University of Swansea

Masters Dissertation

BL1: Interfaces in the 2D Potts model

Author:
Robert James

Supervisor:
Professor Biagio Lucini

March 9, 2015

Abstract

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Chapter 1

Introduction

In the field of Computational Physics, there is a large interest in lattice simulation. One of the most simple models that still exhibits non trivial behaviour is the q-state Potts Model. By Restricting the Potts model to 2 or 1 dimension(s) and the constraining the number of independent states,$q = 2$ you can determine the behaviour at high,low and critical temperatures analytically[1] this is known as the Ising Model.

This dissertation will be looking at directly determining the interface free energy as a ratio of the partition functions.

$$F_I(L) = -\log \frac{\tilde{Z}(L)}{Z(L)} + \log(L) \tag{1.1}$$

From the interface free energy above we can calculate the interface tension σ.

$$\sigma = \lim_{L \to \infty} \frac{F_I(L)}{L^{D-1}} \tag{1.2}$$

To reach the final goal of studying the interface tensions in the q-state Potts Model, there w

Chapter 2

Theory

The Potts Model, a lattice simulation typically performed on a regular euclidean grid. In this model, the number of states per lattice site is given by q. In the code that was written for this project, each lattice point is assigned a value $q = 1, q$. The values that are assigned to the lattice can be visualised as an angle equally distributed in the space.

$$\theta_n = \frac{2\pi n}{q} \tag{2.1}$$

Or to show it visually,

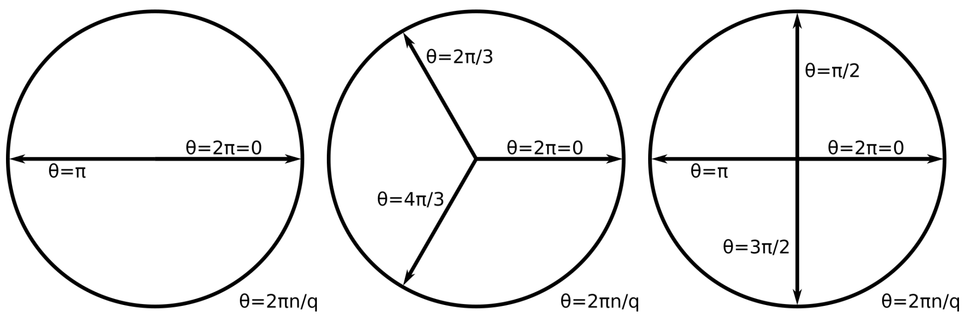


Figure 2.1: Angle representation of q states

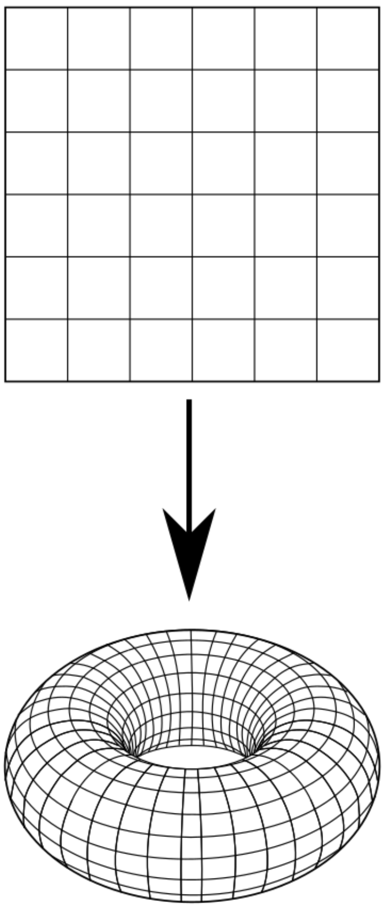
2.1 Lattice

Most lattice simulations try to measure thermodynamic quantities in the Thermodynamic limit. The Thermodynamic limit can be written as

$$N \to \infty, V \to \infty, \frac{N}{V} = const \tag{2.2}$$

In this limit, macroscopic thermodynamics apply.

For small lattice sizes which are reasonably easy to simulate, you will have to account for boundary effects. For small grids, boundary effects can start to dominate the behaviour of the system, because of this, periodic boundary conditions are often implemented to remove the issue. A 2D lattice with periodic boundary conditions can be visualised as a torus like in the diagram below.



2.2 Hamiltonian

$$\mathcal{H} = J_c \sum_{<i,j>} \delta(s_i, s_j) \tag{2.3}$$

Where J_c is a coupling constant, the summation is over the nearest neighbours and a Kronecker delta function which equals one whenever $s_i == s_j$.

2.3 Magnetisation

For a $q = 2$ (Ising) model, the magnetisation is simply the sum of the spin states. Thinking about it in terms of angles, assuming the lattice is completely filled then opposite states will cancel out.

$$\mathcal{M} = \sum_{i}^{N} s_i \tag{2.4}$$

For more complex q we must fully engage in the angle model to calculate magnetisation. Because each of the states $1, q$ has an angle representation and we know that the Magnetisation is a real quantity it was simply the sum of the cosines of the angle.

$$\mathcal{M} = \sum_{i}^{N} \cos s_i \tag{2.5}$$

Onsagers Solution for Spontaneous magnetisation for the 2D Ising Model, (ie/$q = 2$ Potts Model)[1]

$$\mathcal{M} = \left(1 - [\sinh 2\beta J]^{-4}\right)^{\frac{1}{8}} \tag{2.6}$$

With J being coupling strength. For the majority of this project, it is reasonable to assume $J = 1$ because it isn't being used to calculate thermodynamic quantities of real materials.

The existence of an analytical solution allows for direct comparison. To confirm that a generalised q state Potts Model simulation is working correct involves setting the parameters to $d = 2q = 2$ and confirming the accuracy of the analytic solution.

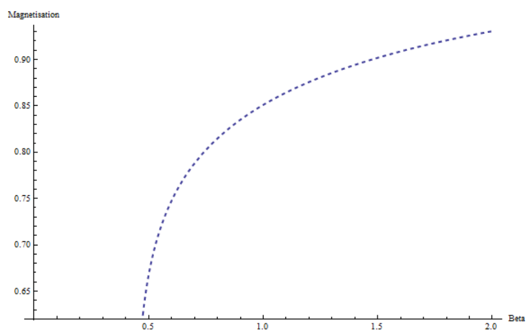


Figure 2.2: Mathematica plot of Osangers exact solution

2.4 Other Thermodynamic Quantities

Chapter 3

Code

Chapter 4

Results

Chapter 5

Discussion of Results

Bibliography

[1] Elliott W. Montroll, Renfrey B. Potts, and John C. Ward. Correlations and spontaneous magnetization of the two dimensional ising model. *Journal of Mathematical Physics*, 4(2):308–322, 1963.