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Simulating the Ising model

Computational Physics

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Date: June 23, 2015

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1. Introduction

In this report we tried to measure the critical exponents for both the 2D and 3D Ising models. We used both the Metropolis algorithm and the Wolff algorithm to simulate the Ising model. The values of the critical exponents ν, γ and the critical temperature T_c were estimated with the finite size scaling method.

2. The Ising model

The Ising model is a simple model that describes ferromagnetic materials. The model consists of a lattice. Each lattice site i has a variable s_i, called the *spin*, which can take the values 1 or -1. These sites can interact with their nearest neighbours. The interaction energy between two neighbouring sites i and j is called J_{ij}. Also at each site an external magnetic field B_i can be applied. The system also interacts with an outside thermal reservoir of fixed temperature T, that acts as noise on the system. The *Hamiltonian*, or energy, of this model is given by:

$$H = -\sum_{\langle i,j \rangle} J_{i,j} s_i s_j - \sum_i B_i s_i, \tag{1}$$

where the notation $\langle i, j \rangle$ indicates that the first sum is taken over all nearest neighbour pairs. The *magnetisation* is defined by:

$$M = \sum_i s_i. \tag{2}$$

In this report we only used differently sized square lattices with periodic boundary conditions. The length of the lattice sides is called L. We have also taken $J_{ij} = 1$ and $B_i = 0$ for all i, j. Since J is taken positive, the lowest Hamiltonian value is achieved when all spins are aligned, and because we have no external magnetic field, the model has no preference for either 1 valued spins or -1 valued spins.

3. The Metropolis algorithm

The first method we used to simulate the Ising model is the Metropolis algorithm. This is a Markov Chain Monte Carlo method that uses the equilibrium distribution of a Markov chain to approximate the Boltzmann distribution. During each time step a random site is selected. Then the energy of the current state, H_{old}, and the energy of the state where the spin of the chosen site is flipped, H_{new}, are computed. Then the new state is accepted with probability

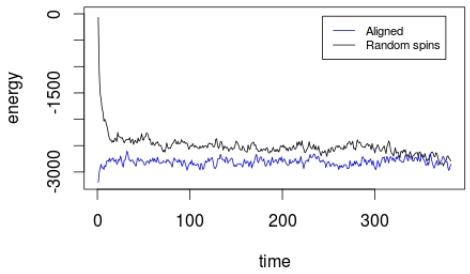
$$P_{change} = \min\{1, e^{\beta(H_{old} - H_{new})}\}, \tag{3}$$

where β is the inverse temperature, $\beta = \frac{1}{T}$. If the new state is rejected, the old state will be used for the next time step. The time is measured in sweeps, or Metropolis time steps per site.

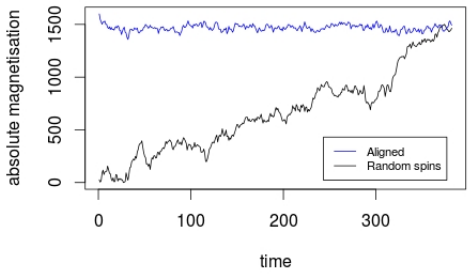
We implemented this algorithm in C++ and measured the energy and magnetisation of our model after each sweep. This data was then analysed using the R language.

3.1. Thermalisation.

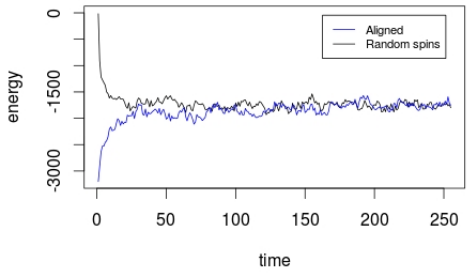
Before we can sample states according to the Boltzmann distribution, we first have to make sure that the model has reached its equilibrium distribution. This process is called *thermalisation*. For our thermalisation criterion two different models were used, one initialized with random spins at each site and one with all aligned spins. After each Metropolis time step the energy and absolute magnetisation of both models were measured. When both the energy values intersect 500 times and the absolute magnetisation values intersect 500 times as well, we assume that the models have thermalised. We have plotted the thermalisation process for different temperatures on a 40×40 lattice.



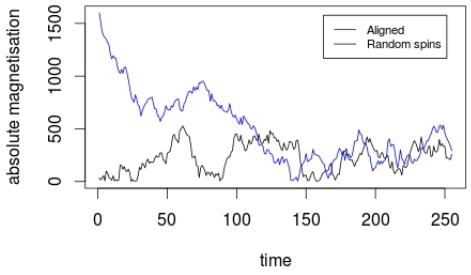
(A) *Energy during thermalisation at temperature* $T = 2.0$.



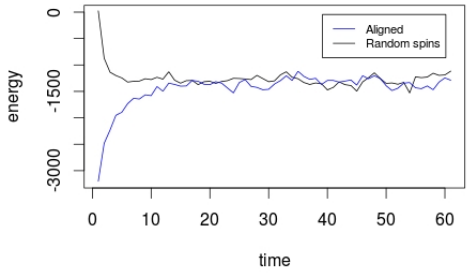
(B) *Absolute magnetisation during thermalisation at temperature* $T = 2.0$.



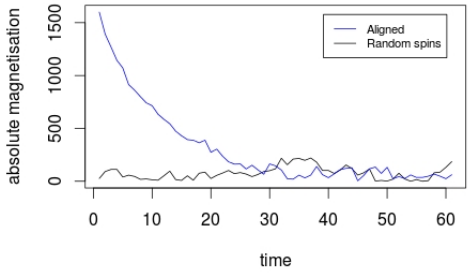
(C) *Energy during thermalisation at temperature* $T = 2.5$.



(D) *Absolute magnetisation during thermalisation at temperature* $T = 2.5$.



(E) *Energy during thermalisation at temperature* $T = 3.0$.



(F) *Absolute magnetisation during thermalisation at temperature* $T = 3.0$.

FIGURE 1. *Energy and absolute magnetisation during thermalisation at different temperatures on a* 40×40 *lattice. Time is measured in sweeps.*

At the end of the thermalisation the energy and magnetisation of both models reach similar levels. This can be seen in figure 1. This indicates that after thermalisation the initial states of our models are no longer relevant for the current state. Therefore, we can assume that our models have reached their equilibrium distribution.

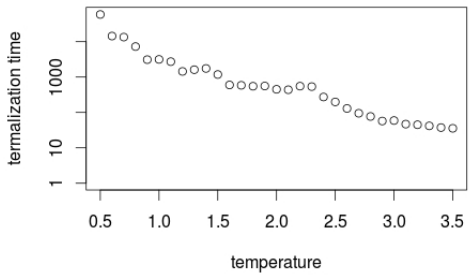


FIGURE 2. *Average thermalisation times in sweeps for different temperatures on a log-scale. The time average for each temperature was taken over 50 measurements on a* 40×40 *lattice.*

As we can see in figure 2, it appears that, using this thermalisation criterion, the thermalisation time increases exponentially as the temperature goes to zero.

3.2. **Correlation time.** Figure 1 also shows that both the absolute magnetisation and the energy of the model only differ slightly after each sweep. This indicates that after a single sweep, the next state is correlated to the first. We wish to sample states from the entire state-space to estimate the behaviour of the model. If all our measurements are correlated, we only sample from a small subset of the state-space, which would give biased estimates. Thus in order for our measurements to be accurate we need to do enough uncorrelated measurements. To do this we introduce the *autocorrelation time* τ of the system. This is a measure for the amount of time it takes the simulation to reach an uncorrelated state. This is the time it takes for the autocorrelation function to drop to $\frac{1}{e}$ of its initial value. We assume that two states are uncorrelated if they are at least 2τ sweeps apart [1].

We also plotted the autocorrelation function of the energy and absolute magnetisation for different temperatures, see figure 3. The autocorrelation indicates the the correlation between two states at different times, one state being Δt sweeps after the first. The autocorrelation function of the absolute magnetisation is given by

$$c_M(\Delta t) = \frac{\langle[(|M(t+\Delta t)| - \mu_{|M|})(|M(t)| - \mu_{|M|})\rangle}{\sigma^2_{|M|}}, \tag{4}$$

and for the energy it is

$$c_H(\Delta t) = \frac{\langle((|H(t+\Delta t)| - \mu_H)(|H(t)| - \mu_H)\rangle}{\sigma^2_H}, \tag{5}$$

where μ is the mean and σ the variance. Since the covariance of a random variable with itself equals its variance, we can rewrite this to

$$c_H(\Delta t) = \frac{\langle((|H(t+\Delta t)| - \mu_H)(|H(t)| - \mu_H)\rangle}{\langle((|H(t)| - \mu_H)(|H(t)| - \mu_H)\rangle}. \tag{6}$$

We assumed that the autocorrelation behaves like $e^{-\frac{\Delta t}{\tau}}$, which means that the log of the autocorrelation behaves like $-\frac{\Delta t}{\tau}$ [1]. We then fitted a straight line through the first linear part of our measurements of $\log(c_H(\Delta t))$ and $\log(c_M(\Delta t))$ using the method of least squares. For the slope s of this line then holds that $-\frac{1}{s} = \tau$. Estimating which part of the log-autocorrelation functions was no longer linear, was done by mere guesswork,

using the graphs of the autocorrelation functions in figure 3. The correlation times we found this way can be seen in table 1.

	Temperature=2.0	Temperature=2.5	Temperature=3.0
Absolute magnetisation	14.273669	41.07734	5.529683
Energy	6.330978	12.37829	2.247598

TABLE 1. *Correlation time in sweeps of the energy and absolute magnetisation at different temperatures on a* 40×40 *lattice.*

We can see that the correlation time increases as the temperature goes to the critical temperature of $T = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$ [2]. Also, our maximal value for τ is $\tau \approx 41$, which means that our measurements should be at least 82 sweeps apart in order for them to be uncorrelated.

3.3. **Equilibrium behaviour.** We simulated the Ising model using the Metropolis algorithm on lattice sizes 40×40 and 100×100 for different temperatures. The temperatures ranged from $T = 1$ to $T = 5$ with step size $\Delta T = 0.01$. For each temperature we simulated 20,000 sweeps after thermalisation and measured the energy and the magnetisation after each sweep. From these measurements we calculated the average absolute magnetisation, $\langle |M| \rangle$, for each temperature. We also calculated the magnetic susceptibility for each temperature

$$\chi = \frac{\beta}{L^2}(\langle M^2 \rangle - \langle |M| \rangle^2), \tag{7}$$

where L^2 is the number of lattice sites.

In figures 4a and 4c we can clearly see signs of a phase transition around $T \approx 2.3$. For lower temperatures $\langle |M| \rangle$ is very close to its maximal value L^2, which means that most of the spins are aligned. For higher temperatures we would expect $\langle |M| \rangle$ to be close to 0, since then all spins are random. This behavior is also observed in figures 4a and 4c. We also see that around $T \approx 2.3$ the magnetic susceptibility increases, which also indicates a phase transition. Note that the phase transition becomes more sudden in the 100×100 lattice, because of the increased size.

However, the magnetic susceptibility appears to be measured very inaccurately, especially in the 40×40 lattice, as can be seen in figure 4b. This becomes on obstacle if we want to use the magnetic susceptibility find the critical exponents using the finite size scaling method.

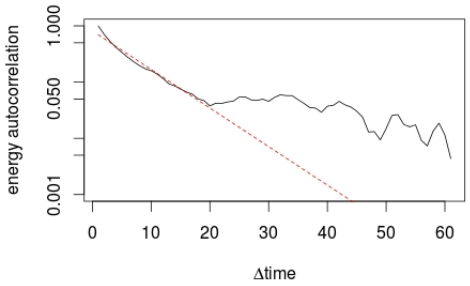
4. THE WOLFF ALGORITHM

The Wolff algorithm is an improvement on the Metropolis algorithm. Like the Metropolis algorithm the Wolff algorithm was designed specifically to simulate the Ising model. The main idea of this algorithm is to flip an entire cluster of equally valued spins, instead of flipping one single spin at a time. We first pick a random lattice site and add it to the cluster. Then for each site we added, we look at all its nearest neighbours and add it to the cluster with probability p_{add}, where

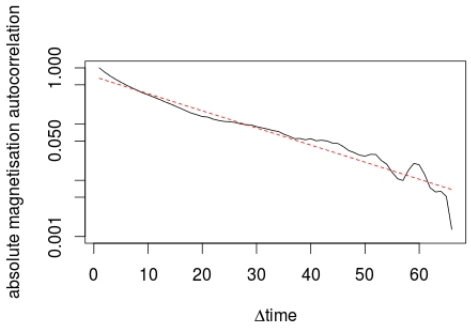
$$p_{add} = \begin{cases} 0 & \text{for } s_i \neq s_j \\ 1 - e^{-\beta J} & \text{otherwise.} \end{cases} \tag{8}$$

We repeat this until we don't add any new sites to the cluster. Then we flip the spins of all sites in the cluster.

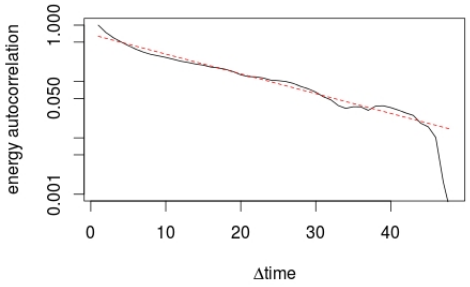
For low temperatures this probability is close to 1, which means that the clusters will be large and lots of spins will we flipped in each step. For high temperatures the clusters



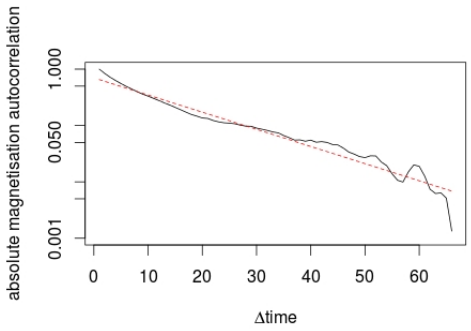
(A) *Autocorrelation of the energy at temperature $T = 2$, with fit through the first 20 measurements.*



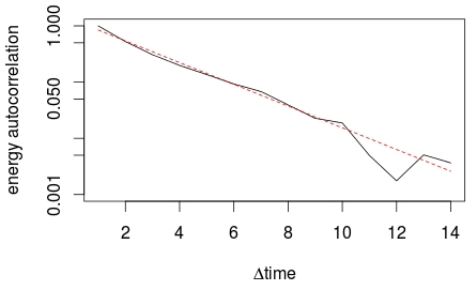
(B) *Autocorrelation of the absolute magnetisation at temperature $T = 2.0$, with fit through the first 35 measurements.*



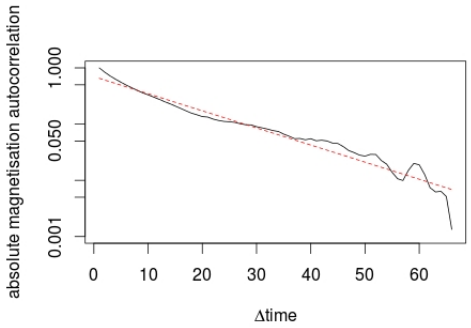
(C) *Autocorrelation of the energy at temperature $T = 2.5$, with fit through the first 40 measurements.*



(D) *Autocorrelation of the absolute magnetisation at temperature $T = 2.5$, with fit through the first 110 measurements.*

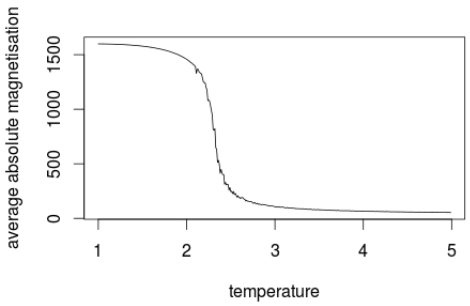


(E) *Autocorrelation of the energy at temperature $T = 3.0$, with fit through the first 9 measurements.*

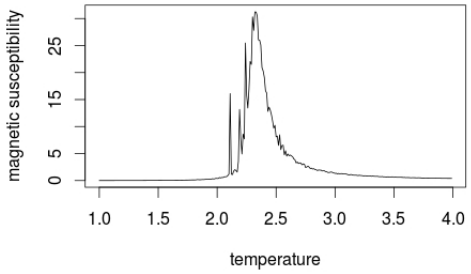


(F) *Autocorrelation of the absolute magnetisation at temperature $T = 3.0$, with fit through the first 21 measurements.*

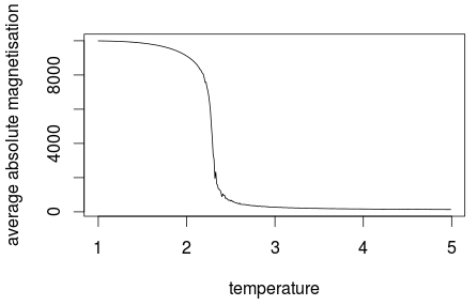
FIGURE 3. *Autocorrelation of the energy and absolute magnetisation at different temperatures on a 40×40 lattice. The red dotted line is a linear fit through the first linear part of the graph.*



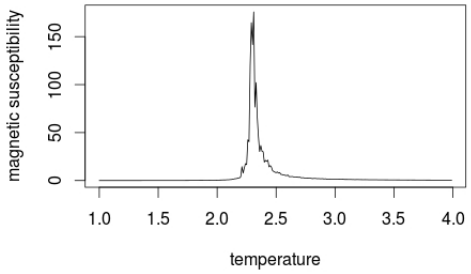
(A) *Average absolute magnetisation on a* 40×40 *lattice.*



(B) *Magnetic susceptibility on a* 40×40 *lattice.*



(C) *Average absolute magnetisation on a* 100×100 *lattice.*



(D) *Magnetic susceptibility on a* 100×100 *lattice.*

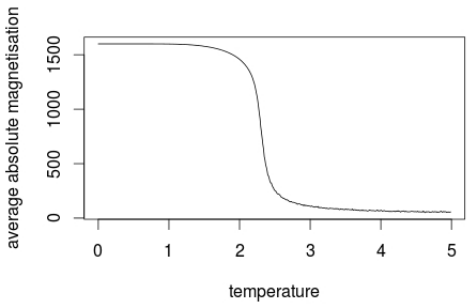
FIGURE 4. *Average absolute magnetisation and magnetic susceptibility as a function of the temperature on a* 40×40 *and* 100×100 *lattice. The averages have been calculated by simulating 20000 sweeps after thermalisation and measuring the magnetisation after each sweep.*

will be small and the Wolff algorithm will perform similar to the Metropolis algorithm. Time is no longer measured in sweeps, but instead in Wolff time steps. One Wolff step equals one cluster flip.

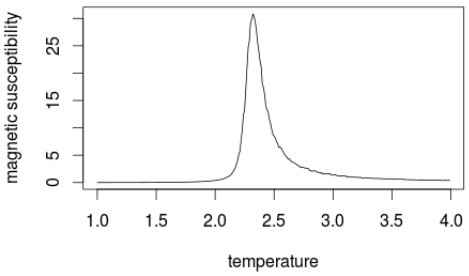
Since the Metropolis algorithm did not produce results that were accurate enough to perform the finite size scaling, we redid our measurements with the Wolff algorithm. We made an implementation in C++, for which we used a recursive function. We then simulated 20,000 Wolff steps after thermalisation for different temperatures. We took our temperatures in the range from $T = 0$, to $T = 5$, with temperature step size $\Delta T = 0.01$. After each Wolff step we measured the magnetisation and the energy. The analysis of this data was done with R.

We again calculated the magnetic susceptibility χ and plotted $\langle |M| \rangle$ and χ as a function of the temperature. As can be seen in figure 5, the general behaviour equals that measured with the metropolis algorithm in figure 4. However, this provided more accurate results then the Metropolis algorithm. The curve of the susceptibility is now as smooth as we would expect.

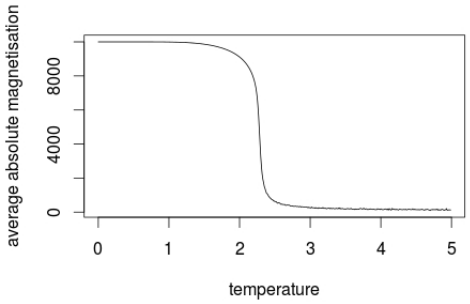
4.1. **Finite size scaling.** To determine the critical exponents ν and γ and the critical temperature T_c of the 2-dimensional Ising model we used the finite size scaling method. This method works by using that around the critical temperature $T = T_c$ the magnetic



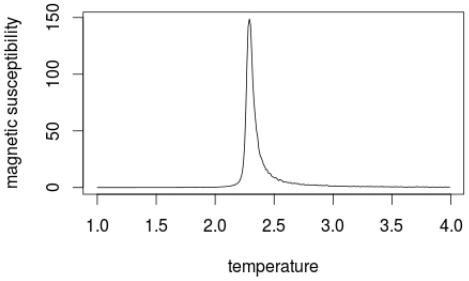
(A) *Average absolute magnetisation on a* 40×40 *lattice.*



(B) *Magnetic susceptibility on a* 40×40 *lattice.*



(C) *Average absolute magnetisation on a* 100×100 *lattice.*



(D) *Magnetic susceptibility on a* 100×100 *lattice.*

FIGURE 5. *Average absolute magnetisation and magnetic susceptibility as a function of the temperature on a* 40×40 *and* 100×100 *lattice. The measurements have been done using the Wolff algorithm. The averages have been calculated by simulating 20000 Wolff steps after thermalisation and measuring the magnetisation after each sweep.*

susceptibility behaves like

$$\chi = L^{\frac{\gamma}{\nu}} \tilde{\chi}(L^{\frac{1}{n}} t), \tag{9}$$

where t is the reduced temperature $t = \frac{T - T_c}{T_c}$ and $\tilde{\chi}$ is the susceptibility scaling function [1]. The susceptibility scaling function is an unknown function that is independent of the lattice size L. This means that if we measure $\tilde{\chi}$ for different lattice sizes the results should stay the same. If we would know the values of ν, γ and T_c we could estimate $\tilde{\chi}$ by using equation (9) and our measurements of χ. Since we measured χ for different lattice sizes, we could make multiple estimates for $\tilde{\chi}$ that should all yield approximately the same values, since $\tilde{\chi}$ does not change with the lattice size. For the correct values of ν, γ and T_c we would expect a data collapse to happen for our different estimates of $\tilde{\chi}$, i.e. the plotted values of the different estimates would overlap. We then guessed the values of ν, γ and T_c and changed our guesses until we observed a data collapse. The best data collapse seemed to occur when $\nu = 1.001$, $\gamma = 1.745$ and $T_c = 2.268$. The values of the critical exponents given by the analytical solution are $\nu = 1$, $\gamma = 1.75$ and $T_c = \frac{2}{\ln(1+\sqrt{2})}$, so our approximated results match the values of the analytical solution incredibly well.

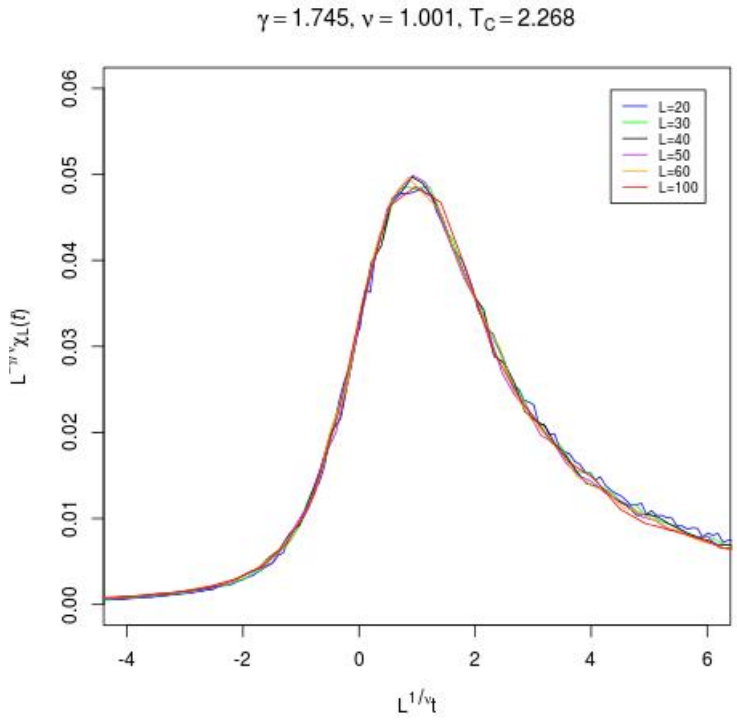


FIGURE 6. *Susceptibility scaling function estimates based on measurements of the susceptibility for six different lattice sizes. The magnetic susceptibility was measured with the Wolff algorithm.*

4.2. **The 3D Ising model.** We were also interested in the critical exponents of the 3-dimensional Ising model. These are not known analytically, but have been estimated at $\nu \approx 0.63$, $\gamma \approx 1.24$ and $T_c \approx 4.5$ [2]. We used a C++ implementation of the Wolff algorithm again to simulate the 3D Ising model. After the thermalisation process, we measured the magnetisation and energy after each of the 20,000 simulated Wolff steps. Because of the increased computational complexity, we used a smaller temperature interval with a larger temperature step size. The temperatures ranged from $T = 3$ to $T = 6$, with step size $\Delta T = 0.05$. We also used smaller lattices for our simulation, with our largest lattice size equal to $L = 40$. Note that in the 3D model, each lattice has L^3 sites.

We used the magnetic susceptibility

$$\chi = \frac{\beta}{L^3}(\langle M^2 \rangle - \langle |M| \rangle^2), \tag{10}$$

for the finite size scaling method. The best results were achieved for $\nu = 0.7$, $\gamma = 1.4$ and $T_c = 4.51$, as can be seen in figure 7. These results are a lot less accurate then the results we got in the 2D case, But this was to be expected since we also used less measurements for our estimation of the scaling function.

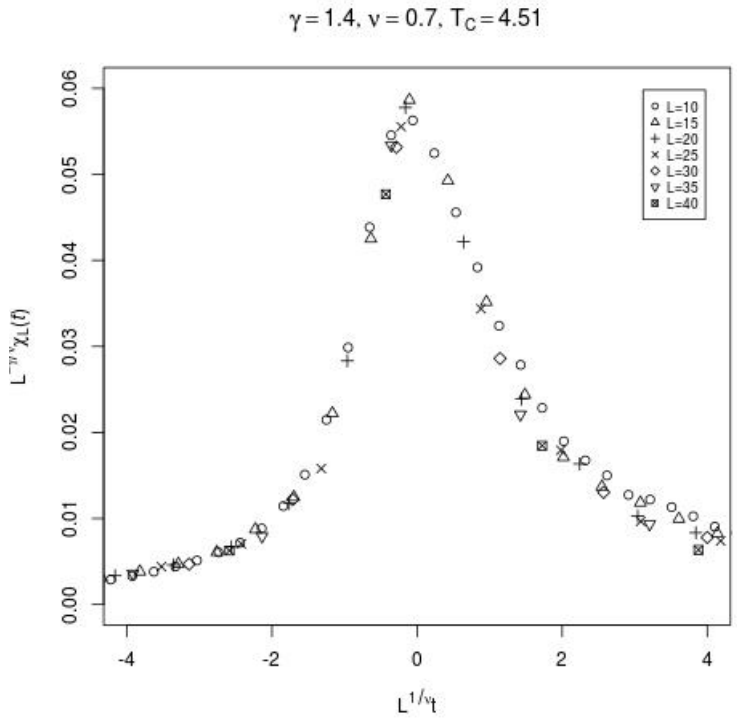


FIGURE 7. *Susceptibility scaling function estimates for the 3D Ising model. These estimates were based on measurements of the susceptibility for seven different small sized lattices. The magnetic susceptibility was measured with the Wolff algorithm.*

5. Conclusion

It is possible to find accurate estimates of the critical exponents of the Ising model. With the Wolff algorithm we found the estimates $\nu = 1.001$, $\gamma = 1.745$ and $T_c = 2.268$, which correspond with the theoretical values [2]. The Metropolis algorithm did not perform well enough to use the finite size scaling method. For the 3-dimensional Ising model the estimates of the critical exponents were less accurate. We found the estimates $\nu = 0.7$, $\gamma = 1.4$ and $T_c = 4.51$. Only the value $T_c = 4.51$ seems to correspond to previous results [2]. This was most likely due to the fact that we also took less measurements in the 3D case.

References

[1] MEJ Newman and GT Barkema. *Monte Carlo Methods in Statistical Physics*. Oxford University Press: New York, USA, 1999.

[2] Andrea Pelissetto and Ettore Vicari. Critical phenomena and renormalization-group theory. *Physics Reports*, 368(6):549 – 727, 2002.