Study of statistical models relevant to QCD phase diagrams

A *project report* submitted by

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Acknowledgement

This project has been one of my best experiences and has shaped my further interest in research in physics. As such, this project will be only half done if I do not begin this report by thanking the people who endured my stupidity at every step, eventually pushing me over the line.

I start by thanking by Professor Rajiv Gavai who has made himself available for discussions on innumerable occasions and helped me clear the doubts I had during the initial days of work. I would also like to thank my fellow colleagues at Department of Theoretical Physics with who I had useful discussions and debates. I would also like to thank Professor Bedanga Mohanty who I often asked for advice during this project. I also want to thank Tata Institute of Fundamental Research for giving me the opportunity to spend a summer at this wonderful campus amongst the best people from around the country.

Finally, it is only fully done when I thank Dr. *Rishi Sharma* for guiding me through the length of this project. I learnt so much about the field of QCD phase diagrams from this project and it wouldn't have been possible without his support. I hope to continue working with him in the near future.

Chapter 1

Introduction

The basic constituents of Quantum Chromodynamics are quarks and gluons that are confined in colourless bound states, hadrons. They exist in "groups", the simplest being mesons (a quark and an anti-quark) and baryons (3 quarks). Recently some tetraquark and pentaquark candidates have been reported too [1]. Hadrons have a limiting volume by virtue of their intrinsic size, hence hadronic matter has a limiting density. Based on production of resonance particles, it has been reasoned that there is an upper limit for the temperature of hadronic matter $T_c \simeq 150 - 200$ MeV [2]. At high temperature and/or densities, quark deconfinement occurs and hadronic matter can turn into a quark-gluon plasma of coloured quarks and gluons as constituents. This is a phase transition to a new state of matter.

For hadrons, their masses have little relevance to the masses of the bare valence quarks, rather, the mass arises from the large amount of energy associated with strong interaction. In vacuum, at $T = 0$, strong force gluons form resonances of massive quarks to form the constituent quarks that form the hadron. Hence, instead of a bare quark mass of $m_q \sim 0$, quarks inside hadrons have $M_q \sim 300$ MeV [3]. In QGP, the quarks and gluons are no longer confined, hence $M_q \to 0$. For massless quarks, the QCD lagrangian is chirally symmetric, hence, in the hadronic matter phase where the quark mass is non-zero, there is spontaneous chiral symmetry breaking. $M_q \to 0$ implies symmetry restoration.

The phase boundary is although, not clear in the $T - \mu_B$ plane. Experiments at

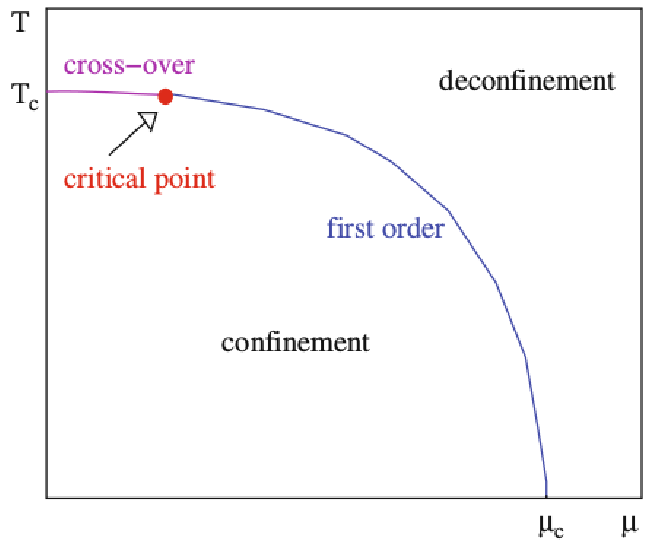

Figure 1.1: *Phase structure in terms of baryon chemical potential.*. **Source:** H. Satz: The Thermodynamics of Quarks and Gluons. Lect. Notes Phys. 785, 121 (2010)

RHIC are trying to map this QCD phase diagram. A first order transition is expected at high μ_B and low T. With decrease of baryon chemical potential and increase of temperature, the first-order phase transition line ends at a critical point, which belongs to the three-dimensional (3D) Ising universality class [4]. Further calculations point to a crossover at vanishing μ [5].

To this end, it is useful to investigate a model belonging to the same universality class as QCD, the Potts model. In this report, I have first summarised the Ising model which is a special case of the generalised Potts model. With insights from that, I have then summarised Potts model while looking at second and third order susceptibilities. Finite scaling has also been discussed, although I am yet to derive the paramters myself.

Chapter 2

Ising Model

2.1 Ferromagnetism

When placed in an external magnetic field, some materials create a magnetic field of their own. It points either in the same direction (paramagnetism) or in the opposite direction (diamagnetism). Ferromagnetism is the ability of a paramagnetic material to retain **spontaneous magnetization** as the external magnetic field is removed. Ferromagnetism involves the spins of electrons of the outer layers. Spontaneous magnetisation always depends on the temperature, typically magnetisation $M(T)$ looks like this.

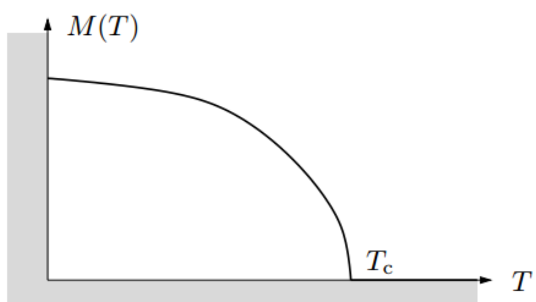

Figure 2.1: *Spontaneous magnetisation for a typical ferromagnet as a function of the temperature.* **Source:** `http://www.ueltschi.org/teaching/chapIsing.pdf`

The critical temperature is the Curie Temperature (T_c) and is a property of the material. As $T \to T_c$, $M(T) \to 0$ following a power law, $M(T) \approx t^{\beta}$ where t is the dimensional reduced temperature, $t = \left|\frac{T-T_c}{T_c}\right|$. β is a **critical exponent** and is nearly identical in all ferromagnetic materials. It is theorised that they depend on general characteristics such as number of dimensions, broken microscopic symmetries,finite size effects, but not on the actual types of lattice or interactions. This phenomenon is called **universality**.

2.2 Model

In the Ising model, we consider a lattice of magnetic moments. On each lattice site, the local magnetic moment is represented by a spin". We assume that the spin has only two possible states, either "up" or "down". We represent the spin at site i by $\sigma_i = \pm 1$. We will consider only nearest-neighbour interactions.

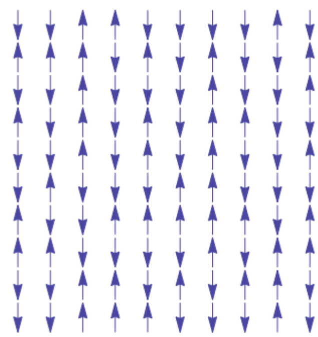

Figure 2.2: *Ising model on a 2D lattice. Up arrows represent +1 and down arrows represent -1.* **Source:** J.V. Selinger, Introduction to the Theory of Soft Matter, Soft and Biological Matter

The energy for the Ising model includes two contributions: the interaction between neighboring spins and the effect of an applied magnetic field on each individual spin. The interaction between neighbouring spins tends to induce parallel alignment of the neighbours. The magnetic field will prefer spins in its direction. Hence the Hamiltonian for the system becomes

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{2.1}$$

To get the magnetic order of the system, we define the "magnetic order parameter" as

$$M = \left\langle \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \right\rangle \tag{2.2}$$

The susceptibilities χ_2 and χ_3 are defined by the 2nd order derivatives of the free energy density and are given by

$$\chi_2 = \frac{1}{V}\left(\langle M^2\rangle - \langle M\rangle^2\right) \tag{2.3}$$

$$\chi_3 = \frac{1}{V}\langle \delta M^3\rangle \tag{2.4}$$

$$= \frac{1}{V}\left(\langle M^3\rangle - 3\langle M^2\rangle\langle M\rangle + 2\langle M\rangle^3\right) \tag{2.5}$$

2.3 Mean-field Theory Solution

Using mean-field theory for the Ising model, we have the interaction energy term as $\left\langle E_{int} \approx -\frac{1}{2}NJqM^2\right\rangle$ where N is the number of sites in the lattice and q is the coordination number of the lattice.

Thus, the free energy becomes

$$\frac{F(M)}{Nk_BT} = -\frac{Jq}{2k_BT}M^2 - \frac{h}{k_BT}M + \frac{1+M}{2}\log\left(\frac{1+M}{2}\right) + \frac{1-M}{2}\log\left(\frac{1-M}{2}\right) \tag{2.6}$$

where we have used Stirling approximation in the thermodynamic limit to write the equation.

At high temperature, the system goes to the state with no magnetic order, M = 0, as favored by entropy. By comparison, at low temperature, the system goes to a state with some magnetic order. This low-temperature state with spontaneous (not induced by field) magnetic order is called a ferromagnetic phase. By contrast, the high-temperature state with no spontaneous magnetic order is called a paramagnetic phase. The change from paramagnetic to ferromagnetic at a specific temperature is a **phase transition**.

The high-temperature paramagnetic phase has a symmetry between up and down, with no preference for either direction. In the low temperature ferromagnetic phase, this symmetry is broken and the system randomly goes one way or the other. This random selection is called *spontaneous symmetry breaking.*

The phase transition temperature can be found by taking the second derivative of the free energy $F(M)$ and equating it to 0 at $M = 0$. This gives $T_c = \frac{Jq}{k_B}$. Furthermore, the extrema of the first derivative gives $M = \tanh\left(\frac{h+JqM}{k_BT}\right)$ which is a transcendental equation and cannot be exactly solved.

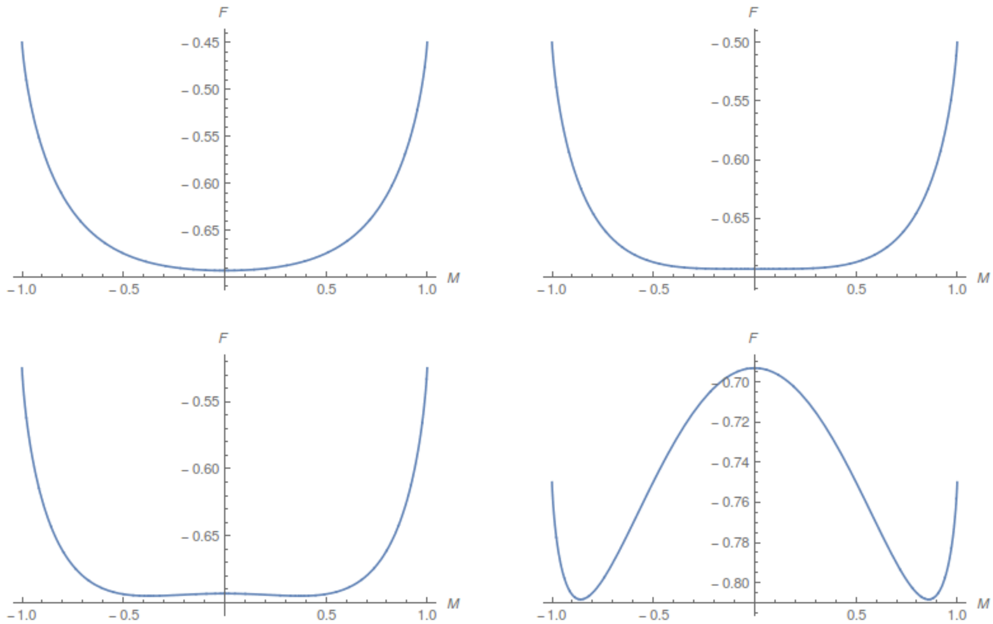

Figure 2.3: Free energy of the interacting Ising Model, with $h = 0$, as a function of M. *Top left:* $Jq/k_BT = 0.9$, *Top right:* $Jq/k_BT = 1.0$, *Bottom left:* $Jq/k_BT = 1.05$, *Bottom right:* $Jq/k_BT = 1.50$

When a magnetic field is applied, the symmetry between $M > 0$ and $M < 0$ is broken. For $T < T_c$, there are two minima in the free energy curve, one of which is deeper, indicating that one is preferred over other. For $T > T_c$, the free energy has one minima only, which is displaced from 0 by the applied field. There is a smooth crossover from $T > T_c$ to $T < T_c$. M has no discontinuity as is seen in Fig. 2.5.

From MFT, the value of β comes out as $\frac{1}{2}$ from the transcendental equation. It is not quite right for 2D and 3D, but that is beyond the scope of this project.

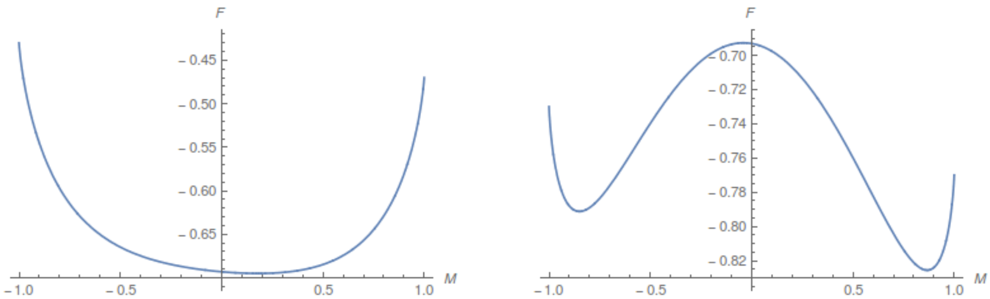

Figure 2.4: Free energy of the interacting Ising Model, with $h = 0.02$, as a function of M. *Left:* $Jq/k_BT = 0.9$, *Right:* $Jq/k_BT = 1.5$

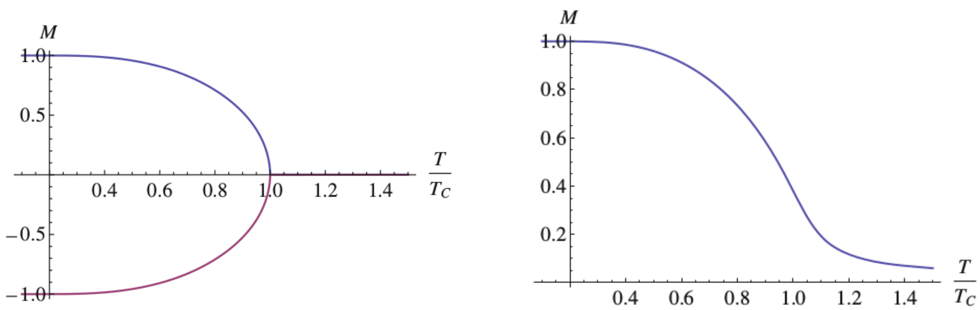

Figure 2.5: Order Parameter for the Ising Model as a function of T. *Left:* $h/k_BT = 0.0$, *Right:* $h/k_BT = 0.02$

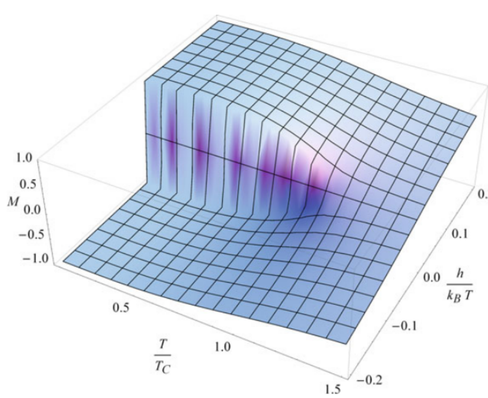

Figure 2.6: *Ising order parameter as a function of H and T*. **Source:** J.V. Selinger, Introduction to the Theory of Soft Matter, Soft and Biological Matter

2.4 Numerical solutions on 3D lattice

There aren't any exact solutions for the Ising model in 3D yet. Some results suggest that it might be impossible to solve owing to the fact that it is NP-complete [6]. Hence, we attempt to numerically solve the Ising model on a 3D lattice. We look at the order parameter and the second and third order susceptibilities near the critical temperature. The simulations have been done using the *Wolff Clustering algorithm* for lattice sizes 20^3, 30^3 and 40^3 using 20000 Monte-Carlo steps.

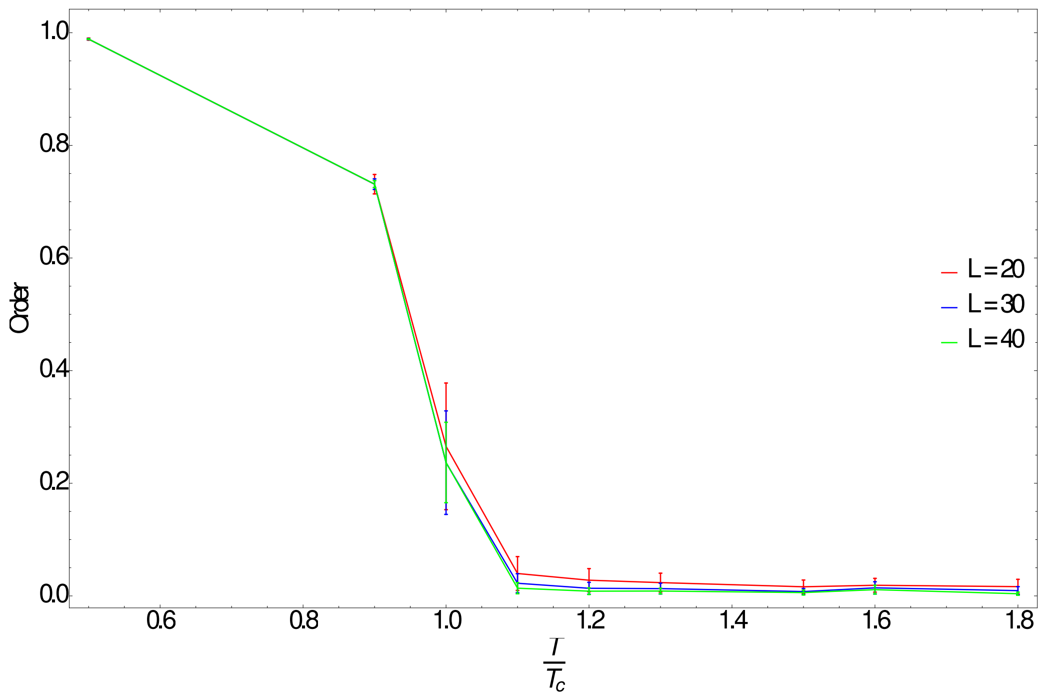

Figure 2.7: Order parameter for different lattice sizes. With increasing linear size, the order parameter approaches the thermodynamic limit becoming discontinuous at T_c.

The second order transition is not very clear in this picture. This is an effect of finite size where it essentially behaves like a crossover. However, the curves become steeper with increasing lattice size. This tells us qualitatively that the observed behaviour is correct and it approaches the infinite volume limit asymptotically where it is a first order transition as was predicted by mean field theory.

From mean field theory, we know that χ is supposed to diverge at $T = T_c$ and fall off as a power law on either sides. That is true in the thermodynamic limit i.e. infinite volume lattice. For finite volumes, χ attains high values near T_c. Qualitatively, the

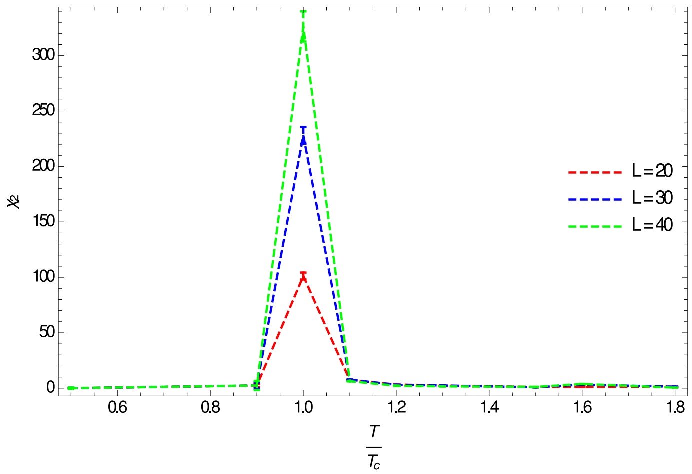

Figure 2.8: χ for different lattice sizes.

peak value increases with the lattice size which can be used to relate to the infinite volume case.

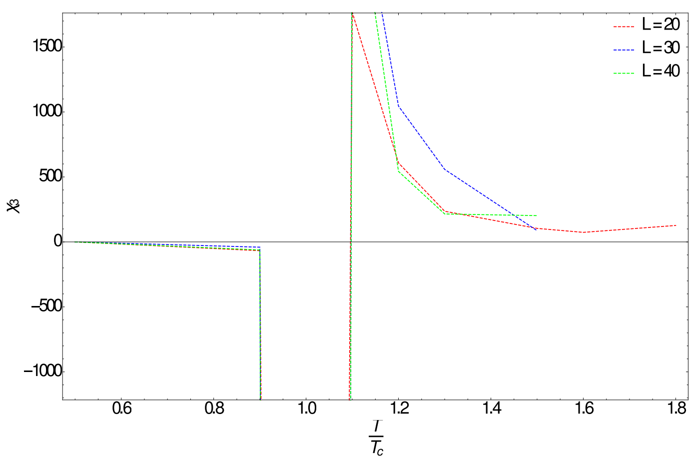

Figure 2.9: χ_3 for different lattice sizes. χ_3 suffers a sign change near the critical point.

When magnetic field is applied, there is no phase transition. This is clear from the variation of order and χ with temperature. The order smoothly decreases and hence it's continuous. χ doesn't have a peak anymore at the critical temperature. For finite lattices, there is still a small peak near the critical temperature, but the magnitude is clearly much less.

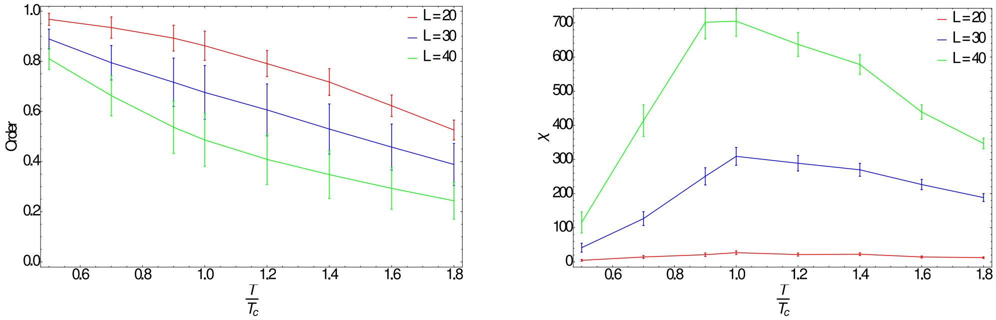

Figure 2.10: Order Parameter and χ for the Ising Model as a function of T at $H = 2$

Ising model is therefore not much helpful to our case of QCD as there is a second order phase transition only at $h = 0$. There is no first order region like the one we encountered in QCD. Nevertheless, it serves as a great model for a couple of physical phenomenon e.g. ferromagnetism and antiferromagnetism. We now turn to the more general Potts model which has a richer phase structure.

Chapter 3

Potts Model

The wide influence of Ising model motivates generalisations like Potts model, vector spin models (O(n) model) among many. In Potts, spins of equal energy tend to co-align. The spins, however can take q possible values instead of ± 1 as in the case of Ising. For $q = 2$, Potts reduces to Ising model. QCD bears resemblance to the 3D 3-state Potts model which is why I have looked into the order parameter and susceptibilities for this model.

The Hamiltonian for the Potts model is given by

$$H = -J \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) - h \sum_i (\sigma_i, \sigma_g) \tag{3.1}$$

The order parameter is defined by the mean of magnetisation

$$m = \frac{3}{2} \frac{\langle M \rangle}{V} - \frac{1}{2} \tag{3.2}$$

This is equivalent to the order parameter in QCD which is given by the Polyakov loop $L(T) \sim \lim_{r \to \infty} \exp(-V(r)/T)$ where $V(r)$ is the potential between a static quark-antiquark pair separated by a distance r. It signals the spontaneous symmery breaking.

For 2D lattices, MFT predicts a critical temperature given by $T_c = \frac{1}{\log(1+\sqrt{(q)})}$ [7].

However, we will numerically solve this model for the given Hamiltonian in 3D using Wolff clustering algorithm. We take the 3 state Potts model. Its phase boundary in temperature and external field plane are shown in figure 3.1. It is comparable to that of the QCD. At vanishing external field, the temperature-driven phase transition has been shown to first-order [8]. With increase of the external field, the first-order phase transition weakens and ends at a critical point ($1/T_c$, h_c) which belongs to the 3D Ising universality class [9]. Beyond the critical point, it is a crossover region. Both transitions of QCD deconfinement and QCD chiral symmetry restoration have the line of first-order phase transition, and end in a second-order endpoint. The baryon chemical potential acts as the external field in the Potts model.

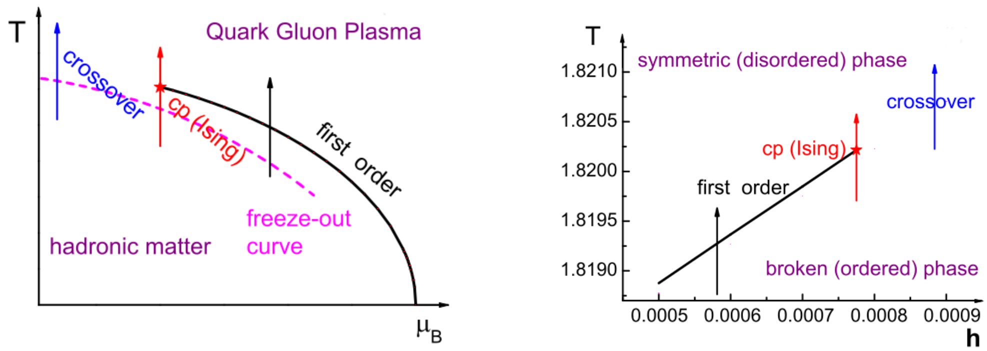

Figure 3.1: Left : Phase diagram for QCD in T vs μ_B plane. Right : Phase diagram for Potts in T vs H plane

In principle, it is uncomplicated to detect the difference between a first-order and a second-order transition by plotting the free energy as a function of temperature. The susceptibility is a δ-function for an infinite system while it is divergent for a second order transition. For a truly infinite size lattice and infinite time simulation, the numerical results should agree with theory. In practice, however, the distinguishing features of each transition become blurred. In the Potts $q < 4$ case, this blurriness is a consequence of the fact that simulations involve finite lattices and finite time simulation runs.

To get rid of this problem, we need to do a finite size scaling, which I haven't done yet. However, we can make some qualitative arguments regarding the nature of phase transitions from the plots for order and susceptibilities.

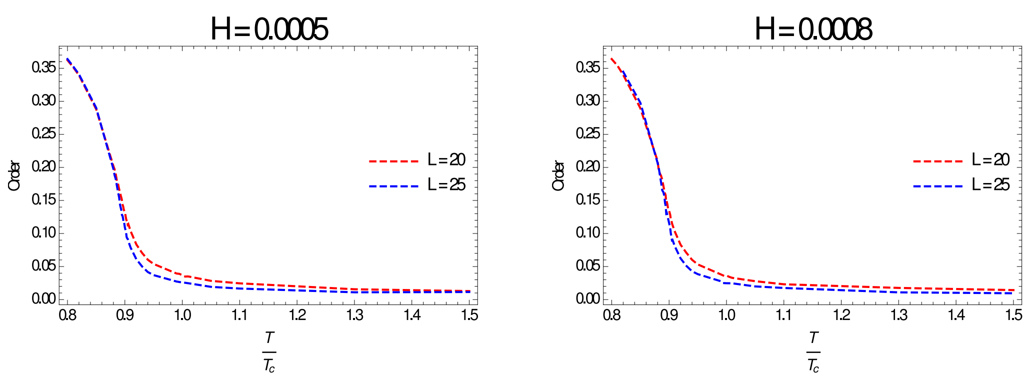

Figure 3.2: Order Parameter for the Potts model at two different values of H. The critical value for H is reported in literature as 0.000775. Here, the plot on the left is from the first order region in Fig 3.1 while the plot on the right is from beyong the critical point, hence the crossover region.

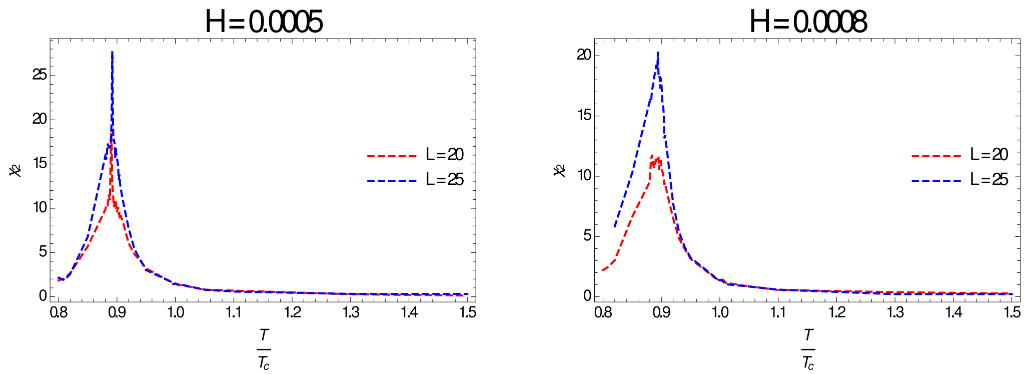

Figure 3.3: χ_2 for the Potts model at two different values of H. The critical value for H is reported in literature as 0.000775. Here, the plot on the left is from the first order region in Fig 3.1 while the plot on the right is from beyong the critical point, hence the crossover region.

χ_2 diverges for a first order transition as we have seen for the Ising case in the thermodynamic limit. Here, however, due to finite size, we have a finite peak. However, the peak value decreases for the magnetic field in the crossover region. This effect will be more pronounced for larger lattice sizes, however, the change from a phase transition to a crossover is clear.

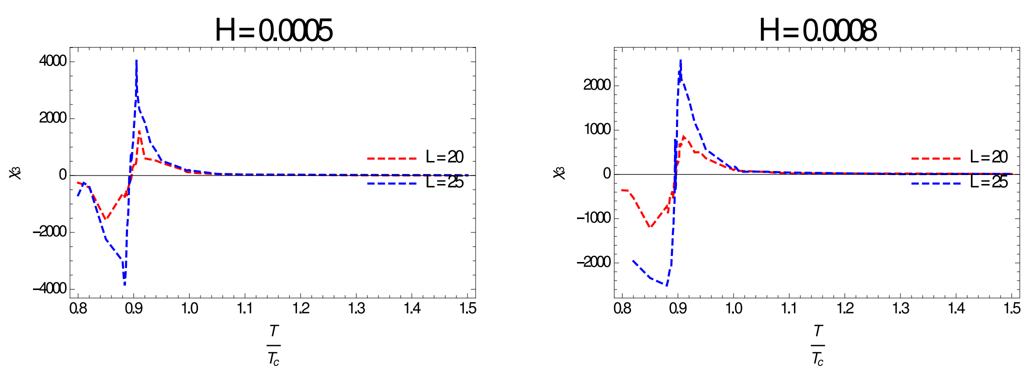

Figure 3.4: χ_3 for the Potts model at two different values of H. The critical value for H is reported in literature as 0.000775. Here, the plot on the left is from the first order region in Fig 3.1 while the plot on the right is from beyong the critical point, hence the crossover region.

Chapter 4

Conclusion

The structure of the second-order susceptibility is similar for both first order and crossover regions, however, the crossover peaks are wider and more blunt as compared to the first order peaks. Also, the peak gets higher with increasing system size, however at higher magnetic fields, the peaks are closer. It indicates that system dependence weakens with increasing magnetic field.

The third order susceptibility χ_3 near the phase transition temperature oscillates from negative to positive when the temperature changes from below T_c to above T_c. The third-order susceptibility fluctuates more frequently and violently near the phase transition temperature than that of the second-order susceptibility. Their dependence on the external field and system size are the same as those of the second-order susceptibility.

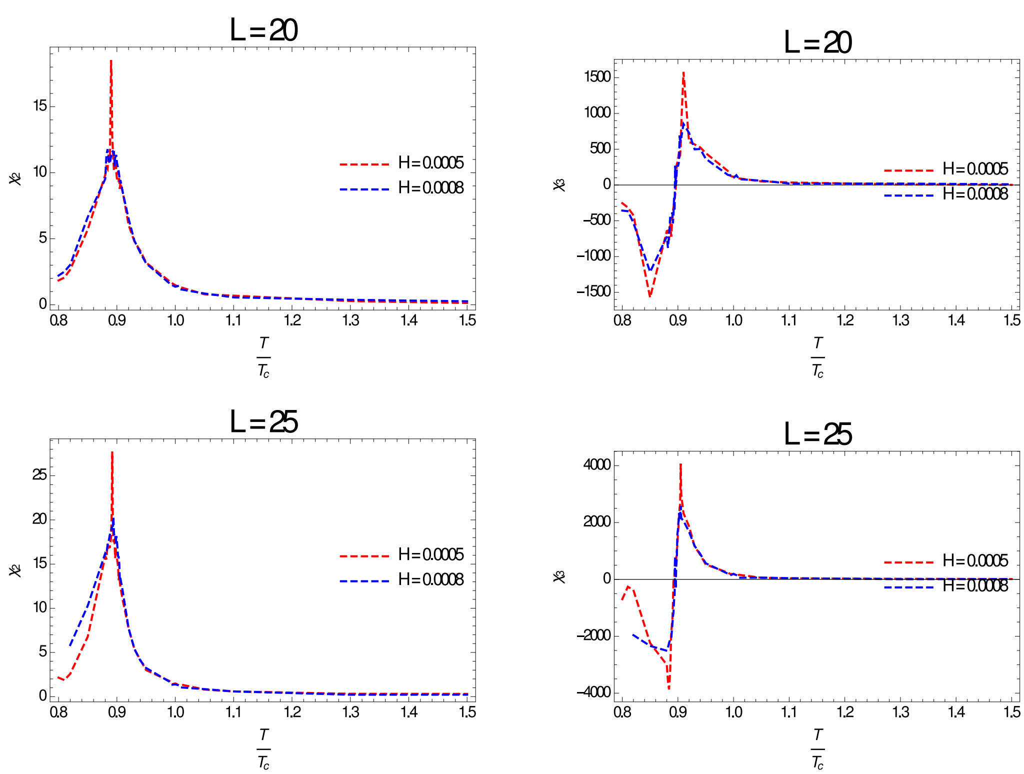

Figure 4.1: **Up** : Susceptibilities at different H for $L = 20$; **Down** : Susceptibilities at different H for $L = 25$

- Further analysis would include finite size scaling and finding the infinite lattice critical parameters from the finite lattice data. Doing that would require finding the critical exponents and fitting with the power law dependences for all the observables like correlation, specific heat etc.

- Finally, it would be useful to find a one-to-one correspondence between μ_B in case of QCD and h in case of Potts.

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