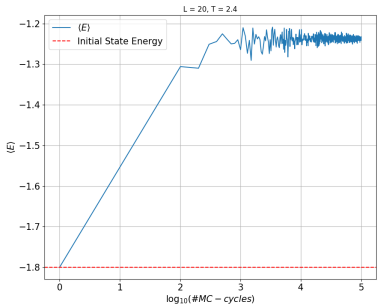
(d)T = 1, energy plot. Initial configuration: random



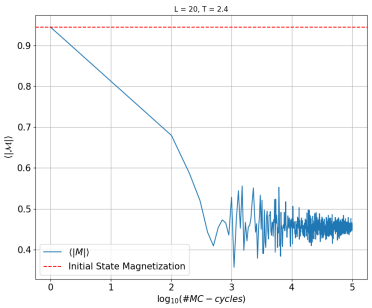
(e)T = 1, magnetization plot. Initial configuration: random



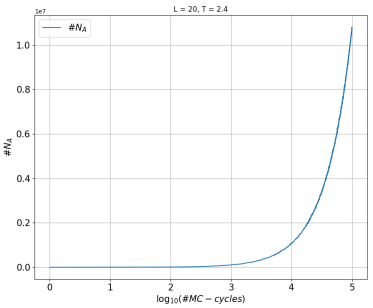
(f)T = 1, #Accepted spins plot. Initial configuration: random



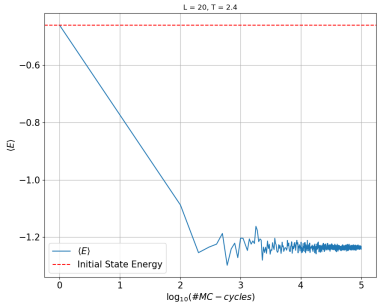
(g)T = 2.4, energy plot. Initial configuration: all up



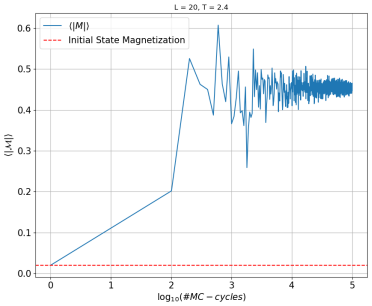
(h)T = 2.4, magnetization plot. Initial configuration: all up



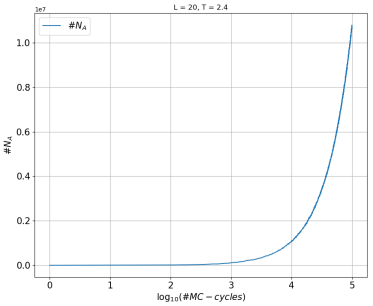
(i)T = 2.4, #Accepted spins plot. Initial configuration: all up



(j)T = 2.4, energy plot. Initial configuration: random



(k)T = 2.4, magnetization plot. Initial configuration: random



(l)T = 2.4, #Accepted spins plot. Initial configuration: random

There are various characteristics observed in the plots, for instance plots (a) shows that the initial energy of the system was lower than the energy in the equilibrated system. While plot (d) shows the opposite of this. This is what is known as respectively; cold and warm starts. An observation to be made is that both cases of non-random initial configurations for T=1 and T=2.4 resulted in a cold start, while the opposite is true for the random initial configurations. The magnetization (middle column of plots (d), (e),(h) and (k)) in the equilibrated states are also non-zero, meaning that neither temperatures are Curie temperatures. The rightmost column of plots: (c),(f) and (i), show an exponential increase of accepted spins as function of #MC-cycles. The middle row of plots (d-f) are particularly noisy, with a close to zero initial magnetization.

When observing all plots, it seems reasonable to assume that the system is at equilibrium at about 10^4 #MC-cycles with perhaps an error margin of $\pm\frac{10^4-10^3}{4}$. This particular error margin is based on, by eye observations of the leftmost and middle columns of plots.

Next the probability distribution of the $L = 20$ lattice is computed by counting the number of times a given energy results from an accepted/declined spin flip in the Monte Carlo iterations for the $T = 1$ and $T = 2.4$ cases with 10^6 #MC-cycles.

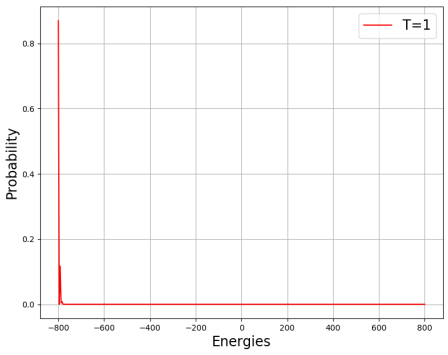


Figure 6: Probability distribution of the $L = 20$ lattice for $T = 1$.

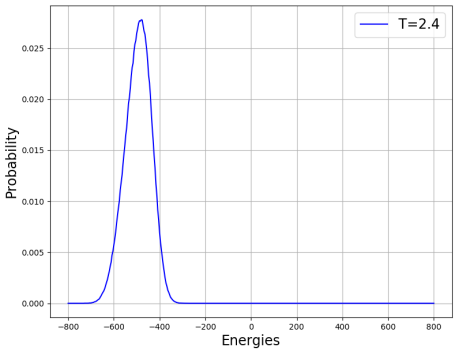


Figure 7: Probability distribution of the $L = 20$ lattice for $T = 2.4$.

As can be studied from the probability distributions, there is a sharp probability for the low temperature distribution, while a more evenly distributed probability for the higher temperature distribution. Computing the maximum probabilities yields

Table VII: The maximum probabilities P_{max} from the probability distribution of the $L = 20$ lattice for temperatures $T = 1$ and $T = 2.4$.

	$T = 1$	$T = 2.4$
P_{max}	0.87	0.03

C. Part III: Phase Transitions

Results for this part stems from the output from *p4sube.py* and *p4subf.py*.

Running with a temperature interval $T \in \{2, 2.5\}$ with a step-size of $h_T = 0.01$ with #MC-cycles $= 10^5$ for each lattice-length $L \in \{40, 60, 80, 100\}$, initial configuration: all spins up.

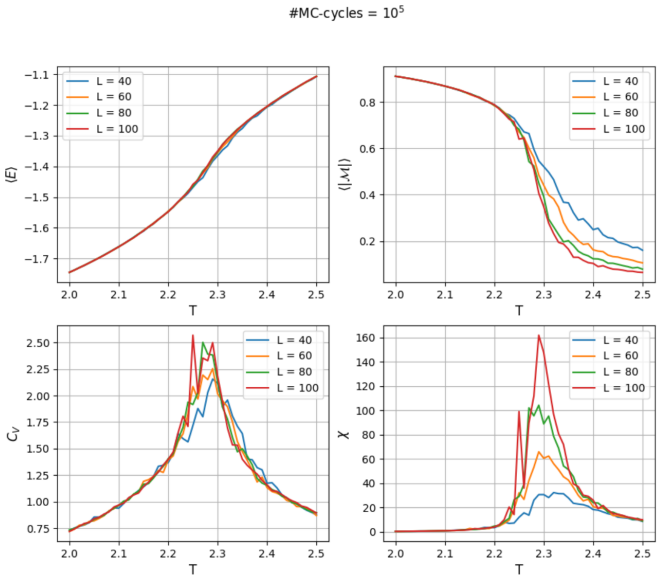


Figure 8: Results of phase transition computation run. Expectation values as functions of temperature.

adding an additional higher precision run with temperatures $T \in \{2.2, 2.3\}$ with step-size $h_T = 0.001$ and #MC-cycles $= 10^6$.

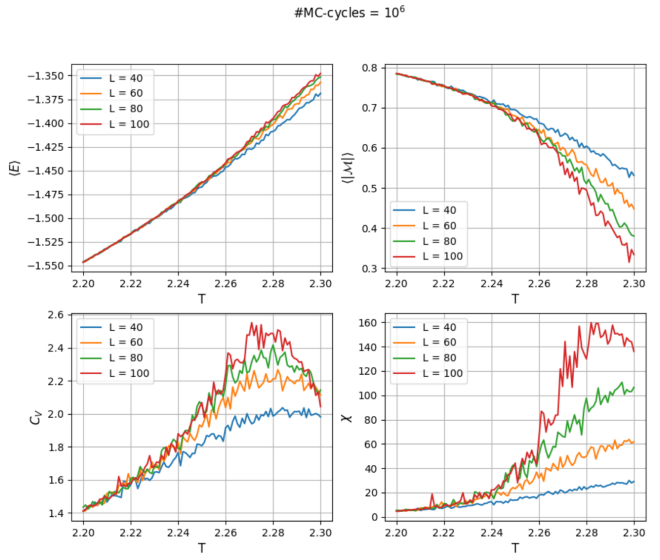


Figure 9: Plots of high precision runs for temperatures $T \in \{2.2, 2.3\}$ with step-size $h_T = 0.001$ and #MC-cycles $= 10^6$.

creating a fourth degree least squares fitting to the heat capacity curves in order to compute the maxima so as to find the approximated Curie temperatures.

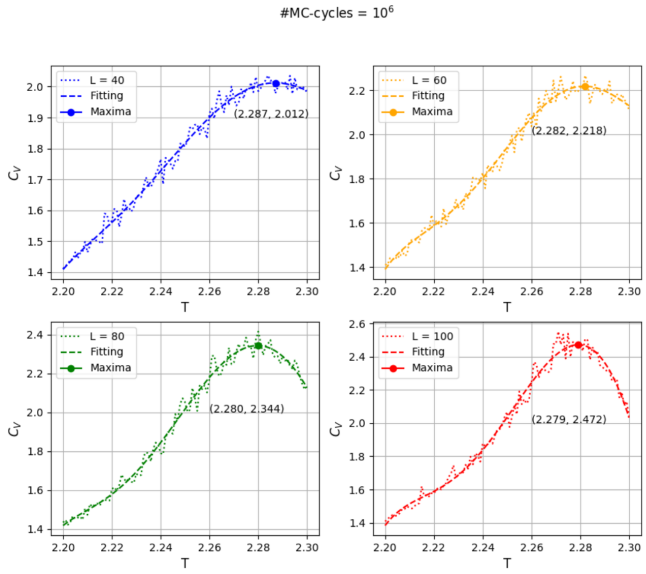


Figure 10: Plots, of high precision runs, of heat capacity, with fourth degree fitting and marked maxima for each expectation value and lattice length.

now extracting the Curie temperatures and performing a least squares fitting of first degree to the finite size scaling model

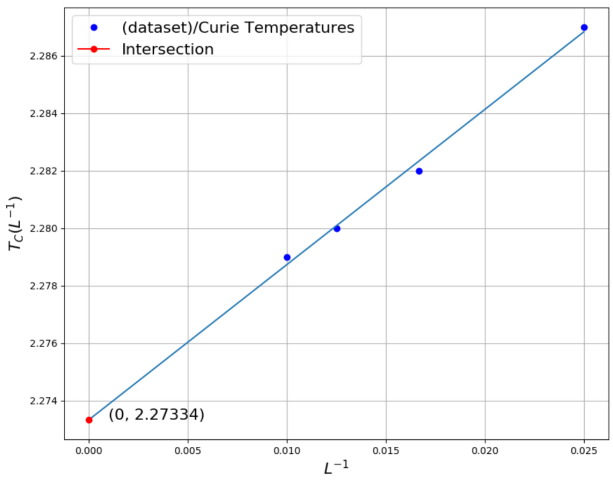


Figure 11: First degree least squares fit of Curie temperatures as function of $1/L$.

V. DISCUSSION

A. Part I: Onsager's Result

In the result section (IV A), plot (5) shows a downward trend with increased sample size for the expectation values. This is what one should expect for a statistical mechanical described system. From the four tables at (III), the energy and the susceptibility have smaller errors than the magnetization and the heat capacity, although all values are within the error margin. Without more data, this will have to be attributed to either a random outcome from the simulation or to unaccounted for causes. An interesting result which would be a good addition, for quantitative reasons, would be to see how the fitted trendlines behave for increasing #MC-cycles. In this case it might be a reasonable assumption that the slopes of the trendlines should become more negatively steep.

B. Part II: Reaching Equilibrium

The observations made in section (IV B) provide several bases for discussion of the plots (a-l) (IV B). Firstly, the fact that both of the random initial configurations resulted in a warm start.

The system should have symmetry in it's microstates about the initial energy of zero, meaning that there should be an equal amount of states, with degeneracies, about the zero energy. This means that without knowing exactly what the equilibration energy is, there is no way of telling whether there is a higher probability for a warm start or a cold start. Based on the computed equilibrium energy for the $L = 20$ lattice, since the energy is negative, a warm start is more probable. Since simply more initial states will be considered warm states.

Secondly, the number of accepted spins N_A increase proportionally to the increase in temperature from $T = 1$ to $T = 2.4$. Specifically, for #MC-cycles 10^5, there is an increase of $\approx 10^7/3 \cdot 10^4 \approx 333$. The functional form of an exponential, however, is the same. Physically this means that the threshold for accepting a spin flip has been lowered. Meaning a proposed spin flip which results in a higher energy is more likely to be accepted by the metropolis algorithm. This means the system will be more likely to transition from a current energy state to a state with higher energy than for a lower temperature. Which seems physically consistent with the expectation of there being more thermal fluctuations in a higher temperature physical system.

The third row of plots in (IV B) show a warm start simulation, where the number of accepted spins N_A greatly fluctuate, meaning that many transitions from low energy states to high energy states are accepted in the metropolis algorithm. This seems to be a highly improbable simulation, due to the fact that such transitions are computed with a probability. This might also be attributed to a faulty computation from a programming error.

In summary, the equilibration time is taken to be $\geq 10^4$ #MC-cycles.

Moving on to the probability distributions (6) and (7).

As can be seen from the probability distributions, and from the computed probabilities in table (VII). The system at lower temperatures, has a very large probability for reaching it's equilibrium energy, when compared to the higher temperature system. An explaination for this might be attributed to the phenomenon of [3]spontaneous magnetization, where the significance of lower spins being aligned, is increased for lower temperatures. Thus causing a certain alignment between the neighbouring spins to become increasingly favourable towards the particular minimized energy. Other factors may also contribute to this. Perhaps the second law of thermodynamics suffices, as the entropy increases with temperature.

C. Part III: Phase Transitions

From the first degree fitting of the Curie temperatures, the result of the Curie temperature in the thermodynamic limit is 2.27334 ± 0.22520, with residuals from the fit. This is extracted from plot (11). When compared to the analytical value of Onsager, ≈ 2.269, it puts the numerical value within the error margin, although with an unsatisfying error magnitude. The magnitude of the error is based on the number and quality of samples, which of there are only four. Thus, a reasonable assumption seems to be that with an increased sample size, this error should decrease. The absolute error of the numerical value and Onsager's value is thus $\sim 10^{-3}$ which happens to be consistent with the step-size of 10^{-3} of the *high precision run*. However, when running the same computation for step size $T \in \{2.0, 2.5\}$ with step-size $h_T = 0.01$ and #MC-cycles $= 10^5$ gives an absolute error for the same comparison of $\sim 2 \cdot 10^{-3}$.

Considering the first plot (8) of the magnetization, there are definite signs of a phase transition. From the theoretical proportionalities, in (II F), the plot shows that respectively, the maximum of the heat capacity and susceptibility have maxima about the Curie temperature. Which is in accordance to the steepest incline and decline, in the plots for the energy and magnetization. Elaborating on this, it can be said that; about the Curie temperature, it is expected to find the largest **change** in magnetization (susceptibility) and energy (heat capacity). A word on the chosen least squares fitting of (11); it was chosen to fit the results with a fifth degree polynomial. This seems reasonably not optimal, due the heat capacity having more similarities with a bell shaped function or a poisson distribution, and not a fifth degree polynomial. This is also a source of error in addition to low #MC-cycles. One could have done a more appropriate fitting of the heat capacity by using better suited methods, such as [1]*Iteratively reweighted least squares*

or [2]cubic-spline interpolation. However for this report's purpose, the acquired results are considered sufficient, in order to demonstrate the phase transitions in ferromagnetic materials using the Ising model.

VI. CONCLUDING REMARKS

From part I, it was found that the absolute error, between Onsager's analytical results and computed results from the Metropolis algorithm, decreased with an increased sample size. Also, the numerical mean value with maximum sample size, when compared to Onsager's results, were in accordance to the seventh decimal for energy and magnetization. While to the sixth decimal, for the heat capacity and susceptibility.

In part II, it was found that the equilibration time of the $L = 20$ lattice was approximately 10^4 and that the system at $T = 1$ had a sharp probability distribution, surrounding the most likely energy, which had a probability of 0.87. While the system with the increased temperature $T = 2.4$, yielded a more evenly distributed probability, where the maximum likely energy had a probability of 0.03.

Lastly, part III showed, that a magnetic phase transition occurs at the temperature $T = 2.27334 \pm 0.22520$. Which, when compared to Onsager's result of the Curie temperature, gave an error of order $\sim 10^{-3}$. Assuming the fitting error is low.

VII. AUTHOR'S REMARKS

Personally, I feel like a lot has been learnt from studying the Ising model, and by applying the Metropolis algorithm. Specifically, just how resource demanding certain physical systems can become and how important it can be to apply efficient algorithms, and to be more *efficient-minded* while doing the actual programming.

I think for sure that, if Metropolis, would be alive today , that he would be highly impressed with just how many fields of not just science, that the Metropolis algorithm has been applied to.

VIII. GITHUB-REPOSITORY

`https://github.com/nhofield/fys3150Projects.git` The programs for this report are found in the folder named, Prosjekt 4.

[1] C Sidney Burrus, *LaTeX: Iterative Reweighted Least Squares.* `file:///C:/Users/meg/Downloads/iterative-reweighted-least-squares-12.pdf`

[2] Qinyang Li, Nengchao Wang, Dayi yi., *LaTeX: Numerical Analysis*

[3] Morten Hjorth-Jensen, *LaTeX: FYS3150 Lecture Notes, chapter 5* `http://stp.clarku.edu/notes/chap5.pdf`

[4] Fowler, Michael, *LaTeX: Historical Beginnings of Theories of Electricity and Magnetism*

[5] Metropolis, Rosenbluth, Rosenbluth, Teller & Teller, *LaTeX: Equation of State Calculations by Fast Computing Machines* `https://bayes.wustl.edu/Manual/EquationOfState.pdf`

[6] Thomas Ising, Folk, Kenna, Berche & Holovatch, *The Fate of Ernst Ising and the Fate of his Model* `https://arxiv.org/pdf/1706.01764.pdf`

[7] Pavel Dvorak, *LaTeX: Ising Model in Finance* `file:///C:/Users/meg/Downloads/bptx_2010_2__0_292817_0_110160.pdf`

[8] D. Stauffer, *LaTeX: Social applications of two-dimensional Ising models* `https://arxiv.org/abs/0706.3983`

[9] G. G. Cabrera, R. Jullien, *LaTeX: Role of boundary conditions in the finite-size Ising model*

[10] Footnote: In the general Ising model the constant $J \rightarrow J_{kl}$ within the sum, but a simplified model will be studied in this report.