Master's Degree in Physics of Complex Systems

2D Ising Model Simulations

11292 - Cooperative and Critical Phenomena

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Contents

1 Introduction

In this report, we study the 2D **Ising model** (with null magnetic field). The hamiltonian of the system is given by:

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

where J is the coupling constant, $s_i \in \{\pm 1\}$ is the spin at site i and $\langle i, j \rangle$ denotes the sum over nearest neighbours. We measure the temperature T in units[1] of J/k so that we do not have to bother of the J and k factors. In practice, we take $k = J = 1$.

In particular, we study the system through numerical simulations, using the *Metropolis Algorithm*. We start all the simulations from a random configuration of spins at some T. Let the system thermalize `MCS0` *Monte Carlo Steps* (MCS) until it reaches an equilibrium state. Then, we take n measurements with `MCS` in between. For the next temperature, we take the last configuration of the previous temperature as the initial configuration. We repeat this process until we reach the last temperature. This procedure of taking the last configuration as the initial of the next steps enhances efficiency [1, pp. 140, 141].

From statistical mechanics, we know that the observable quantities O are given by the **Thermal Average** $\langle O \rangle$. Numerically, we approximate the expected value by [1, pp. 100–103]:

$$\langle O \rangle \approx \mu_n[O] \pm \sigma_n[O] \sqrt{\frac{2\tau_O + 1}{n}}, \tag{2}$$

where μ_n is the common **Sample Average** over the n measurements, $\sigma_n[O]$ is the sample standard deviation and τ_O is the **Autocorrelation Time** of the observable O:

$$\mu_n[O] = \frac{1}{n} \sum_{i}^{n} O_i, \qquad \sigma_n^2[O] = \left(\frac{1}{n} \sum_{i=1}^{n} O_i^2 - \mu_n^2[O] \right), \qquad \tau_O = \sum_{k=1}^{n-1} \left(1 - \frac{k}{n} \right) \rho_O(k) \tag{3}$$

being $\rho_O(k)$ the normalized correlation function:

$$\rho_O(k) = \frac{\langle O_i O_{i+k} \rangle - \langle O_i \rangle \langle O_{i+k} \rangle}{\sigma^2[O]}.$$

In this practice, we have taken the exponential decay approximation of:

$$\tau_O \approx \frac{\rho_O(1)}{1 - \rho_O(1)}. \tag{4}$$

When calculating the errors of the physical quantities that depend on other observables $q(x_1, \ldots, x_N)$, we have propagated errors using the upper bound [2]:

$$\delta q = \sum_{i}^{N} \left| \frac{\partial q}{\partial x_i} \right| \delta x_i, \tag{5}$$

where δx_i is the uncertainty of x_i. The *relative error* of a quantity v approximated by v_{approx} is given by $\eta := |v - v_{\text{approx}}|/v \times 100\%$.

[1] Throughout the text, we have not explicitly written the J/k units in every temperature for clearness.

Parameters

We have considered a regular square lattice of size $L \times L$ with periodic boundary conditions. Lattices of sizes $L \in \{4, 8, 16, 32, 64\}$. For a better performance, we have divided the temperature interval $T \in [0.1, 5]$ in 2 regions, the extremum intervals $[0.1, T_c^{\min}] \cup [T_c^{\max}, 5]$ and the critical interval $[T_c^{\min}, T_c^{\max}] = [2.1, 2.6]$. In the extremum intervals, we have taken $\Delta T_1 = 0.1$, `MCS1 = 50`. While, for the critical interval[2] , we have taken $\Delta T_2 = 0.05$ and `MCS2 = 500`. We have thermalized the system `MCS0 = 2000` and taken $n = 1000$ measurements. We refer to this choice of parameters as the *default parameters*. Unless stated otherwise, we have used the *default parameters* in all the simulations. If we do not specify the index 1 or 2, it means that we have not made such partition of the temperature interval.

2 Basic Measurements

In this section, we have computed the energy, magnetization, specific heat and susceptibility per spin:

$$u := \frac{\langle H \rangle}{N}, \qquad m := \frac{\langle M \rangle}{N}, \qquad c_v := \frac{C_v}{N}, \qquad x = \frac{\chi}{N},$$

where $N = L^2$ and:

$$M = \sum_i^N \sigma_i, \qquad C_v = \beta^2 \sigma^2[H], \qquad \chi = \beta \sigma^2[M],$$

with $\beta = 1/T$, $\sigma^2[O] = \langle O^2 \rangle - \langle O \rangle^2$. The errors of C_v and χ are given by eq. (5):

$$\delta C_v = \beta^2 \left[\delta \langle H \rangle + \delta \langle H^2 \rangle \right], \qquad \delta \chi = \beta \left[\delta \langle M \rangle + \delta \langle M^2 \rangle \right].$$

The obtained results, adjust to the expected behaviour as shown in fig. 1.

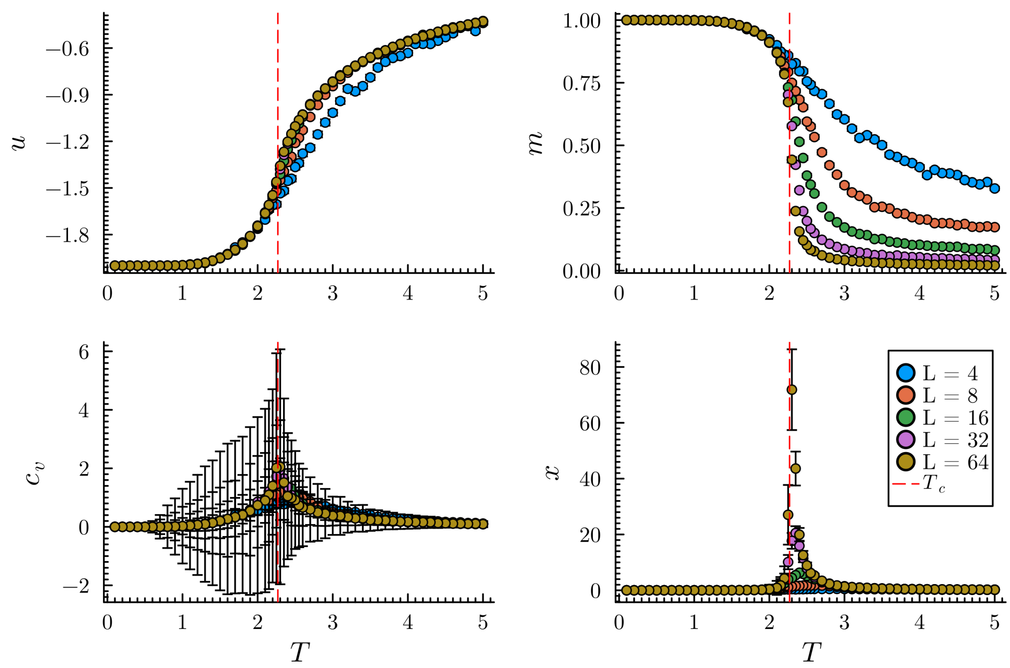


Figure 1: Basic measurements for different values of L. Default parameters.

[2]See the autocorrelation time fig. 4 in §5 for the justification.

3 Critical Temperature

In this section, we compute the critical temperature T_c by the *Binder Cumulant* which is defined as [1, p. 160]:

$$U_4(T, L) \equiv 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2}. \tag{6}$$

The finite-size scaling behavior of the fourth-order cumulant is given by:

$$U_4(T, L) = \bar{U}_4 \left[(1 - T/T_c)\, L^{1/\nu} \right].$$

Therefore, as $U_4(T_c, L) = \bar{U}_4(0) = \text{cte}$, the critical temperature can be determined by the common intersection of the curves $U_4(T, L)$ for different values of L. The obtained results are shown in fig. 2.

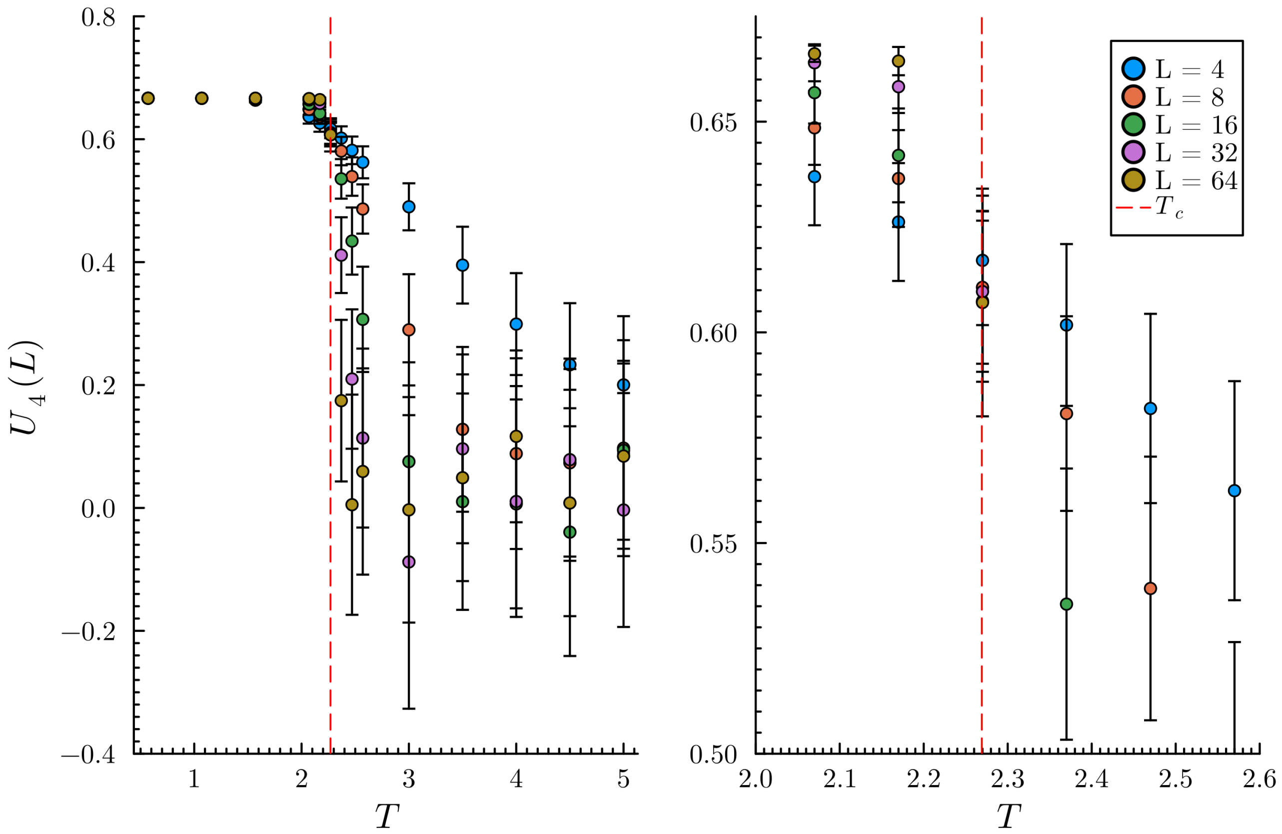


Figure 2: Binder cumulant for different values of L. Default parameters, changing: $T_c^{\min} = 2.07, T_c^{\max} = 2.57, \Delta T_1 = 0.5, \Delta T_2 = 0.1$.

However, for obtaining a precise value of T_c, we have performed a finer run with $\Delta T_2 = 0.001$, obtaining:

$$T_c = 2.264 \pm 0.001$$

where the error is given by the integration step. The theoretical value of T_c is:

$$T_c = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.269.$$

Getting a relative error of 0.2%, which is very accurate.

4 Critical Exponents

Theoretically, the critical exponents are defined by:

$$m \sim |t|^{\beta}, \qquad c_v \sim |t|^{-\alpha}, \qquad x \sim |t|^{-\gamma}, \qquad \xi \sim |t|^{-\nu}, \tag{7}$$

where ξ is the *Correlation Length* and $t := \big(T/T_c\big) - 1$ is the *Reduced Temperature*. The theoretical values of the critical exponents for the 2D Ising model are:

$$\alpha = 0, \qquad \beta = 0.125, \qquad \gamma = 1.75, \qquad \nu = 1.$$

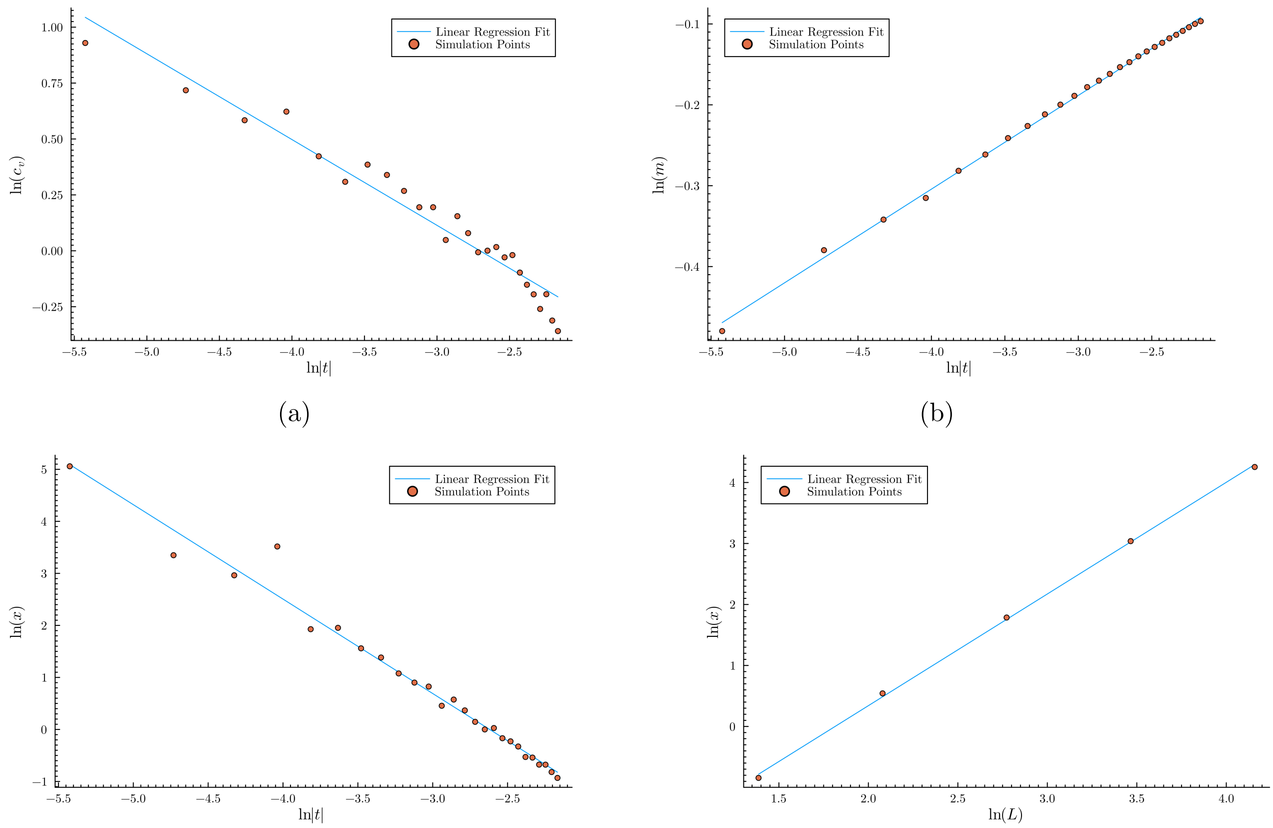
Doing our simulations we have obtained:

$$\begin{aligned} \alpha &= 0.38 \pm 0.02, & (\eta &= \varnothing), & \beta &= 0.1159 \pm 0.0009, & (\eta &= 7.2\%), \\ \gamma &= 1.81 \pm 0.06, & (\eta &= 3.31\%), & \nu &= 0.97 \pm 0.02, & (\eta &= 3\%). \end{aligned}$$

Regarding α, β and γ, we have computed the critical exponents by eq. (7) for $L = 180$. However, for ν, we have used the fact that $\xi \sim L$ at T_c, therefore:

$$x \sim L^{\gamma/\nu}, \qquad (T = T_c).$$

The obtained results are shown in fig. 3.



(a) (b)

(c) (d)

Figure 3: Critical Exponents. For 3a, 3b, 3c we took $L = 180$, $T \in [2, T_c]$ and $\Delta T = 0.01$. For 3d $T \in [2.1, 2.5]$ and $\Delta T = 0.1$. In both cases, we took `MCS = 500`.

5 Correlation Time & Length

The autocorrelation time is given by eq. (4). The magnetization[3] autocorrelation time is shown in fig. 4.

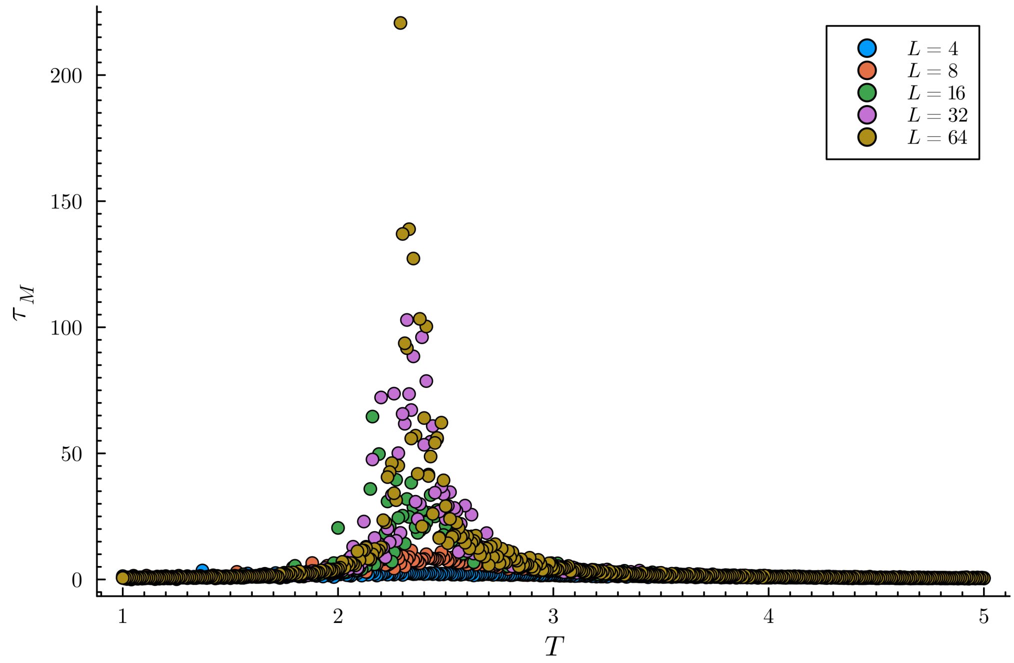


Figure 4: Autocorrelation time. Default parameters for $T \in [1, 5]$ with $\Delta T = 0.01$ setting `MCS = 1`.

This plot motivates the election of `MCS1 = 50` and `MCS2 = 500` outside and inside the critical region.

Regarding the correlation length ξ, we know that the correlation function is given by:

$$g(r) = \langle (s_i - m)(s_j - m) \rangle \,, \qquad r = |\vec{r}_i - \vec{r}_j|, \tag{8}$$

where $\vec{r}_i$ denotes the position vector of the spin i. It is well know that $g(r)$ decays exponentially with the distance as:

$$g(r) \sim e^{-r/\xi}. \tag{9}$$

From this relation, we obtain the correlation length ξ by fitting the correlation function to eq. (9). For efficiency purposes, we have assumed the lattice to be homogeneous and computed $g(r) = \langle (s_1 - m)(s_j - m) \rangle$ instead[4]. r denotes the euclidean distance:

$$r = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2},$$

taking into account the periodic boundary conditions. The correlation length for $L = 32$ is shown in fig. 5. We see how the correlation length diverges at T_c as expected.

[3] We considered the magnetization because the autocorrelation time of the energy H was smaller.

[4] Here, we checked the independence of the results in the i choice, which supports the homogeneous assumption.

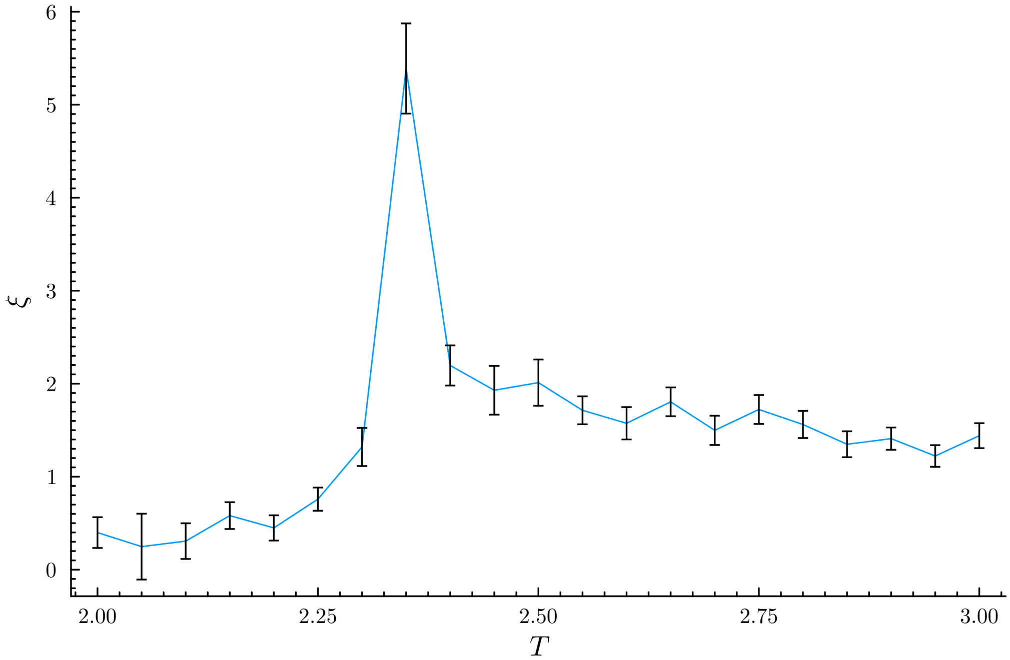


Figure 5: Correlation length. Default parameters for $T \in [2, 3]$ taking $\Delta T = 0.05$.

Moreover, as $\xi \sim L$ at T_c, we can compute $\xi(T_c)$ for different values of L and find that ξ scales linearly with L. The obtained slope was 0.73 ± 0.16.

6 Universal Scaling

Finally, we check the data collapse in fig. 6.

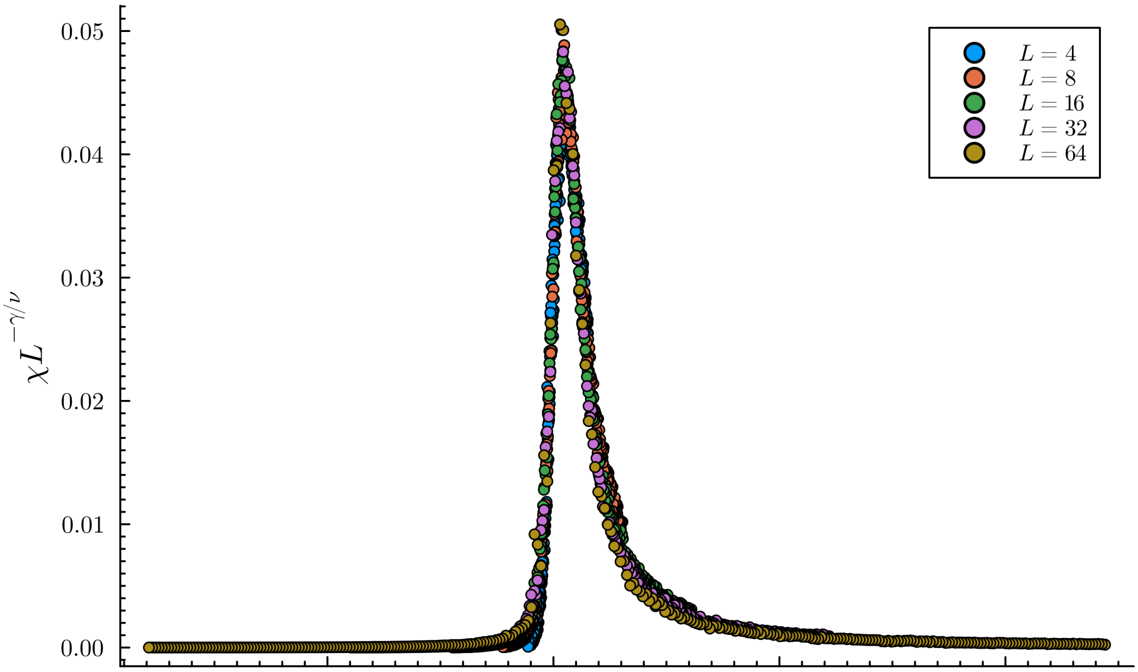


Figure 6: Universal Scaling. Default parameters for $T \in [1, 4]$ with $\Delta T = 0.01$. γ and ν are the theoretical values.

References

[1] Raúl Toral and Pere Colet. *Stochastic Numerical Methods: An Introduction for Students and Scientists*. Physics Textbook. Weinheim: Wiley-VCH, 2014. 402 pp. ISBN: 978-3-527-41149-8 (cit. on pp. 1, 3).

[2] John R. Taylor. *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements*. Third edition. New York: University Science Books, 2022. 371 pp. ISBN: 978-1-940380-09-4 978-1-940380-08-7 978-1-940380-14-8 (cit. on p. 1).