KTH Royal Institute of Technology

Project 25: Wang-Landau simulations and Lee-Kosterlitz method to study discontinuous phase transitions

João Pedro Ferreira Biu

13th of December 2024

Computational Physics SI2530 ..... Professor Jack Lidmar

Abstract

In this work, we implemented two computational methods to study phase transitions in lattice models. Specifically, we implemented the Wang-Landau algorithm, which is used to compute the density of states of the model, and the Lee-Kosterlitz method, used to determine the order of phase transitions in systems that are computationally simulated. The model studied was the Potts Model with $q = 8$ possible states for each lattice point. The results presented in this work agree with the system's finite-size scaling properties, and confirm that this model undergoes a discontinuous phase transition (first-order). This was shown by verifying the increase of the free-energy barrier that separates the two phases of the system during the phase transition with the increase of the system size, as it was expected by previous works.

1 Introduction

Statistical physics provides us with methods to study the collective behavior of particles that interact with each other. While for many systems these methods can be studied analytically, there are still some cases where the system's complexity poses a problem to analytical methods. In the field of condensed matter physics, which investigates microscopic and macroscopic properties of matter, highly complex many-body systems with many interactions among their constituents are often encountered. These range from superconductors to spin liquids, and to obtain information about properties such as their thermodynamic quantities, density of states, or phase transitions, computational methods are a powerful tool [1, 2, 3]. One type of system that is typically studied using computational methods are systems of multiple particles with spins, arranged in a lattice, such as the Ising model [4], the Potts model [5] or the XY model [6]. These systems are often studied using Monte-Carlo methods, computational algorithms that use repeated random sampling to compute integrals numerically, or, as in this case, to sample quantities from a specific probability distribution [7].

In this work, phase transitions of the Potts model in two dimensions are studied. The Potts model is a lattice model where each constituent interacts with its nearest neighbors. To study this model a Monte-Carlo algorithm was used, the Wang-Landau algorithm [8, 9] to compute the density of states of the system, from which we can compute the probability distribution function. After this, the Lee-Kosterlitz [10] method was used to determine the order of the phase transition in the data obtained of the density of states for different sizes of the system. Further details of this model and methods will be explained in the next sections.

This work is organized as follows. In Section 2 the theoretical aspects of the model studied and the computational methods used are explained, and in Section 3 the implementation details are then explored. In Section 4 the results obtained are presented and discussed, and Section 5 contains the conclusion of this work. Finally, in Appendix A, it is possible to find the plots of the density of states and free energy for the system sizes used.

2 Theoretical Background

2.1 Potts Model

The Potts Model is a model of interacting spins on a lattice described by the Hamiltonian

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

where $\langle ij \rangle$ means that sum is over nearest neighbors, $s_i \in \{1, ..., q\}$ are the discrete states of each lattice point, and δ_{s_i,s_j} is the Kronecker delta defined as

$$\delta_{s_i,s_j} = \begin{cases} 1 & \text{if } s_i = s_j \\ 0 & \text{otherwise} \end{cases}. \tag{2}$$

The Potts model can be thought of as a generalization of the Ising model, that we can recover by considering $q = 2$. This model can be used to study the behavior of ferromagnets, and it is particularly relevant for the study of phase transitions since the 2D Potts model has phase transitions for $q \geq 1$. In 2D, for $1 \leq q \leq 4$ the phase transition is continuous, or of second order, and for $q > 4$ this model has discontinuous phase transitions, or, first-order phase transitions. In this work, we are focused on detecting and classifying first-order phase transitions, and for that purpose, a value $q = 8$ is used to guarantee the existence of highly discontinuous phase transitions, and the systems used are two-dimensional squares of side L, meaning that the number of lattice points is L^2.

From the Hamiltonian in Eq. (1) one can deduce that the ground level has energy $E_{ground} = -2JL^2$, which corresponds to all the lattice points being in the same state q, and the highest energy value is $E_{max} = 0$, which corresponds to no lattice point having a neighbor in the same state. From this fact, we can also conclude that the density of states for the ground level is equal to the value of q, which in our case is 8.

2.2 Wang-Landau Algorithm

The Wang-Landau algorithm is a Monte-Carlo method used to iteratively obtain the density of states $\Omega(E)$ of a system, this is, the number of microstates that correspond to a value of energy E. The density of states of a system is an important quantity to understand the system's behavior, and from it, its thermodynamic quantities can be extracted. One advantage that this method has is that contrary to the Metropolis-Hastings algorithm [11], which allows us to extract information about the simulated system at a specific temperature, from the density of states obtained using the Wang-Landau algorithm we can extract thermodynamic quantities for various values of temperature.

Considering the phase space of the system's configurations as Γ, the Wang-Landau algorithm works as follows:

1. We initialize all the density of states of all energy values as 1, $\Omega(E) = 1$, a histogram of the visited energies as zero, $H(E) = 0$, and a multiplicative factor f as $f = e^1$.

2. We choose a random configuration, $x \in \Gamma$, of the system and compute its energy $E(x)$.

3. We change the state of a randomly chosen lattice point to a state $s_i \in 1, ..., q$, once again randomly.

4. This new state with energy $E(x')$ is accepted according to the acceptance probability

$$r < A(x' \leftarrow x) = \min\left(1, \frac{\Omega[E(x)]}{\Omega[E(x')]}\right), \tag{3}$$

with r being a random number sampled from a uniform distribution, $r \sim U[0, 1)$. We repeat this process the number of times that we define as the number of samples for our Monte-Carlo method, since this is similar to the Metropolis-Hastings method but with a different acceptance probability.

5. Each time a state with energy E is visited we update the density of states and the histogram H at that energy value as

$$\Omega(E) \leftarrow \Omega(E) \cdot f, \tag{4}$$

$$H(E) = H(E) + 1. \tag{5}$$

6. When the histogram H is sufficiently flat according to an implemented criteria that in our case will be the minimum value H_{min} being greater than 95% of the average of the histogram bins, $H_{min} > 0.95\,\bar{H}$, we reset all the bins of the histogram to $H(E) = 0$ and update the multiplicative factor by $f \leftarrow \sqrt{f}$.

7. We continue this steps until f meets a certain criteria, in our case, until $f < \exp(10^{-8})$.

Eventually, Ω converges to a density of states relative to the true density of states of the system by a scalar factor. Finally, since we know that the density of states of the ground states is equal to q, we normalize Ω so that $\Omega(E_{ground}) = q$, obtaining an approximation of the true density of states of the system. This algorithm can be improved for example by computing the logarithm of the quantities, as we will further develop in Section 3. Once we have these results, we can then apply the Lee-Kosterlitz method to study our system.

2.3 Lee-Kosterlitz method

Jooyoung Lee and J.M. Kosterlitz first presented the Lee-Kosterlitz method in [10]. This method consists of a data analysis process to detect first-order (discontinuous) phase transitions on numerical simulations. While phase transitions are one of the most interesting phenomena to study from numerical simulations of statistical mechanics systems, the behavior of a system near its critical points is not always the easiest to study: we can have first-order phase transitions with discontinuity in order parameters, or second-order continuous phase transitions with non-analytic behavior of the order parameters near the critical point. Therefore, having a systematic method to apply to simulation data in order to classify the type of phase transitions is very important.

Lee-Kosterlitz's method is able to identify first-order phase transitions by studying the probability distribution of the system's states, knowing that these phase transitions have free energy barriers between the phases. The free energy barriers have finite-size scaling properties that provide a way to determine the order of the phase transition. As described in the original work where this model was developed, by considering a system with periodic boundary conditions on a d-dimensional cube of side L, with a first-order phase transition, we can write the free energy as

$$F(\beta, L) \simeq L^d f_0(\beta) + L^{d-1} f_1(\beta), \tag{6}$$

where f_0 is the free energy density in the thermodynamic limit and f_1 is related to the free energy per unit area of a domain wall between the coexisting phases. The first term is a minimum and is constant, and the second term will have a maximum, making the resulting free energy have a local maximum between two minima, separated by a height

$$\Delta F(t, L) = A(t)L^{d-1} + O(L^{d-2}), \tag{7}$$

where $t = \beta/\beta_c - 1$, with β_c being the critical inverse temperature.

Due to the finite size scaling properties of the system, ΔF increases with L in the case of the first-order transition. With this said, to classify the order of the transition we need to compute ΔF from our simulations and observe how it varies with the dimension of the system.

To do this we start with the probability distribution of the system,

$$P(E, \beta, L) = \Omega(E, L)\frac{e^{-\beta E}}{Z(\beta, L)} \equiv \exp(-A(E, \beta, L)), \tag{8}$$

and from this, we can obtain the value of ΔF by measuring the difference between $A(E, \beta, L)$ minima and maximum. Finally, by assessing if ΔF increases with L, we conclude if the phase transition is of first-order or not.

3 Implementation

The implementation of this work was mainly made in two parts, the first one consisting of the implementation of the Wang-Landau algorithm to obtain the density of states of the Potts model, and the second one consisting of the implementation of the Lee-Kosterlitz method to the data previously acquired.

3.1 Potts model and Wang-Landau algorithm implementation

This part of the work was developed in C++ due to the complexity of the algorithm. This allowed for a faster and more efficient code and to study larger systems, since the size of the system and the number of microstates q for each lattice point have a direct impact on the code's running time.

The two-dimensional Potts model lattice is implemented as a class, `PottsLattice`, that stores the lattice configuration as a two-dimensional vector array, and has methods to obtain the minimum and maximum energy value, to access and print the lattice configuration, and to obtain the energy for the configuration, according to Eq. (1). To avoid double counting, when computing the energy of the system only the interactions of a lattice point with two of its nearest neighbors are counted, e.g. the lattice point to the right and below, in a two-dimensional system. The lattice is initialized with $L \times L$ random values between 1 and q. In this work, we always use $q = 8$ and $J = 1$, the factor in the Hamiltonian in Eq. (1).

The Wang-Landau algorithm was implemented as a method that takes a `PottsLattice` object and computes the density of states of the model. To do so, the algorithm described in Section 2.2 is implemented in its logarithmic form to avoid numerical overflows. To do this we need to make some small changes such as

- We initialize $\log(\Omega(E)) = 0$ and $f = 1$.

- The acceptance criterion is now

$$r < A(x' \leftarrow x) = \min\left(0, \exp\left(\log[E(x)] - \log[E(x')]\right)\right) \tag{9}$$

- The density states is updated as $\log(\Omega(E)) \leftarrow \log(\Omega(E)) + f$ and the multiplicative factor is updated as $f \leftarrow f/2$.

- The algorithm is run until it meets the criteria $f < 10^{-8}$.

All the other steps remain the same.

3.2 Lee-Kosterlitz method implementation

The implementation of this method was done in Python since this language is more user-friendly for visualization and data analysis. This model consists of a systematic application of transformations to the data of the logarithm of the density of states, $\log(\Omega(E))$ obtained from the Wang-Landau algorithm. The first thing that is done is normalizing the data knowing that the ground state, has q number of configurations - in our case, $q = 8$ - since this corresponds to all the lattice sites having the same microstate. After that, to obtain ΔF we first need to obtain $A(E, \beta, L)$, which can be computed as

$$A(E, \beta, L) = -\log(\Omega(E)) + \beta E - \log(Z(\beta, L)). \tag{10}$$

The first term on the right-hand side of Eq. (10) comes from the simulation data, as well as the energies E. By fixing β we can compute the second term by multiplying it with the energy values, and finally, we can compute the third term as

$$Z(\beta, L) = \sum_E \Omega(E) e^{-\beta E} \Leftrightarrow \log(Z(\beta, L)) = \log\left(\sum_E e^{\log(\Omega)) - \beta E}\right). \tag{11}$$

The only missing component to compute these quantities is then the value of β at the critical point, β_c. Since we know that on the critical point we expect $A(E, \beta_c, L)$ to have a local maximum in the middle of two minima and that these minima should have the same value, we implemented a minimization algorithm that for each value of β computes the difference between the values of A on the two minima, $A_{\text{difference}} = |A(E_{min1}, \beta, L) - A(E_{min2}, \beta, L)|$, and obtains the value of β for which $A_{\text{difference}}$ is closer to 0. This minimization process needs an initial guess to search values close to it. As an initial guess, we use $\tilde{\beta} = \log(1+\sqrt{q})$, which corresponds to the analytical value of β_c. The value of β obtained with the minimization will be used as the inverse temperature value for which the phase transition occurs, β_c.

Once we define our value of β_c we just compute de difference between the minima and local maximum of $A(E, \beta, L)$, ΔF, so that we can analyze how it varies with L. If the value of the difference ΔF increases with the system's dimension, the phase transition is discontinuous. In Fig. 1 it is possible to see the plot of $A(E, \beta, L)$ and the points needed to compute ΔF, and what it represents, using $L = 16$ and $q = 8$.

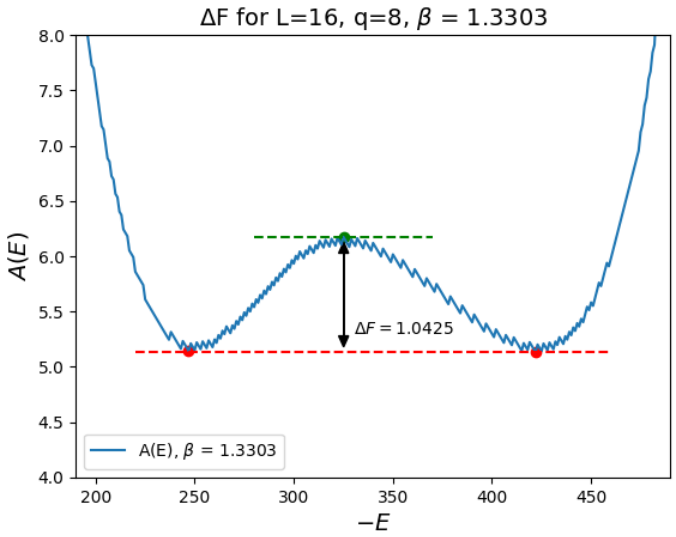


Figure 1: Plot of $A(E, \beta, L)$ with maximum and minima identified. The difference between the minima and the maximum is ΔF, the value needed to use the Lee-Kosterlitz method to identify first-order phase transitions.

4 Results

To obtain our results we simulated a lattice Potts model system with $q = 8$, this is, with possible microstates $s_i = 1, ..., 8$, and a coupling constant $J = 1$. We simulated this system for the dimensions $L = \{9, 10, 11, 12, 14, 16\}$. First, we applied the Wang-Landau algorithm to the lattice model, obtaining the logarithm of the density of states, $\log[\Omega(E)]$. To normalize the results we need to guarantee that the ground state has a density of states equal to $q = 8$. We used a flatness criterion $H_{min} > 0.95\bar{H}$ and convergence criterion $\log(f) < 10^{-8}$, where $\bar{H}$ is the average of the histogram entries. It is possible to find the plot of the normalized logarithm of the density of states in Fig. 2, for $L = 16$.

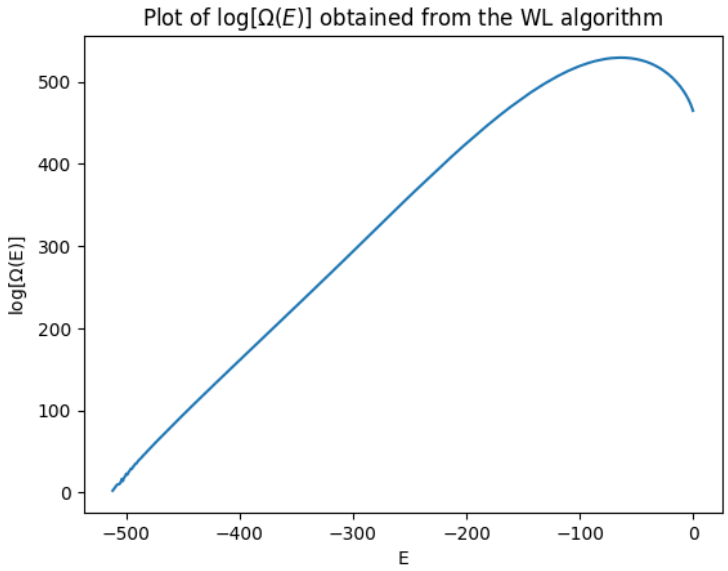


Figure 2: Normalized logarithm of the density of states for the Potts model with $L = 16$, obtained using the Wang-Landau algorithm.

The states with lower energy have more fluctuations since these states are less accessed during the simulation, as we can assess from the plot. This proves to be a challenge for computing the ΔF in systems with small L. Once we have $\log[\Omega]$ we can then compute $A(E)$ using Eq. (10), and use the minimization algorithm to obtain the value of β_c that makes the minima have the same value $A(E_{min1}) = A(E_{min2}) = A_{min}$. In Table 1 it is possible to find the values of β_c obtained for each system size L.

L	9	10	11	12	14	16
β_c	1.310322	1.315127	1.319131	1.322134	1.327339	1.330342

Table 1: Values of β_c obtained for each value of the system's size L.

Using the value of Table 1 for $L = 16$, we can plot $A(E)$, as it can be found in Fig. 3

After obtaining the value of β_c we need to compute the value of $A(E)$ for the minima and the local maximum, A_{min} and $A_{l.max}$. Since we have two minima, we use the average of their value of A, since they differ by a small value of the order of 10^{-3}. Once we have all the values needed, we can then obtain ΔF. The values for $A(E)$ in its minima and local maximum, as well as ΔF can be found in Table 2 for the values of L studied.

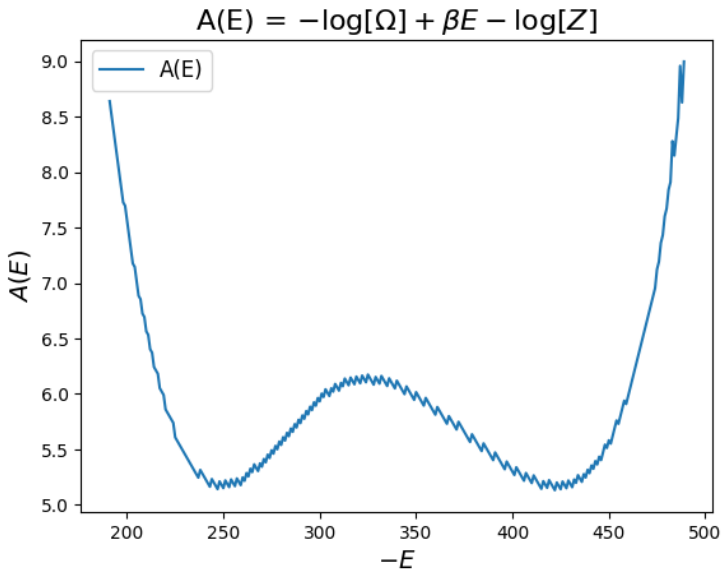


Figure 3: Plot of $A(E)$ for $L = 16$, using $\beta = \beta_{c,16} = 1.330342$.

L	A_{min}	$A_{l.max}$	ΔF
9	4.322914	4.959009	0.636096
10	4.475482	5.175053	0.699571
11	4.594812	5.361751	0.766939
12	4.724227	5.531382	0.807156
14	4.933760	5.875694	0.941934
16	5.133961	6.176438	1.042477

Table 2: Values of $A(E)$ in its minima and local maximum, and value of ΔF for each value of L.

Using the values of Table 2 we can now plot the variation of ΔF by the system's size L, allowing us to conclude the order of the phase transition. This can be found in Fig. 4. As we can see in the plot in Fig. 4 the value of ΔF increases with the system's size L, which, according to the Lee-Kosterlitz method, means that this system, the two-dimensional Potts model with $q = 8$, has indeed a first-order, discontinuous, phase transition. From the plots in Appendix A, we can see that the larger the system is, the better the resolution of the function $A(E)$. For larger systems, there are much more energy levels, and the $A(E)$ is much closer to what is expected - described in Section 3.2 - and the maximum and minima are easily detected.

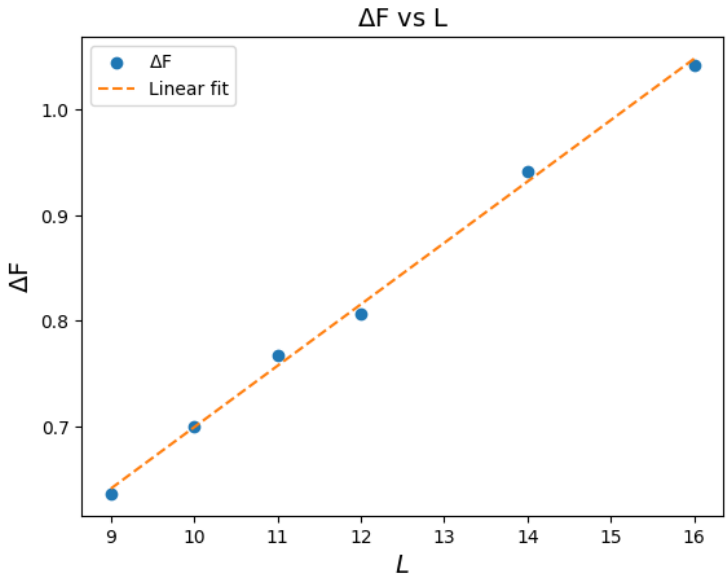


Figure 4: Variation of ΔF with L.

Fitting the data to a linear function, we obtain that $\Delta F = [(5.823 \pm 0.153) \times 10^{-2}]L + (1.171 \pm 0.188) \times 10^{-1}$, from which we can conclude that $\Delta F \propto L$. This is expected from Eq. (7), which states that $\Delta F \propto L^{d-1}$, and for our case, $d = 2$.

5 Conclusion

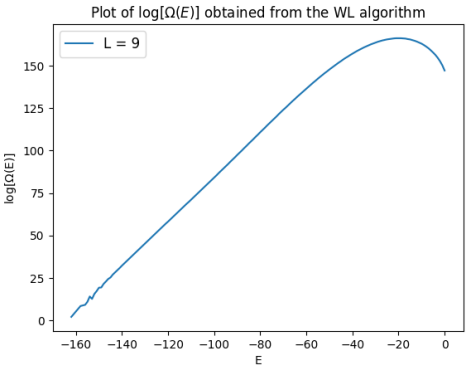
In this work, we explored and implemented methods to study condensed matter physics lattice models, namely the Wang-Landau algorithm to compute the density of states of the system and the Lee-Kosterlitz method to determine the order of the phase transition. To do so it was developed two codes, in C++ for the first algorithm and in Python for the data analysis required to apply the Lee-Kosterlitz method. By doing so, we took advantage of a compiled language aligned with techniques like multiprocessing and changes such as computing the logarithm of quantities required, speeding the run-time of the algorithm, and also took advantage of an easy-to-use language with libraries dedicated to data analysis such as Pandas, SciPy, and NumPy.

For this project, we studied the case of the Potts Model, Eq. (1), with $q = 8$. This model is a generalization of the Ising Model and can approximate the behavior of ferromagnetic materials, and it is used a lot in phase transition studies since for $q > 1$ this model has phase transitions.

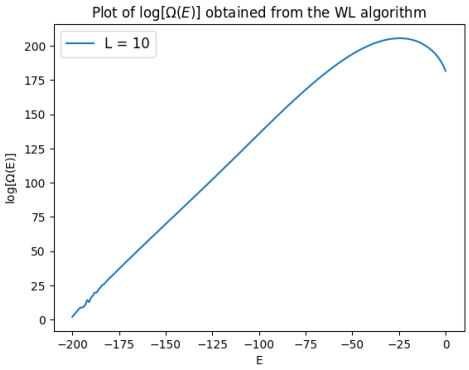
With the code implemented, we verified that this system goes under a phase transition of the first order, this is, discontinuous, as was expected since the free-energy interval increases with the size of the system, a property that comes from the finite size scaling properties of the Potts Model for a finite lattice, as our case. This behavior is represented in Fig. 4. We verified that the free energy barrier ΔF varied proportionally to L, which agrees with the expected behavior described by Eq. (7).

This code could be generalized for different models, given that the lattices and the Hamiltonian that describe the system are implemented accordingly since both the Wang-Landau algorithm and the Lee-Kosterlitz method do not depend on the model used. The possibility of generalization is one of the reasons why object-oriented programming was used.

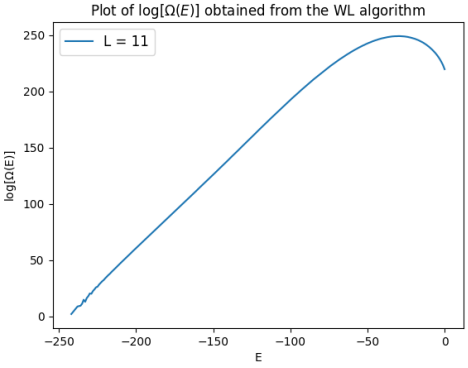
A Appendix - Plots for all system sizes



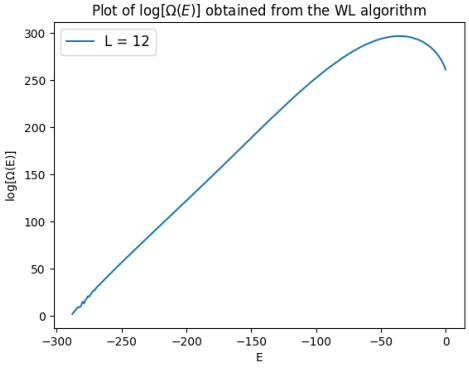
(a) $L = 9$.



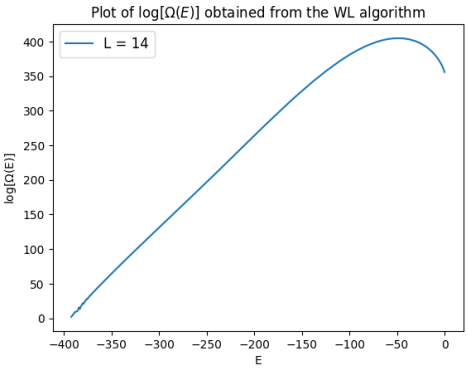
(b) $L = 10$



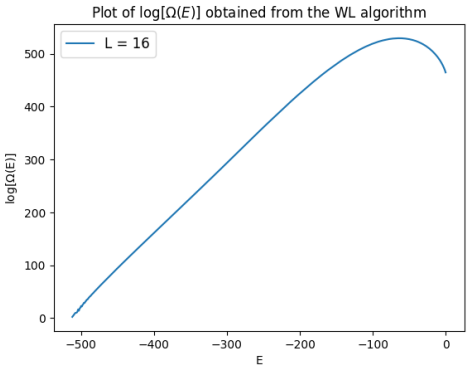
(c) $L = 11$



(d) $L = 12$

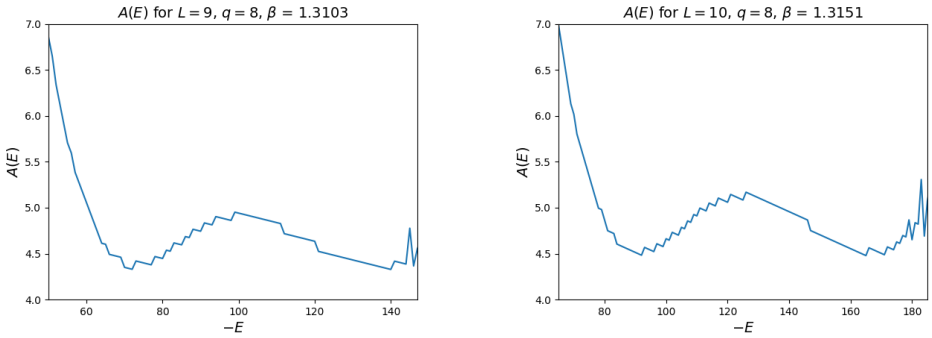


(e) $L = 14$



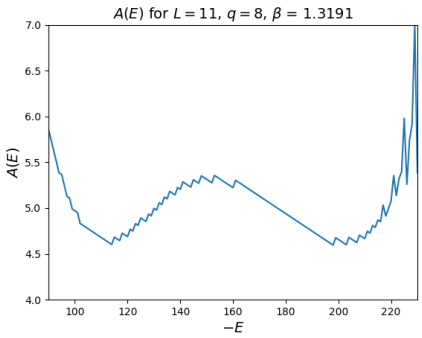
(f) $L = 16$

Figure 5: Logarithm of the density of states of the Potts Model for various values of system size L.

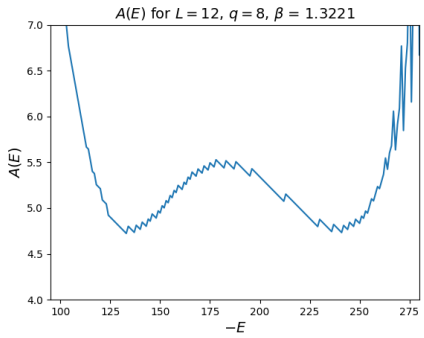


(a) $L = 9$.

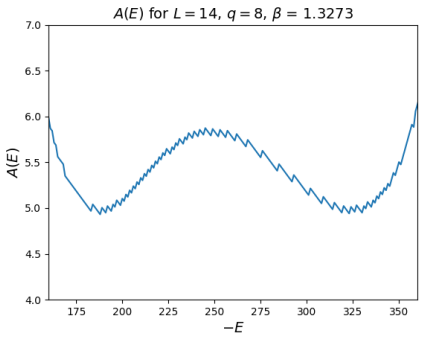
(b) $L = 10$



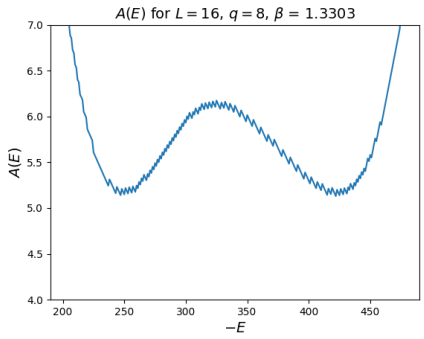
(c) $L = 11$



(d) $L = 12$



(e) $L = 14$



(f) $L = 16$

Figure 6: Plots of $A(E)$ for the Potts Model with various values of system size L.

References

[1] Johannes Arnoldus Delport, Kyle Jackman, Paul Le Roux, and Coenrad Johann Fourie. Josim - superconductor spice simulator. *IEEE Transactions on Applied Superconductivity*, 29, 8 2019. ISSN 15582515. doi: 10.1109/TASC.2019.2897312.

[2] S. Ryu, S. Doniach, Guy Deutscher, and A. Kapitulnik. Monte carlo simulation of flux lattice melting in a model high-tc superconductor. *Physical Review Letters*, 68:710, 2 1992. ISSN 00319007. doi: 10.1103/PhysRevLett.68.710. URL https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.68.710.

[3] Lucile Savary and Leon Balents. Quantum spin liquids: a review. *Reports on Progress in Physics*, 80:016502, 11 2016. ISSN 0034-4885. doi: 10.1088/0034-4885/80/1/016502. URL https://iopscience.iop.org/article/10.1088/0034-4885/80/1/016502https://iopscience.iop.org/article/10.1088/0034-4885/80/1/016502/meta.

[4] Ernst Ising. Contribution to the Theory of Ferromagnetism. *Z. Phys.*, 31:253–258, 1925. doi: 10.1007/BF02980577.

[5] R. B. Potts. Some generalized order-disorder transformations. *Mathematical Proceedings of the Cambridge Philosophical Society*, 48(1):106–109, 1952. doi: 10.1017/S0305004100027419.

[6] Elliott Lieb, Theodore Schultz, and Daniel Mattis. Two soluble models of an antiferromagnetic chain. *Annals of Physics*, 16(3):407–466, 1961. ISSN 0003-4916. doi: https://doi.org/10.1016/0003-4916(61)90115-4. URL https://www.sciencedirect.com/science/article/pii/0003491661901154.

[7] David P. Landau and Kurt Binder. *A Guide to Monte Carlo Simulations in Statistical Physics*. Cambridge University Press, 3 edition, 2009.

[8] Fugao Wang and D. P. Landau. Efficient, multiple-range random walk algorithm to calculate the density of states. *Physical Review Letters*, 86:2050, 3 2001. ISSN 00319007. doi: 10.1103/PhysRevLett.86.2050. URL https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.86.2050.

[9] Fugao Wang and D. P. Landau. Determining the density of states for classical statistical models: A random walk algorithm to produce a flat histogram. *Physical Review E*, 64:056101, 10 2001. ISSN 1063651X. doi: 10.1103/PhysRevE.64.056101. URL https://journals.aps.org/pre/abstract/10.1103/PhysRevE.64.056101.

[10] Jooyoung Lee and J. M. Kosterlitz. New numerical method to study phase transitions. *Physical Review Letters*, 65:137, 7 1990. ISSN 00319007. doi: 10.1103/PhysRevLett.65.137. URL https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.65.137.

[11] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller. Equation of state calculations by fast computing machines. *The Journal of Chemical Physics*, 21:1087–1092, 6 1953. ISSN 0021-9606. doi: 10.1063/1.1699114. URL /aip/jcp/article/21/6/1087/202680/Equation-of-State-Calculations-by-Fast-Computing.