Studying Phase Transitions In The q-state Potts Model

A computational study using the Lee-Kosterlitz approach

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Abstract

The project attempts to simulate the q-state potts model for a two dimensional square lattice using the Metropolis algorithm. Different q_s correspond to different possibilities for phase transitions. This project utilizes the Lee Kosterlitz algorithm and the histogram method of extrapolation to predict- whether a phase transition exists for a given q, and if it exists, characterise it. The results of the code were first verified using the critical temperature values obtained from analytic results. The phase transitions near critical temperatures for $q = 2, 3, 5, 10$ were studied.

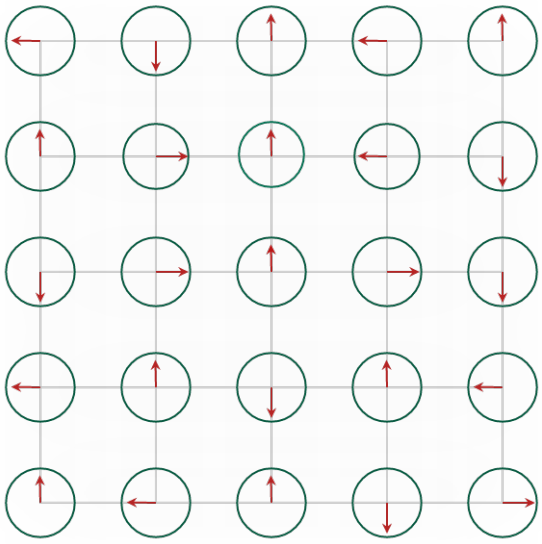


Figure 1: The analogy for the potts model where each spin site can be compared to a clock's hand pointing in q directions. This diagram shows a $q = 4$ model where spins can point in one of the four directions

1. Introduction

1.1. Problem Description

The Potts model is a statistical thermodynamic model where spins are placed on a lattice. Unlike the Ising spin model where each spin site (point on a lattice) can host a $+1$ spin or a -1 spin, the Potts model sites can host integer values of spins from 1 to q. Therefore a site for $q = 3$ can have any value from $1, 2, 3$. These interactions can be understood by the analogy of placing a clock on each lattice site. The hour hand on the clock can point in any of q directions. We consider the energy interactions between two neighbouring clocks to give an interaction energy of $-J$ when their hour hand points in the same direction, i.e. when their spin is the same. For all other cases when neighbouring clocks have hour hands pointing in different directions, their spins being different, they do not interact, giving 0 energy.

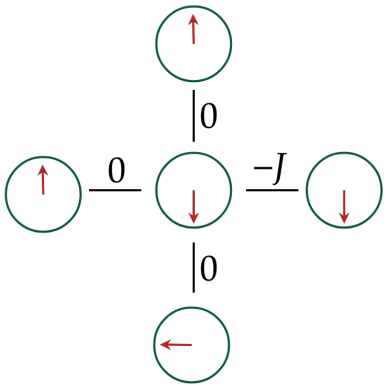


Figure 2: The right bond where two clocks point in the same direction gives an interaction energy of $-J$. Therefore the Hamiltonian for the entire near neighbour interaction is just $-J$ since all other neighbours are pointing in different directions

This implies that the Hamiltonian takes the form:

$$H = -J \sum_{\langle i,j \rangle} \delta_{ij}$$

Where i, j are neighbouring interactions, J is the interaction energy (for this project $J = 1$) and δ_{ij} is the Kronecker delta function. For the q states model, a thermodynamics phase transition occurs

for all values of $q \geq 1$ The analytical solution for the critical temperature T_c for a given q where a phase transition occurs is given by:

$$T_c = \frac{1}{\ln(1+\sqrt{q})}$$

The phase transition that occurs in these systems near the critical temperature can be categorised in two segments depending on their behaviour as we vary the size of our lattice. This method of categorising was suggested by Lee and Kosterlitz. Consider simulating a lattice of size $L \times L$ with a spin q_i placed in each lattice site. These spins interact with one another over time (in our case known as a montecarlo sweep) giving us an idea of the total energy of the system at any given instant. In this regard, we can obtain energy as a function of time. In the case of a Monte-Carlo simulation, we can essentially obtain energy as a function of each Monte-Carlo sweep. For discrete spin systems such as the potts model, the energy values will also be discrete. Lee and Kosterlitz proposed to create a histogram $H(E)$ of these energies, or in other words, bin these energy values and count how many times each energy value bin is repeated. They proposed that if a system is simulated close to some inverse temperature β which is very close to the critical temperature β_0 and we obtain the histogram $H(E)$, we can estimate the change in free energy ΔF. This expression is given as:

$$F(E) \propto -\ln H(E) + (\beta - \beta_0)\, E$$

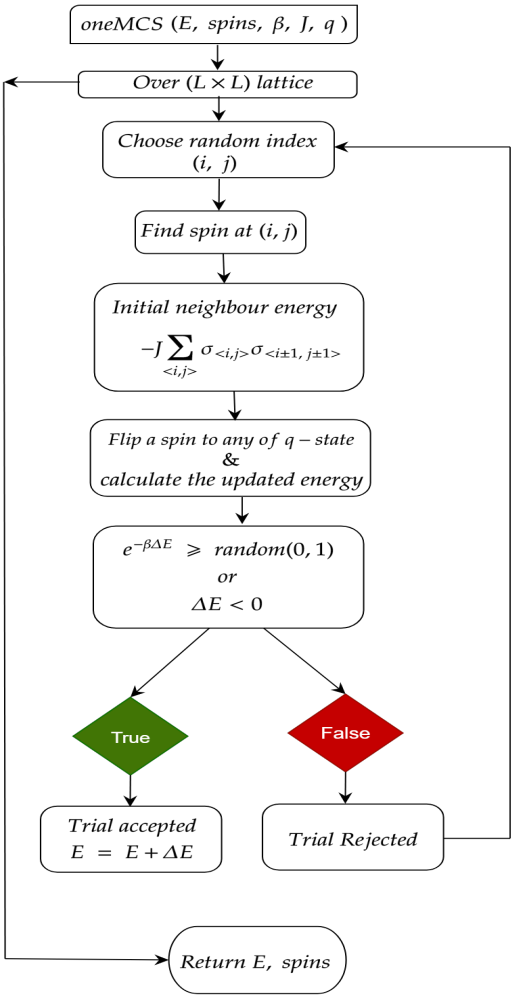
When we plot the energy as a function of the free energy, we obtain a double minima structure. The double minima structure is a consequence of the fact that for systems where a phase transition occurs, the free energy is essentially equal for the two phases. This allows us to make two inferences. In the systems where there are no phase transitions, there will only be a single free energy minimum. For systems that do have a phase transition, we can use the double minima to estimate the critical temperature for finite size lattices. When we simulate the system at the analytically found critical temperature β_0 and plot $F(E)$ against E we will obtain two unequal minima. We can keep guessing the value of β until we obtain two equal minima. The inverse temperature β at which these minima become equal is the *Critical temperature* for that lattice size L. Now that we have an estimate of the free energy of a $L \times L$ lattice for a given q we can characterise its phase transition.

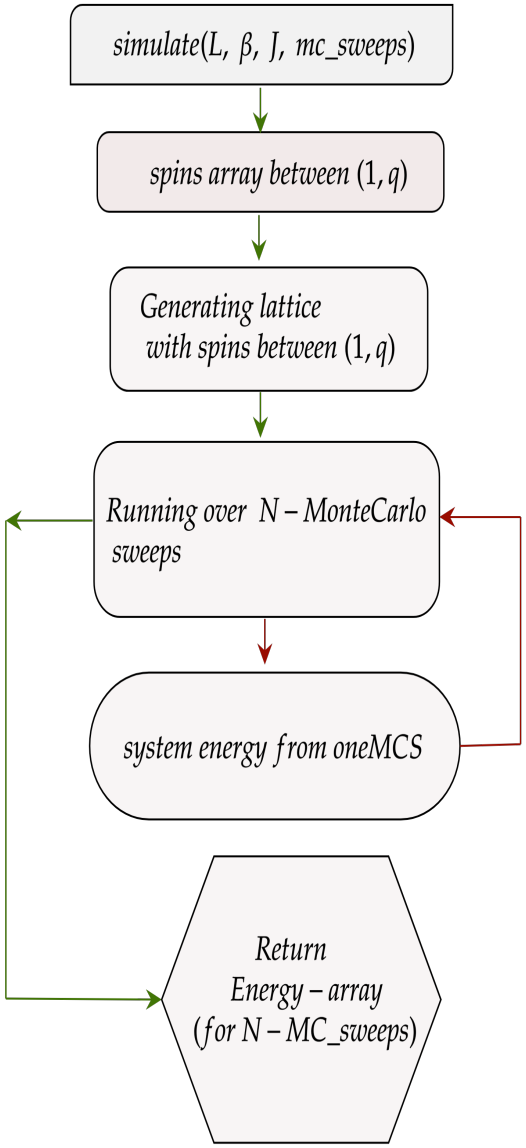
If we look at ΔF, calculated using the difference between the minima and the peak of the $F(E)$ vs E curve for different lattice sizes and we find that ΔF increases as the size of the lattice increases, we can classify it as a first order transition. The increasing ΔF term for these transition indicates the increasing of the potential barrier for the transition. For transitions where the term ΔF remains the same irrespective of the lattice size, the transition can be characterised as continuous.

2. Methods

2.1. Simulating the q-state lattice

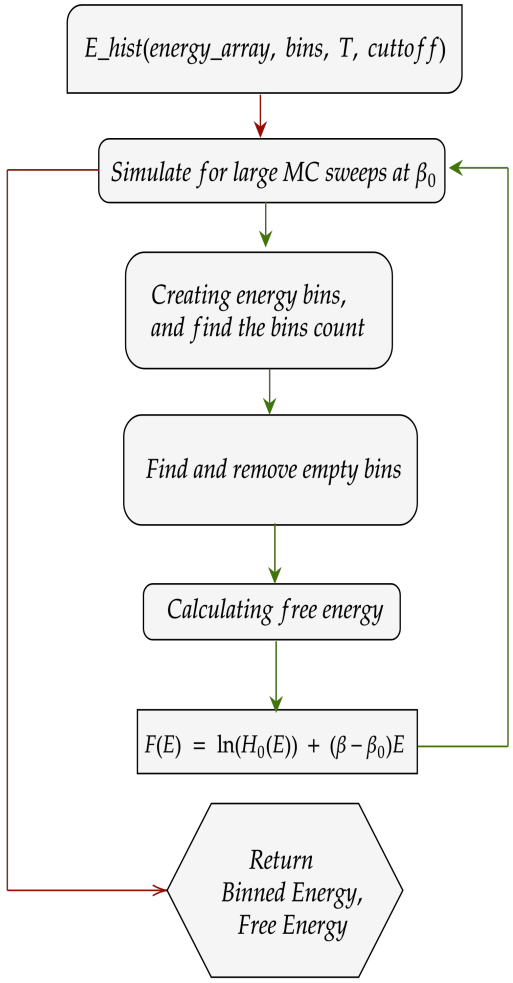
The Metropolis algorithm is a method of importance sampling where certain trials are accepted on the basis of a desired probability distribution. The q-state potts model uses a single flip dynamic where a random spin site is chosen, and its spin is flipped form q_0 to some q_{new}. The energy change is then calculated, on the basis of which one decides whether to accept or reject this flip. This process was repeated for n montecarlo steps (n_{mcs}) which represent a unit of time. The following shows the flowchart for calculating energy for one trial:





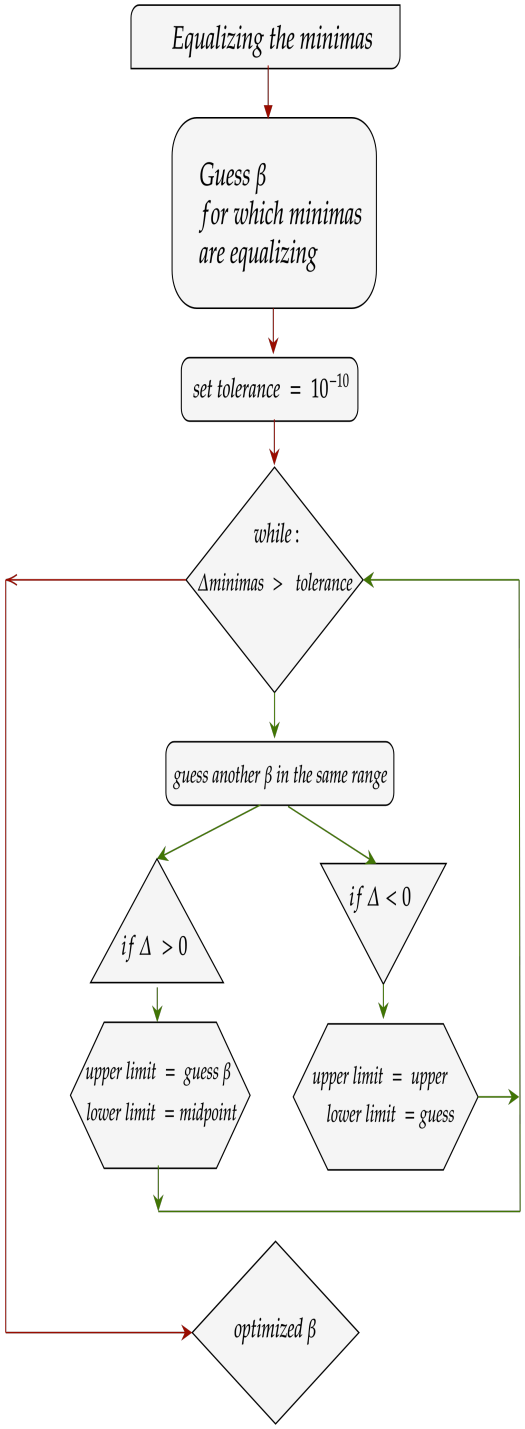
2.2. Creating a histogram to calculate F(E)

Once we have a list of energies that are obtained for multiple Monte Carlo sweeps for a given value of β we can bin these energies according to their unique values and calculate $H(E)$, an array that gives the energy degeneracy, i.e. how many times a particular energy is repeated. This can be used to calculate the free energy of the system whose equation was mentioned previously. For the simulations presented in this report, about 60 bins were enough to obtain reliable results for the double minima. It should be noted that the binning needs to be done in such a way that no energy has a zero count. The following flowchart indicates the procedure used for binning:



2.3. Estimating the finite-size critical temperature

Now that we have established a double minima structure it is important to realise that these double minima are not always equal. This is because the critical temperature of a finite varies from the analytically found critical temperature for an infinite lattice. Hence we must *guess* a value of the finite critical temperature. This guessing can be made computationally more efficient by using a bisection algorithm where we guess a range between which the temperature must fall. We then look at the graph for the midpoint value of the range. If the first minima is higher than the second minima then we choose an inverse temperature value to be between our lower range and the midpoint. If the second minima is higher than the first, then we choose the new guess to be between the midpoint and the higher range. Repeating this until our difference between the peaks is lesser than a set tolerance limit (10^{-10}) yields a minima structure with two equal minima.



2.4. Characterising a Phase Transition

Once we have equalised our minima, we attempt to classify the transition that takes place. For this, we obtain the double minima structure graph for different lattice sizes ($L = 32, 64, 128$) and then look at the difference in free energy between the peak and the minima. The peak of the free energy curve lies between the two equal minima. Note that we need to get accurate values for the minima and the peak, we do a polynomial best fit of the 8th order. Looking at this difference between the two minima and the maxima that lies in between these two, we estimate the nature of the phase transition. A direct correlation between the size of the lattice and the difference in free energy indicates a first nature behaviour.

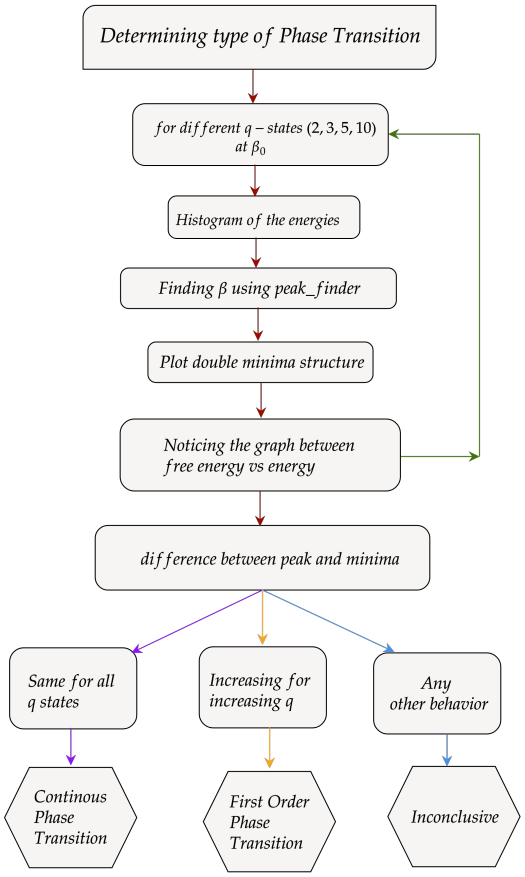


Figure 3: For finding the phase transition for different $q - states$

3. Results

3.1. Parameters in the model

Parameter	Value/Explanation
Interaction energy J	1
Monte Carlo Sweeps	25,00,000
L	Length of Lattice
Spins	2D array of $(L \times L)$
q state	[2,3,5,10]
allowed states	`{1,2,3...q}`
β	Inverse temperature

Table 1: Parameters in the Project

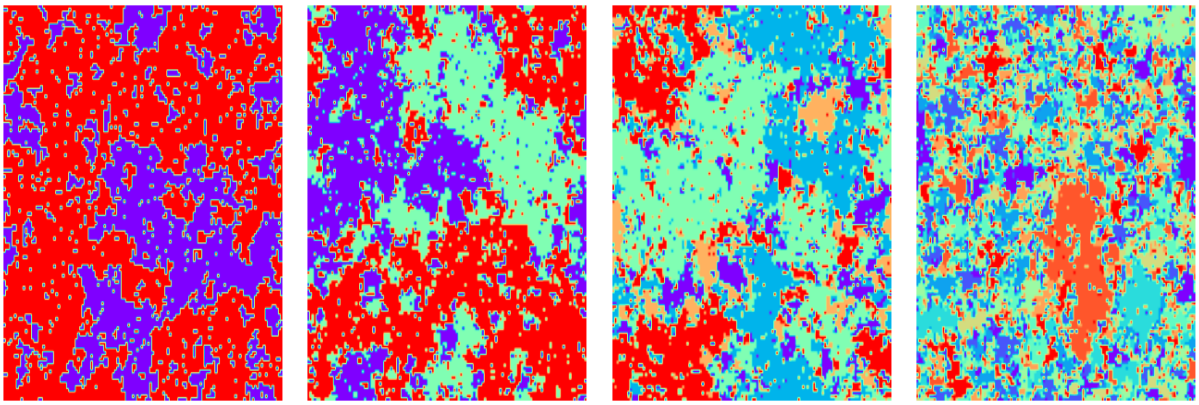


Figure 4: For states $q = 2$, $q = 3$, $q = 5$, and $q = 10$ respectively. Notice the reduced domain sizes for $q = 5, 10$

3.2. Qualitative observations at analytically found critical temperatures

If we run the simulation for the q-potts model for a (128×128) lattice for 5000 monte-carlo steps to see the behaviour of the system at low temperatures (below analytically found critical temperatures) we can obtain some hints for what the system might behave like. In fig(4) we see two very different behaviours. For $q = 2, q = 3$ we can clearly see individual domains where there are regions of similar spins indicated by their similar colours. At the same time if we look at the lattices for $q = 5$ and $q = 10$ we do not see a precise demarcation between the domains. The colours are much more dispersed in the higher q lattices and their individual domains are also much smaller than $q = 2, 3$. This alludes to the fact that the phase transitions for $q = 2, 3$ are of a different kind than that of $q = 5, 10$. Now this could be more empirically verified via the use of the Lee Kosterlitz algorithm discussed in the later parts of the report.

3.3. Behaviour of the specific heat

The specific heat curve produced for $50,000$ Monte Carlo sweeps with a (32×32) lattice suggests the possibility of a thermodynamic phase transition for every value of q indicated by the peaking of the specific heat close to the analytical solution. This indicates that the code used in the project works. The temperature values that are found using the specific heat maximum will be utilised as the simulation temperature for the histogram method in the later sections of the report.

As the value of q is increased, the peak temperature shifts to the left. The left most peak corresponds to $q = 10$ while the rightmost corresponds to $q = 2$. The vertical lines indicate that the analytic solutions are close to the theoretically found values from the simulation.

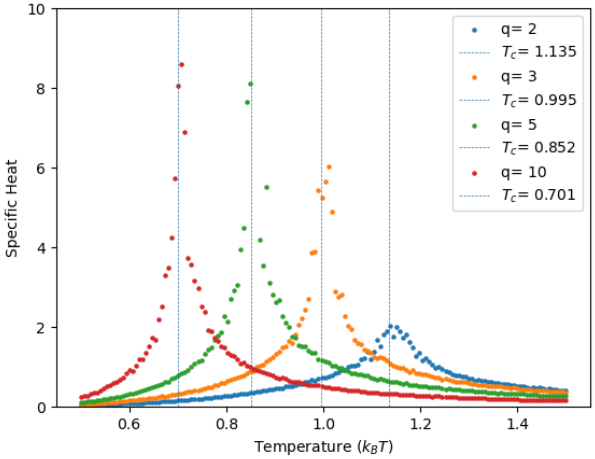


Figure 5: Specific heat curve simulated for different values of q

3.4. Double minima structures

The Lee Kosterlitz Algorithm was implemented to equate both minima. The difference between the minima and the maxima were estimated in some cases by the best fit graph while for other cases, the directly simulated values were used (depending on the noise). The following is showed in fig(6) and fig(7).

3.5. Difference in free energy

For a first order phase transition, we observe a linear relationship between free energy and the lattice size. We computed the change in free energy for $q = 5$, and $q = 10$ state of the Potts model, and plotted it against the respective lattice sizes. Figure 8 indicates this behaviour. The graphs corroborate the fact that for $q = 5$ and $q = 10$ states, there is an assured first order transition. This is due to the fact that increasing lattice sizes leads to increasing change in free energy indicated by the

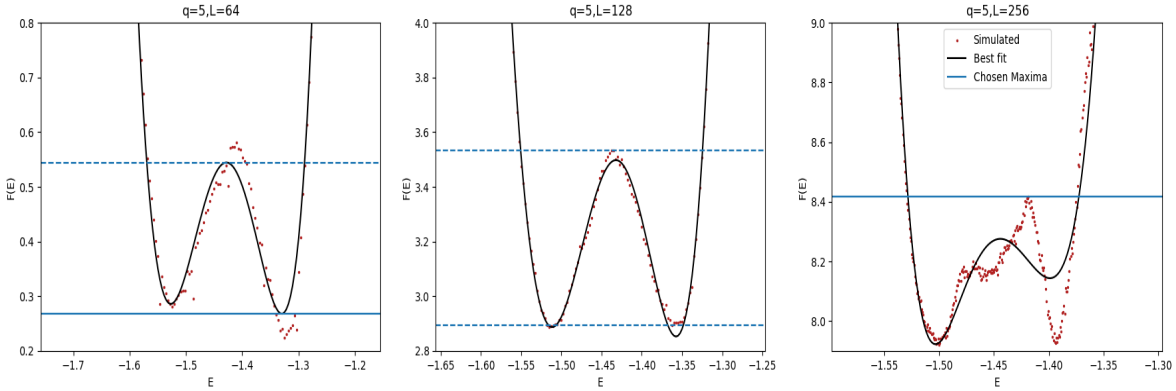


Figure 6: The double minima structure observed while plotting the Free Energy of different lattices of the same q-state Potts model. The graph is for $L = [64, 128, 256]$ for $q = 5$. These graphs were then used to find the maxima, and minima values which provides us with the change in free energy for the respective lattices. For $L = 64$, the curve of best fit was used to find the values of maxima and minima points. For $L = 128$, the simulated value was used to find the maxima and minima points as it gave a better estimate than the best fit curve values. Similarly, for $L = 256$ the minima point was taken according to the simulated values, as the peaks were equalized easily at the simulated values rather than the best fit curve values. The location of these maxima, and minima changes with the bin-count, however the difference between them stays constant irrespective of the bins used.

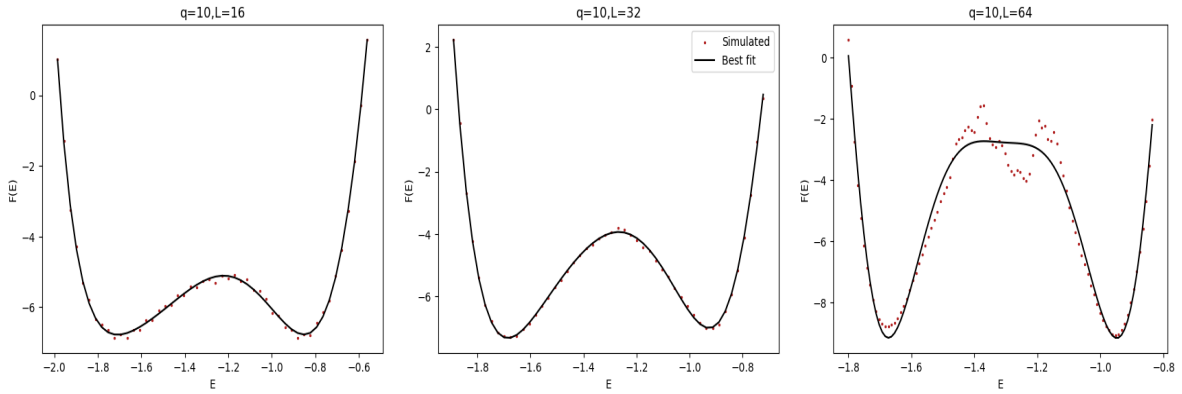


Figure 7: The double minima structure observed while plotting the Free Energy of different lattices of the same q-state Potts model. The graph is for $L = [16, 32, 64]$ for $q = 5$. These graphs were then used to find the maxima, and minima values which provides us with the change in free energy for the respective lattices. For all the lattice sizes, we used the best fit curve to find the maxima and minima values, which was then used to find the difference in free energies with varying lattice sizes.

linear best fit in fig(8). There are however some caveats to this result. Although the line was linear for $q = 10$ nd $q = 5$ the results were inconclusive for $q = 2, 3$ This possibly occurs as a consequence of the negligible difference between the minima and maxima in their case. The non existence of the double minima from our graph for both $q = 2, 3$ can be shown from the Free energy relations in both the cases.

Notice the fact that for $q = 3$ there is a platform of sorts in the middle rather than one single minima. This means there are a range of minima values closely packed with one another. The inconclusive nature of our results for $q = 2, 3$ can be attributed to the fact that bins may not have been proper or that the system may not have achieved equilibrium yet, leading to noise in the data. The noise in the data and its contribution is made more evident by the necklace like jagged patterns in the data-points in fig(9). A filter to reduce the noise in the data may lead to a better minima structure. One hint that suggests that $q = 2, 3$ go through continuous transition comes from the unchanging shape of the graph with increasing the sizes of the lattice L as shown in fig(9).

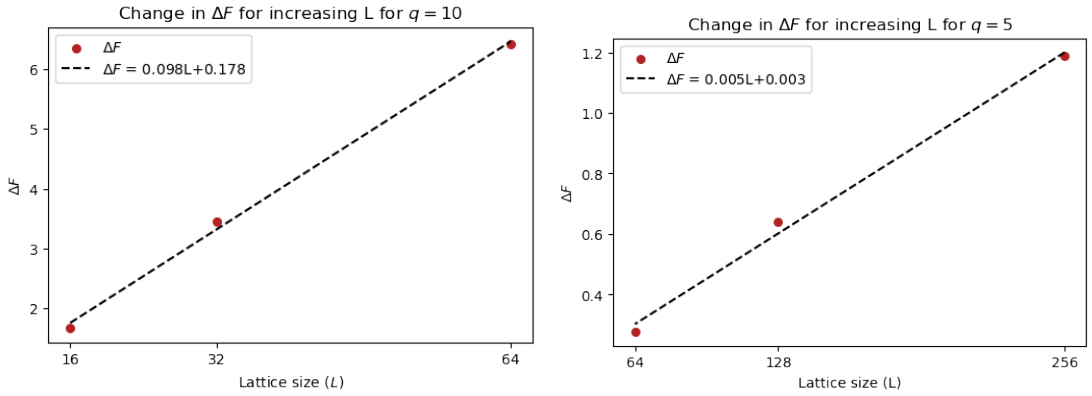


Figure 8: Change in free energy with increasing lattice size for $q = 5$ and $q = 10$ states. This linear behavior suggests a first order phase transition is occurring for the observed $q = 5$, and $q = 10$ state of Potts model.

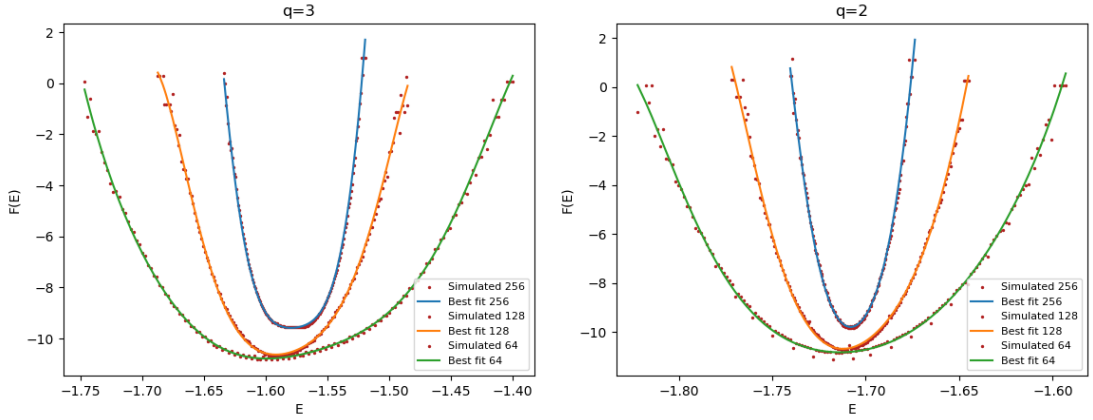


Figure 9: Change in free energy with increasing lattice size for $q = 2$ and $q = 3$ states indicating the absence of a double minima structure

3.6. Finite size critical temperatures

The points at which the two minima are equal for the Free energy we get an estimate of the critical temperature for that lattice dimension. This should ideally be equal to the peak of the specific heat and hence be marginally different from the analytically found critical temperature. All of these should be 99% similar to the analytical solution. Note that the lattice sizes for q were different. The data can be found in Table(2), and Table(3).

L	T_{finite}	$T_{\text{finite}}/T_{\text{c}}$
64	0.8528	0.9984
128	0.8519	0.9995
256	0.8516	0.9998

Table 2: For $q = 5$, and $L = [64, 128, 256]$ the table contains the value of the finite temperature was found from the simulations, and the critical temperature for the q^{th}-state is given as, $T_{\text{c}} = \ln(1 + \sqrt{q})$, and the ratio of finite temperature to the critical temperature was found.

L	T_{finite}	$T_{\text{finite}}/T_{\text{c}}$
16	0.7066	0.9923
32	0.7027	0.9978
64	0.7015	0.9996

Table 3: For $q = 10$, and $L = [16, 32, 64]$ the table contains the value of the finite temperature that were found from the simulations, and the critical temperature for the q^{th}-state is given as,$T_{\text{c}} = \ln(1 + \sqrt{q})$, The ratio was also computed

4. Discussion

The results in this project can be evaluated in manifold ways. It is important to realise that for the transitions that occur solely as a result of temperature (what we studied in this project) we must simulate the system for a long enough time (at least $10,00,000$ sweeps for a good histogram) so that we actually obtain enough unique values for energy for a double minima fit. Similarly it is also

important to note that it is not only about the sweeps but also about reaching the equilibrium. Simply binning values for which equilibrium has not been reached leads to extra noise in the histogram. This could be avoided by only taking the energy values after equilibrium has been met. For the sake of this project, we arbitrarily discarded at least half of our montecarlo sweeps hoping that the system would have reached equilibrium. For most plots the first $10,000$ values were discarded assuming they were non equilibrium states. Devising a more precise method for knowing when equilibrium is achieved would not only save computational time, but would also reduce the noise in the data.

Another limitation of this project is the limitation in data collected. The project only analysed $q = 2, 3, 5, 10$ for which we only simulated 3/4 different lattice sizes. Considering how small the actual difference in the free energy is, as a result of changing lattice sizes, making presice deductions on the nature of phase transition becomes a difficult task. Something that we have not considered for this project is a way to find the error bars associated with the change in free energy,the error bars would allow the experimenter to understand whether there is an actual possibility for there to be a first order transition. One way to make the functions more smooth would be to use a spline fit instead of a polynomial fit. Cubic splines are generally smoother and for interpolation, they do not have an oscillatory behavior that is common for higher-order degree polynomials associated with interpolation. For various double you see in this project,there was an ad-hoc approach that was taken to calculate the temperature for which both minima were equal. In many cases, just the best fit line was chosen, while for many cases just the simulated values were chosen. The experimenter should decide which ones to choose depending on how much noise they obtain from the data. The guessing function used in this project through the bisection method was too sensitive to noises and it incorrectly classified certain peaks, hence for various trials the guessing function was abandoned to calculate the minima directly through guesses.

Another limitation of the code is associated with its time complexity. The `OneMCS` function in the code takes a long time to run for higher lattice sizes and even longer when we increase the q. While the scaling of time is expected with increasing lattice sizes, we do should not expect as much change with just changing the value of q. While we have only taken a theoretical approach, applying the potts model to adsorption sites, for instance, the graphite-helium interaction would be something interesting to look at.

5. Conclusion

This project studied the possibility of a phase transition in the q state Potts model and classify its transition via the Lee Kosterlitz algorithm. The Project concludes that the Potts model goes through a thermodynamic phase transition. The first hint of a transition came from the graph of the specific heat which showed a discontinuity at a given temperature in the form of a sharp peak. The temperature of the peak matched with the analytically deduced critical temperature for a given q . Furthermore the presence of a phase transition was established by the presence of a double minima structure in $q = 5, 10$ while for $q = 2, 3$ we get a hint of a transition through the presence of a bench (a row of minima values)in the free energy. This also corroborates the idea that transitions for $q = 2, 3$ are fundamentally different than those of $q = 5, 10$. It was further concluded that the transitions for $q = 5, 10$ are first order transitions as inferred from the relation between the change in free energy as as function of changing lattice sizes. The qualitative images in the project indicate a formation of domains for lower values of q while for $q = 5, 10$ the domains are almost non-existent with greater mixing.

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