2D Ising model

1. Introduction

This report has been developed from the study of the behaviour of a two-dimensional lattice model. Specifically, we have worked with the so-called Ising model. In our case, we will consider a model where its spins can take two values $s_i = \pm 1$. This model is defined by an Ising-type Hamiltonian with two terms. The first term representing the interaction of one of the spins with its first neighbours and the second term indicates the interaction of this spin with an external field h.

However, the application of this model is not simple at all. Even though in our case its resolution is analytically possible (using mean field approximations) we will use computational physics to solve it as it requires a large amount of time to do it.

We have also made some simplifications which do not significantly interfere with the study of this model. The first is that our Hamiltonian only considers interactions with its first neighbours (it is important to note that we have had to resort to periodic boundary conditions for the case of border spins). On the other hand, the second simplification has been to consider that the external field was null i.e. we have only considered the first term of the Hamiltonian. So, this one is like:

$$\mathcal{H} = -J \sum_{ij}^{neighbour} s_i s_j$$

With this Hamiltonian we have applied what is known as the Metropolis algorithm. Thus, when a change in one of the random spins provokes a minimization of the energy the change is accepted otherwise, we will call a random number U (0,1). If this one is less than the Boltzmann factor corresponding to this temperature (the Boltzmann factor can be expressed as $\exp(-\Delta H / K_B T)$) is also accepted if not, the change will be rejected, and another spin change is proposed. Because this algorithm is performed so many times, we can ensure that we will work with the entire lattice of spins.

To calculate quantities such as energy or magnetization we will use the Monte Carlo method. This method involves using the central limit theorem. So, we will be able to calculate integrals by evaluating the function to integrate in N different points between the integration boundaries. If we do this a large enough number of times the average of these points will give us the value of the integral.

Finally, it should be noted that simulations of the Monte Carlo method consume many random numbers. Therefore, it is necessary that these have the least possible correlation. This makes simple random methods useless to us so we will be using the mt19937 generator to generate our random numbers.

2. Temporal evolution of magnetizations and energies at different temperatures

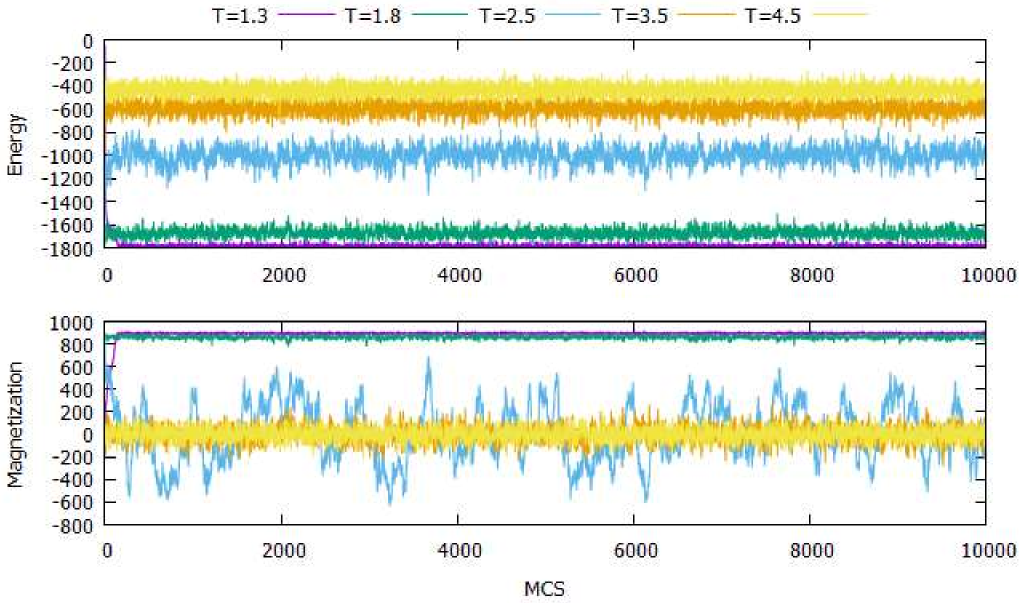

Figure 1. Temporal evolution of energy and magnetization by 5 different temperatures.

In the chart above us we have plotted how magnetization and energy vary for 5 different temperatures. Hence, we can see that from a certain number of Montecarlo steps the magnitudes tend to converge even though they have a certain fluctuation.

We can also observe that in the case of T = 2.5 this convergence does not occur this must be because we are close to a critical point. That is why the farther we are from these points the smaller the fluctuations are and the faster the variables will converge.

Finally, we can see that this phase transition consists of a shift of our spins from a ferromagnetic behavior (temperatures T = 1.3 and T = 1.8) to a paramagnetic behavior (temperatures T = 3.5 and T = 4.5). This can be seen with the values of magnetization and energy as in the ferromagnetic phase we will have the spins aligned and in the paramagnetic phase will be arranged randomly (we can see that for T = 3.5 and T = 4.5 the magnetization fluctuates around 0).

3. System behavior for L=30.

For L = 30 we have carried out a detailed study of the system. In it we have studied the temporal evolution of different variables between T = 1.4 and T = 3.4 with an interval of 0.01. This is done in order to study the behavior at the points close to the critical point appropriately.

Having L = 30 means that we are operating with a 900-spin system, large enough so the effects of periodicity do not affect it too much. We must keep in mind that as we increase the L the time it takes our program to run increases considerably.

Let us now represent the variables that we have calculated in our program.

Let's start with energy by spin. At low temperatures, ie at the ferromagnetic phase as the spins are aligned the value is expected to be -2. On the other hand, at high temperatures the energy by spin value will be close to zero as the spins are randomly oriented.

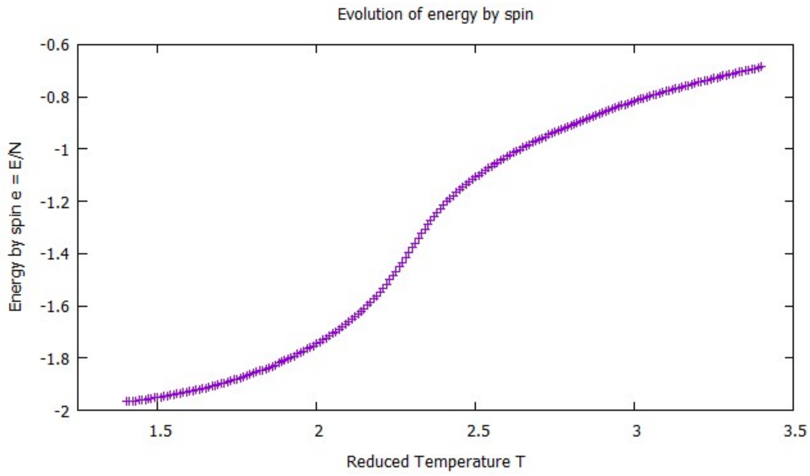

Figure 2. Energy by spin representation as a function of the temperature.

In Figure 2 we can see that although for low temperatures the system behaves like the ideal approximation for high temperatures this does not happen. The reason for it is the periodicity of the lattice. So, in case we wanted an ideal behavior we would have to operate with a lattice of $L \rightarrow \infty$.

In the case of the magnetization by spin, at low temperatures (ferromagnetic phase) we expect it to have a value around 1. On the other hand, once the critical temperature is exceeded the magnetization should become zero (paramagnetic phase).

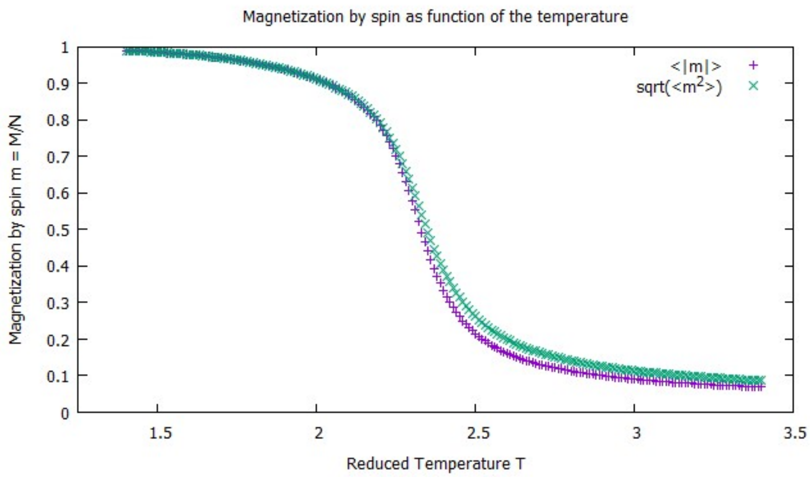

Figure 3. Magnetization by spin evolution as a function of the temperature.

We can notice that the behavior despite looking somewhat like the expected is not exactly the same. We should see how the curve intersects at the T_C and then the magnetization becomes 0. Instead, we have a much smoother behavior as a result of the finite size of our lattice.

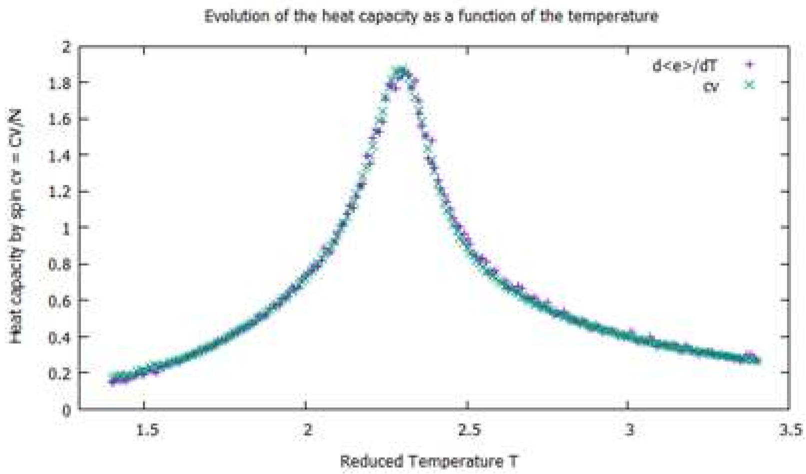

Figure 4. Heat capacity by spin calculated in two different ways.

The heat capacity behavior is as expected either if it is calculated from the fluctuations of the energy or from the derivative of <e> with respect to T. We can see that it presents a peak corresponding to the critical temperature. The value of this point should be around $T_C = 2.3$.

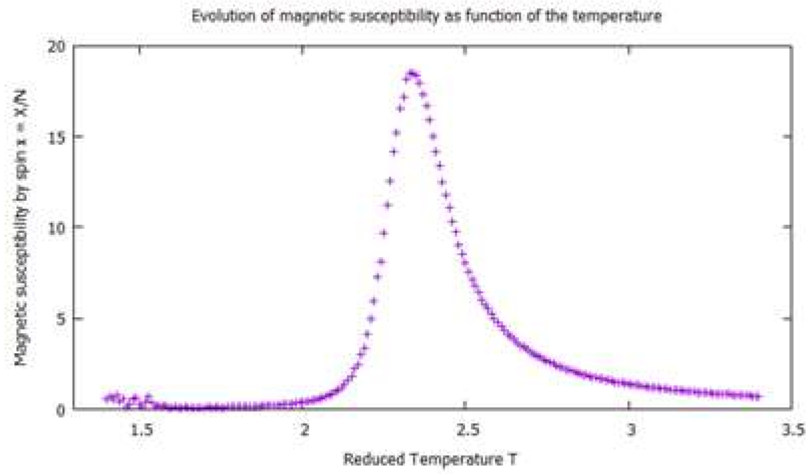

Figure 5. Magnetic susceptibility by spin representation as a function of the temperature.

The behavior of the magnetic susceptibility by spin also has the expected form. We can observe how it also has a critical temperature around the point $T_C \approx 2.3$.

4. Effect of varying the value of L

As we have mentioned before as we increase the value of L the system gets closer to its ideal behavior. This is because the periodicity we have imposed on the system is decreasing.

However, increasing the value of L is a major disadvantage, as the CPU time is drastically increased.

We have run our program for L = 15, 30 and 60. In order to reduce the number of temperatures we have limited the study around the critical temperature and thus minimizing the execution time of the program which was very large for L = 60.

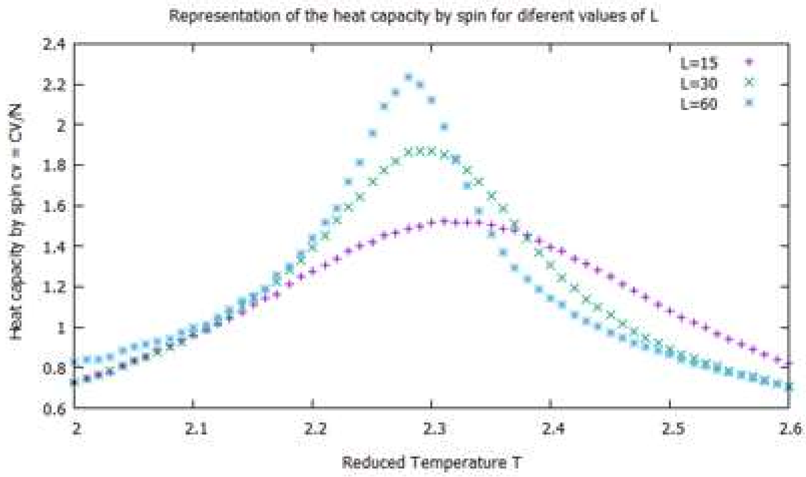

Figure 6. Heat capacity representation for different values of L.

We can see that as we increase the value of L the heat capacity per spin increases whereas the critical temperature decreases. This makes us doubt whether the critical temperature would really be $T_C \approx 2.3$ in an ideal system (when $L \rightarrow \infty$).

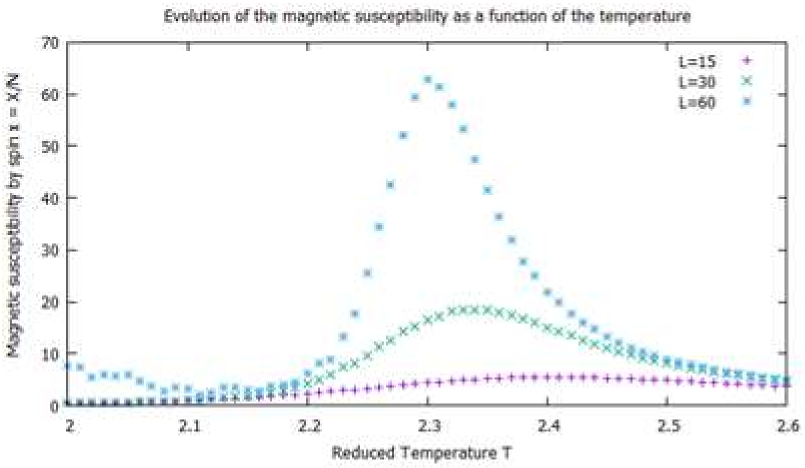

Figure 7. Magnetic susceptibility representation for different values of L.

We can observe that at low temperatures and for larger values of L in particular for L = 60 the system behaves in a strange way. Despite this the behavior is as expected but we again have the same problem as with the heat capacity, the critical temperature decreases as the size of the system lattice increases.

So, what is the value of the critical temperature? We will try to answer this in the next segment.

5. Determination of the critical temperature T_C

We have seen that the critical temperature does not have a strict value as it decreases its value as we increase the size of our lattice.

Now in order to find the critical temperature at which this system converges we are going to represent the T_C points that we have found for the heat capacity and magnetization:

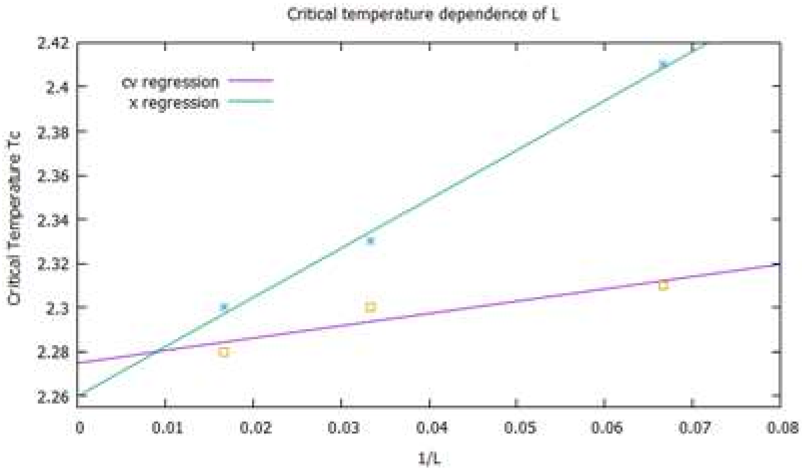

Figure 8. Critical temperature evolution as a function of 1/L

If we make a linear regression, we find that for the heat capacity we have:

$$T_C = 0{,}5571\frac{1}{L} + 2{,}275$$

Doing an extrapolation to the infinite (L →∞) we get that: T_C=2,275

Instead the linear regression of the magnetic susceptibility by spin is:

$$T_C = 2{,}2286\frac{1}{L} + 2{,}260$$

Now doing the same we will get that T_C =2,260

Therefore, the value of the critical temperature is: T_C= 2,27 ±0,01

6. Determination of the critical exponents

We have been able to observe how the critical temperature decreases as we make our lattice bigger. So, we have had to do an extrapolation in or order to calculate T_C. This is because in finite systems critical behavior does not exist as such what we observe are pseudocritical phenomena at temperature called pseudocritical temperature or T_{CL}.

These are given by the formula

$$A|T - T_C|^{-\nu} = KL$$

Operating,

$$T_{CL} = T_c + DL^{-\nu}$$

Where D=K/A

Now we are going to estimate ν. If we want to do that, we will have to represent log (T_{CL} -T_C) as a function of ln(L). So, we will have:

$$\log(T_{CL} - T_C) = \log(D) - \frac{1}{\nu}\log(L)$$

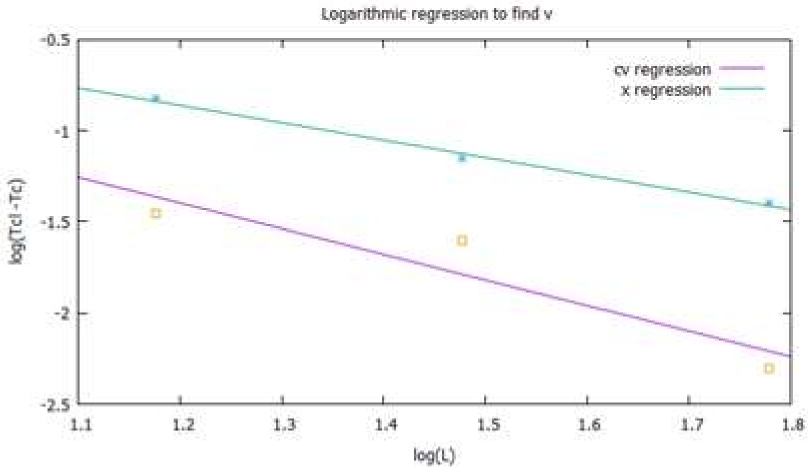

Figure 9. Representation of a logarithmic regression used to find v.

The heat capacity per spin regression is:

$$\log(T_{CL} - T_C) \ = -1{,}4037 \cdot \log(L) + 0{,}2871$$

In the case of magnetic susceptibility per spin we have:

$$\log(T_{CL} - T_C) = -\,0{,}9534 \cdot \log(L) + 0{,}2828$$

Therefore: $\left(\frac{1}{v}\right)_1 = 1{,}4037 \qquad \left(\frac{1}{v}\right)_2 = 0{,}9534$

We see that in the heat capacity case we are moving away from the behavior that we expected. This must be due that we only have 3 pseudocritical points. If we had more significant points the behavior would be most probably corrected.

$v_1 = 0{,}712 \qquad v_2 = 1{,}049 \qquad \rightarrow v = 0.9 \pm 0.2$

Where the theorical value is $v = 1$

In the case of γ we will estimate it from the pseudocritical behavior of the magnetic susceptibility.

$$X = A|T - T_C|^{-\gamma}$$

Operating we have that:

$$X = A|T - T_C|^{-\gamma} = A\left(CL^{-\frac{1}{v}}\right)^{-\gamma} = BL^{\frac{\gamma}{v}}$$

Where B is a constant.

Hence, we will have:

$$\log(X) = logB + \frac{\gamma}{v}\log(L)$$

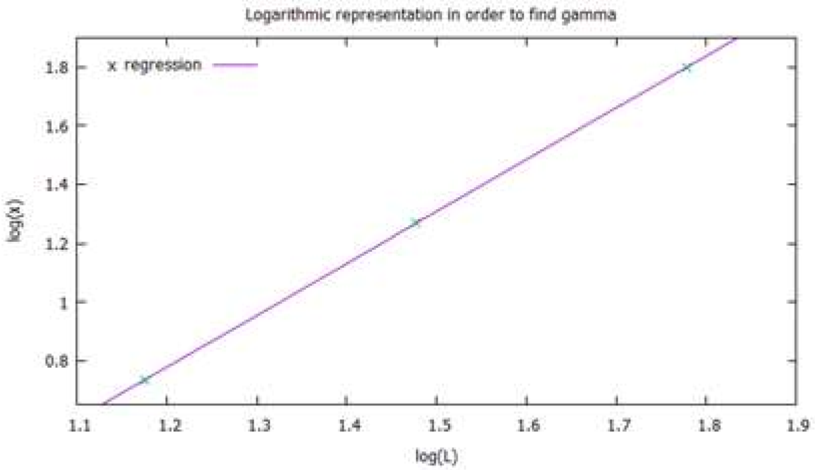

Figure 10. Representation to find ϒ.

The regression in this case is:

$$\log(\mathrm{x}) = 1{,}766\log(L) - 1{,}3413$$

Then $\frac{\gamma}{v} = 1{,}766$

Which is close to the expected value $\frac{\gamma}{v} = 1{,}75$

Now we can continue the calculus of critical exponents with the α exponent.

We can do that similarly to what we have done to calculate γ. Therefore, we will have:

$$c_v = A|T - T_C|^{-\alpha} = BL^{\frac{\alpha}{v}}$$

Operating this will result in:

$$\log(c_v) = logB + \frac{\alpha}{v}\log(L)$$

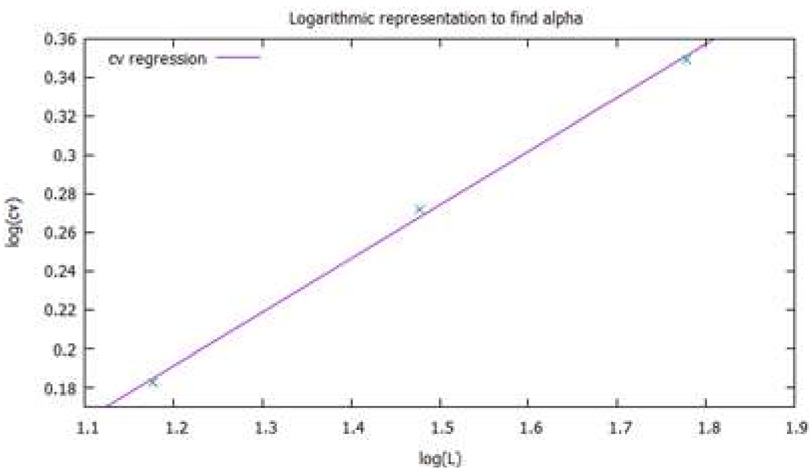

Figure 11. Representation to find β .

The resulting regression is:

$$\log(c_v) = 0{,}2769\log(L) - 0{,}1411$$

With $\frac{\alpha}{v} = 0{,}2769$

The theoretical value of $\frac{\alpha}{v}$ is 0 so we have an important deviation.

Finally, we have the β exponent which can be calculate from:

$$m = A|T - T_C|^{-\beta} = BL^{-\frac{\beta}{v}}$$

Operating we can obtain the function that will allow us to obtain β when we represent it graphically.

$$\log(m) = logB - \frac{\beta}{v}\log(L)$$

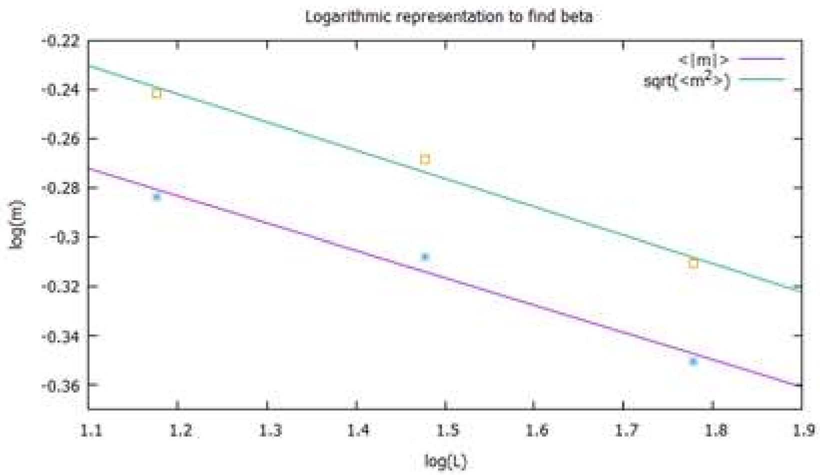

Figure 11. Representation to find α

We have represented the two ways that we have to calculate the magnetization: with the absolute value and with the root of the magnetization squared.

The regression in the absolute value case is.

$$\log(m) = -0{,}1109\log(L) - 0{,}1502$$

On the other hand, for the root of the magnetization squared we will have:

$$\log(m) = -0{,}1149\log(L) - 0{,}1039$$

Operating then we will have:

$$\frac{\beta}{v} = 0{,}113 \pm 0{,}002$$

That is very close to the ideal value of $\beta = 0{,}125$.

7. Conclusions

When studying the two-dimensional Ising model we made two simplifications. These two were that the Hamiltonian only considered interactions with its first neighbours and that that the external field h was null. We also must take in count that we have been working with a finite lattice, so we added some periodicity to our system. However, as we made the graphical representation of energy, magnetization, heat capacity or susceptibility we have not found any major changes to its ideal representation. As a result, we can say that the simplifications we have made have resulted to be correct.

We can see that at both limits of low and high temperatures the results fit perfectly with the theory. On the other hand, when studying the system by varying the value of L we have observed that as we increase this value, we get closer to the thermodynamic limit. Considering this and making an extrapolation to the infinite we have been able to graphically calculate the value of the critical temperature $T_C = 2.26 \pm 0.01$

Finally, we have obtained the critical exponents by means of plotting the functions that define them. Thus, we have found $v = 0.9 \pm 0.2$, $\gamma / v = 1.766$, $\beta / v = 0.113$ and $\alpha / v = 0.2769$. The value of α, however, is the only one that has not given us a result close to the theory, probably due to some of the simplifications made.