Critical and Cooperative Phenomena: The Ising Model

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1. Magnitudes representation for different lattice sizes

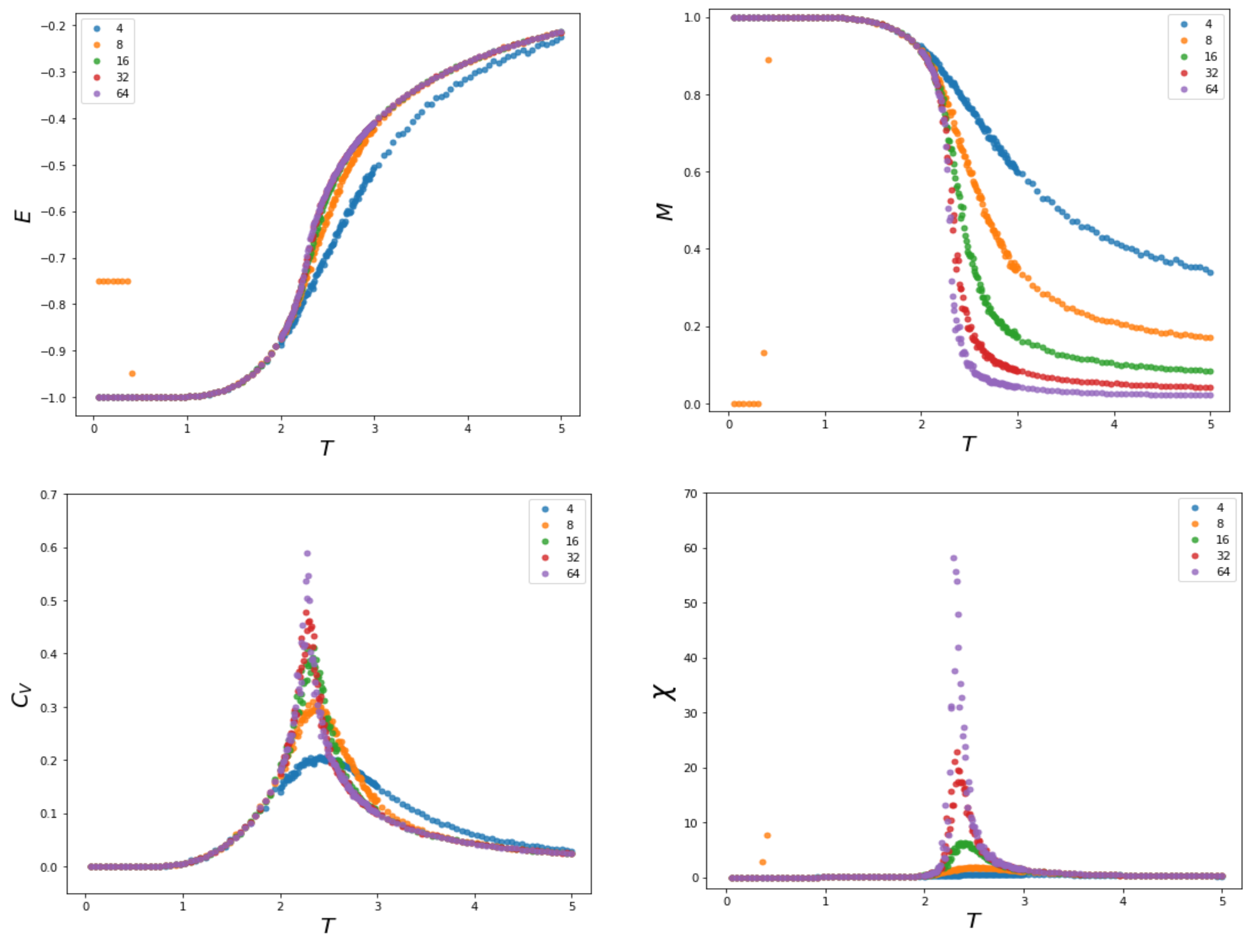


Figure 1: Energy, magnetization, specific heat and susceptibility for different lattices sizes L. The temperature T is in units of J/k_B.

The four plots above have been generated with a temperature interval $\Delta T = 0.05$ outside the critical region, i.e in the intervals $(0, 2)$ and $(3, 5)$, while in the range $(2, 3)$ I took 100 measures (that is, every $\Delta T = 0.01$). Thus, for every L I took 179 measures for each magnitude and this high number of measures was necessary above all for high dimensions L in order to get enough points in the critical region.

On the other hand, for each temperature the number of equilibrium steps was 1000 and the number of Monte Carlo steps was 15000. That is, once the system was at equilibrium I took 15000 measures separated by one Monte Carlo step ($L \times L$ Metropolis steps) and

I finally computed the average. The updating process was done sequentially: instead of choosing a random site (i, j) $L \times L$ times for each Monte Carlo step and then applying the Metropolis algorithm, I directly applied this Metropolis algorithm by rows. Finally, for the next temperature T I did not initialize the system with a random configuration but I rather took the final system of the previous temperature. This allowed me reduce the fluctuations. Regarding the computational time, the four plots only took me 40 minutes thanks to the *numba* package in Python.

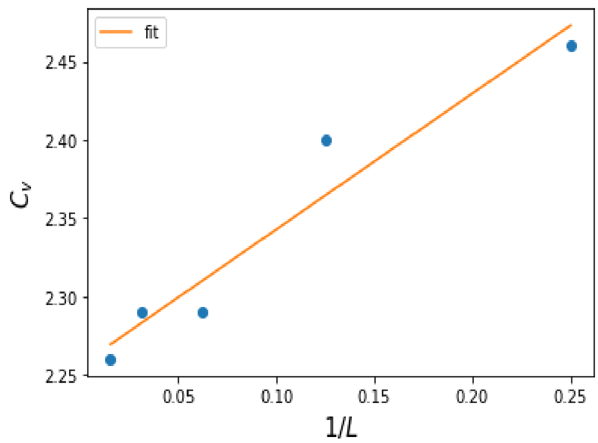
2. Critical Temperature Calculation

In Figure 2 I show a method of computing the critical temperature. Since this critical temperature is defined in the thermodynamic limit $L \to \infty$, for every lattice size L we simply have to plot the temperatures for which there is a peak in the specific heat and the susceptibility in terms of $1/L$. The intersection of the linear regression with the y axis will be the critical temperature. From the specific heat and the susceptibility I got, respectively, the following critical temperatures:

$$Tc = 2.259 \pm 0.055$$

$$Tc = 2.247 \pm 0.011$$

These results are quite satisfying, above all the first one, which is compatible with the theoretical one $T_c = 2.269$ taking into account the errors.



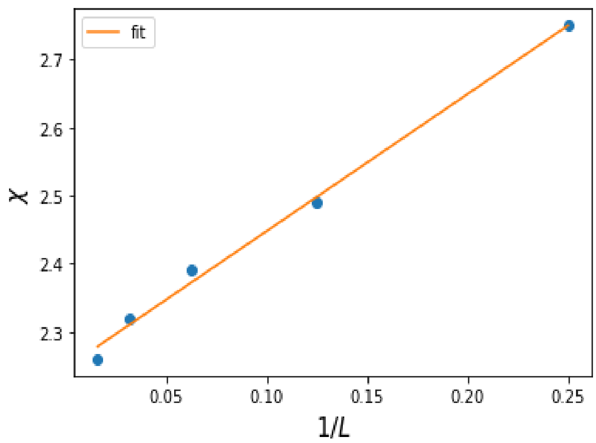


Figure 2: On the y axis I plot the argument (temperature) of the specific heat and susceptibility peaks in terms of $1/L$. The critical temperature is the intersection of the linear fit with the y axis.

3. Critical Exponents

For the critical exponents I took into account the following well-known theoretical results:

$$\begin{aligned} E(T) &\sim |T - T_c|^{-\nu} \sim L \\ M(T) &\sim |T - T_c|^{\beta} \sim L^{-\beta/\nu} \\ C_v(T) &\sim |T - T_c|^{-\alpha} \sim L^{\alpha/\nu} \\ \xi(T) &\sim |T - T_c|^{-\gamma} \sim L^{\gamma/\nu} \end{aligned}$$

This comes from the fact $L \sim |T_c(L=\infty) - T_c(L)|^{-\nu}$ (as the lattice size is increased, the difference $|T - T_c|$ tends to 0). This simplifies a lot the calculations of the critical exponents because, supposing $\nu = 1$, the critical exponents are the slopes of the linear fits in logarithm scale. More specifically, I plot the peaks of C_V and χ in terms of L in log-scale. Since for the energy there is no peak, I plot the values of the energy for $T = 2.269$ and I make the same linear regression once I take the logarithms. The fittings are shown in Figures 3 and 4 and the results for the critical exponents are:

$$\alpha = 0.365 \pm 0.040$$
$$\beta = 0.1157 \pm 0.0024$$
$$\gamma = 1.64 \pm 0.32$$

My results for β and γ are precise given the interval defined by the errors (they are both compatible with the theoretical results $\beta = 0.125$ and $\gamma = 1.75$). However, I could not get a reasonable result for α, whose theoretical value is $\alpha = 0$.

a) α calculation b) β calculation

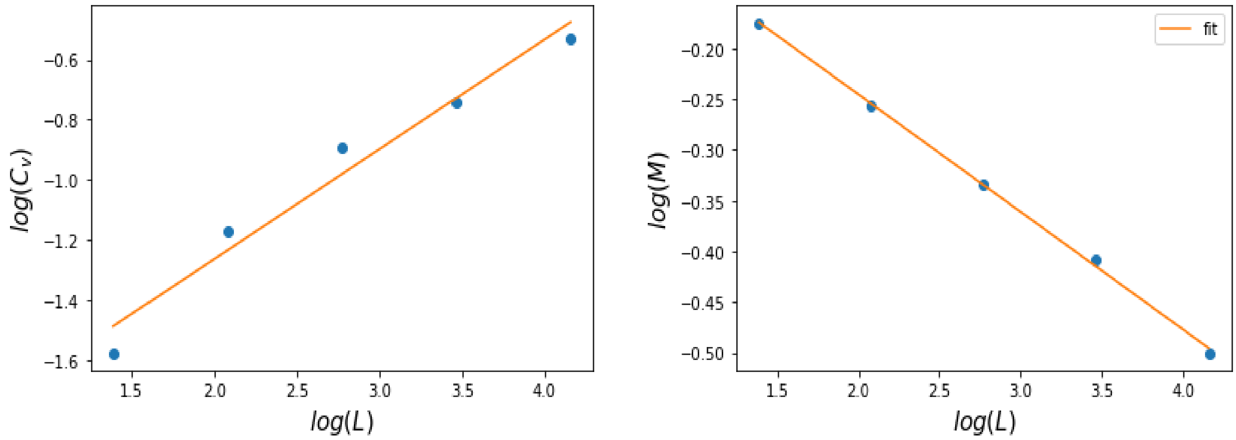


Figure 3: For each graph I plot the peak of the magnitude for every size L in log-scale and the respective critical exponent is the slope of the linear regression.

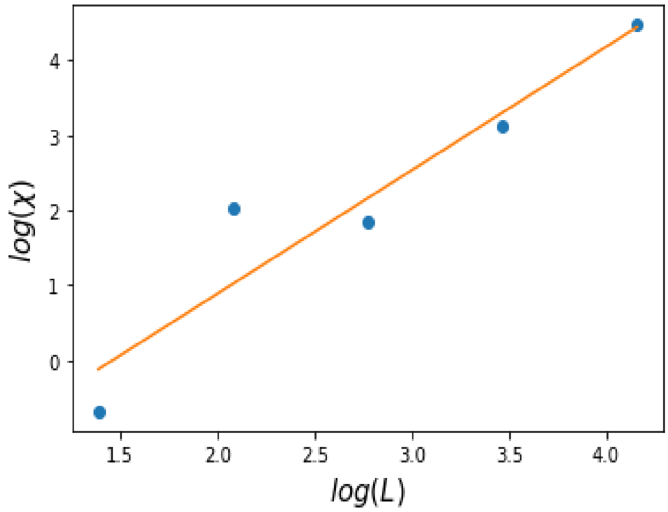


Figure 4: γ calculation. The graph represents the peak of the susceptibility for each size L in logarithmic scale. γ is simply the slope of the linear fit.

4. Correlation time, Correlation Length and ν calculation

For the correlation time I considered $L = 32$ and 3 temperatures, being one of them the critical one, and for each temperature I calculated the correlation function over 1000 measures of the magnetization with 10000 previous equilibrium steps. I define the correlation as usual: $C(t,T) = \langle M(t)M(t+t')\rangle_{t'} - \langle M\rangle^2$. In other words, for each of the 1000 measures of the magnetization, I analyze how correlated the i-th measure is with the rest of measures. The correlation function, as expected, decays exponentially and the decay is much slower at the critical temperature (*critical slowing down*).

Since the correlation function decays exponentially ($C(t,T) \sim e^{-t/\tau}$), the correlation time τ can be estimated as minus the inverse of the slope in logarithmic scale. However, in order to avoid the fluctuations, I do this fit for the first 5 values of each curve for better results. The correlation times are thus:

$$\tau(T = 1.8) = 3.1$$
$$\tau(T = 2.269) = 128.7$$
$$\tau(T = 5) = 1.8$$

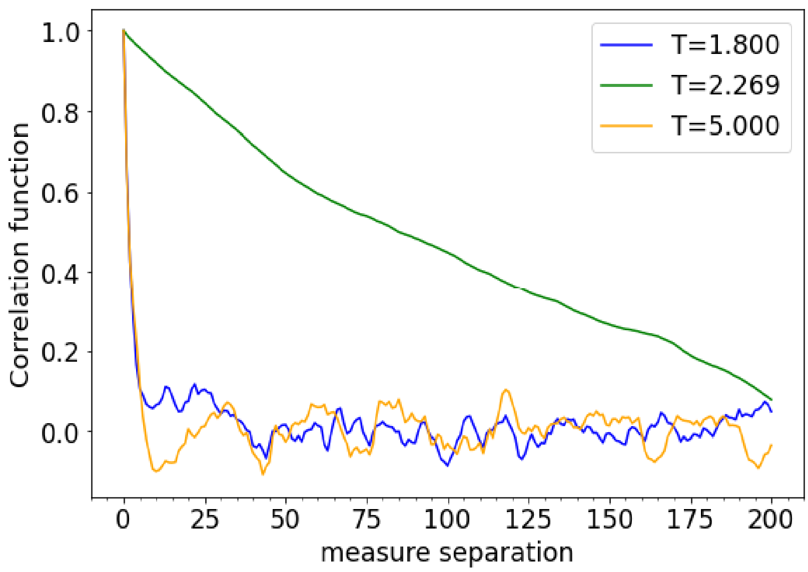


Figure 5: Correlation function for the susceptibility measures for 3 temperatures.

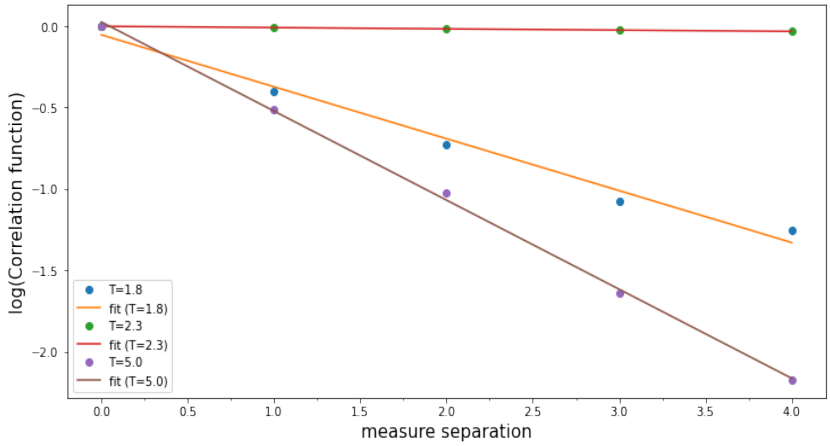


Figure 6: Correlation time estimation for different temperatures.

To compute the correlation length I do something similar, but for $L = 16$: for every temperature I make 1000 equilibrium steps and once I get the spin configuration in a $L \times L$ matrix I compute the correlation for different spin distances $|i - j|$ along the 4 directions. The correlation is $C(i - j) = \langle \sigma_i \sigma_j \rangle$ and, since it decays exponentially with a rate equal to minus the inverse of the correlation length, I estimate this correlation length, again, with a linear fit in log-scale but just taking the first 3 values of each curve (otherwise I get a wrong tendency: the correlation lengths increases with T). The correlation length decays for higher temperatures and it ranges from $\xi(T = 3) = 0.78$ to $\xi(T = 5) = 0.39$. Finally, with these 5 values of ξ we can estimate ν by means of another linear fit between $log(\xi)$ and $log(T - T_c)$, since $\xi(T) \sim |T - Tc|^{-\nu}$. However, I get a non-accurate value of ν, far from 1:

$$\nu = 0.43 \pm 0.16$$

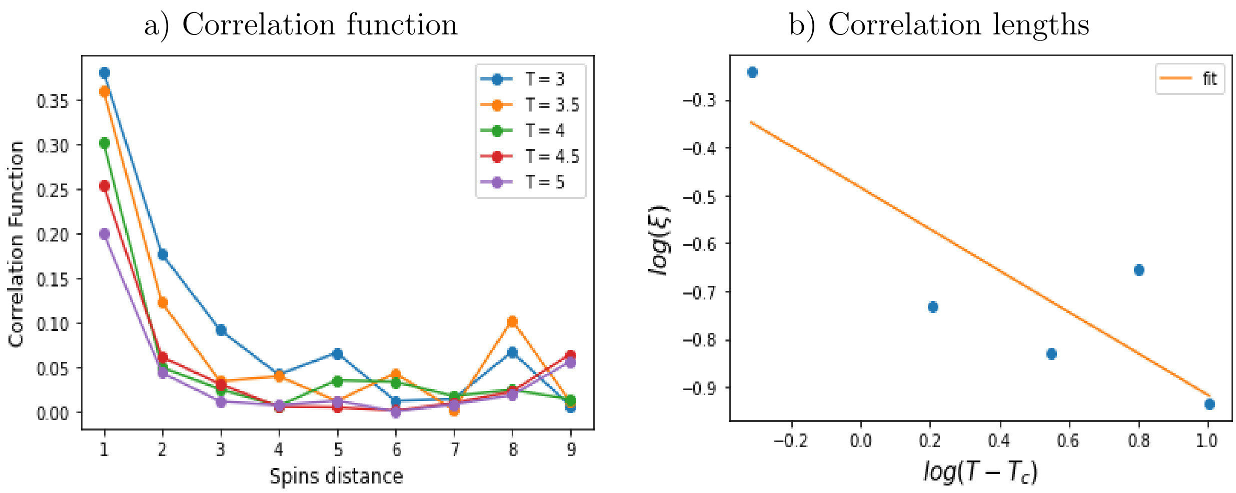


Figure 7: Once the correlation function is computed for every T (Figure a), an exponential fitting is made to estimate the correlation length ξ (Figure b).

5. Finite size and Scaling

The re-scaling is done according to what is shown in the axes in the figures below, hence the scaling is done with the critical exponents. τ is $T_c - T$ and for each temperature it was considered 1000 equilibrium steps and 15000 Monte Carlo steps for the magnetization and susceptibility calculations. The lengths L are the same as in the first section and the number of temperature points is not the same for every L: for L=4 it was enough to consider 50 points in the interval (0,5), and for the next dimension L this number was increased in 25 units until $L = 64$, for which I used 150 temperature points. The results are quite satisfactory: for all sizes the functions collapse at the critical point.

a) Magnetization scaling b) Susceptibility scaling

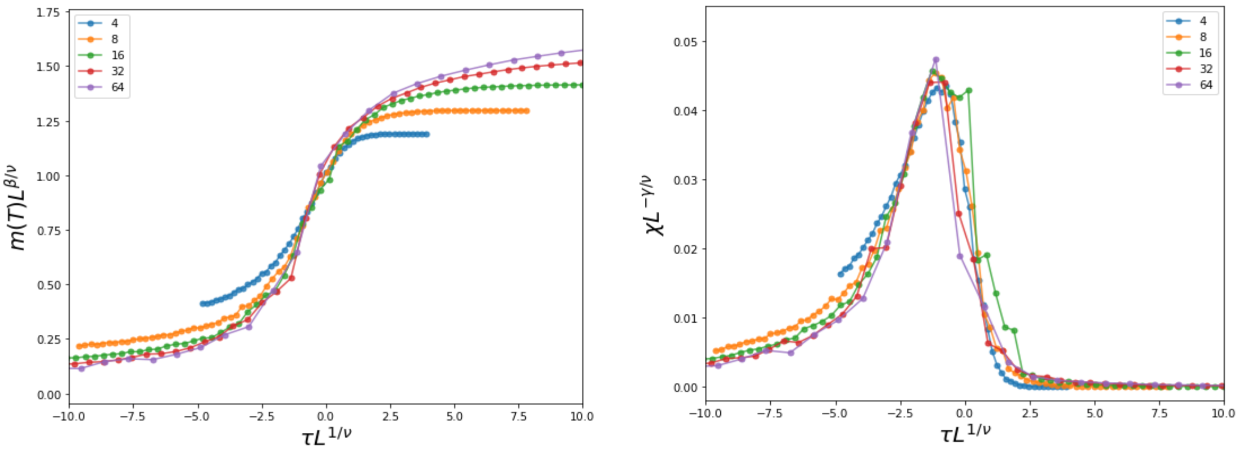


Figure 8: Re-scaled magnetization and susceptibility for different system sizes L.