

# QCD at Finite Density with Taylor Expansion

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## MASTER OF SCIENCE

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## DECLARATION

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# Abstract

Studying the phase diagram of strongly interacting matter requires to us to understand QCD at a finite density of fermionic particles QCD at finite density which introduces a non-zero chemical potential  $\mu$  into the fermionic part of the QCD action which allows the system to have finite number density of fermions of a kind (say baryons or quarks). Solving QCD at finite density poses a computational challenge known as the 'sign problem'; to overcome it one of the methods used is the Taylor expansion. A new resummation scheme proposed for the Taylor expansion shows improved convergence and better capturing of the sign problem's severity. Due to omission of certain terms the series becomes biased at cost of resumming upto all orders, hence we introduce modified schemes of exponential resummation with the chemical potential basis and cumulant basis to give more unbiased estimates.

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# Chapter 1

## QCD at Finite Density

### 1.1 Motivation

A theoretical analysis of Quantum Chromodynamics in the non-perturbative regime is a difficult task. Due to its non-abelian nature gluons have the property of self-interaction. In fact, the hadronic matter that makes up most of the mass of the universe exists due to the peculiar properties of QCD such as color confinement, asymptotic freedom and spontaneous breaking of chiral symmetry.

But this hadronic matter that we observe exists under certain ranges of temperature  $T$  and chemical potential  $\mu$ . Only within these conditions do the quarks remain confined and hence all we get to see are colorless baryons and pions. At different values of these one can find that  $T$  and  $\mu$  the strength of interaction between them changes which can cause the formation of a variety of phases of QCD matter such as the quark gluon plasma, color flavor locked phase, etc.

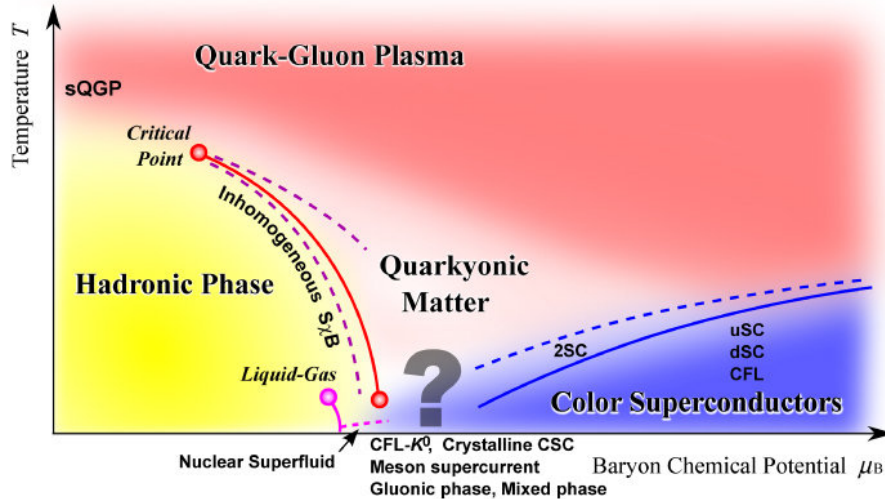


Fig. 1.1: Different phases of QCD on the  $T$ - $\mu$  plane

Experimentally one resorts to heavy ion collisions to study QCD matter at high energies. The theoretical study of such a variety of phases and to reconcile theory with experimental results calls for the study of non-perturbative physics. The applications of this range of from defining the QCD phase diagram and equation of state to neutron star matter to cosmology. Since there are no established ways to analytically study non-perturbative QCD, we must resort to brute force simulations on the lattice (discretized space-time). We already have well developed



ways of dealing with matter at finite temperature on the lattice that are actively used (in conjunction with experimental data) to produce results such as the critical temperature, etc. However introducing a finite density of particles brings into the question of defining the chemical potential on the lattice in a meaningful way. Naively, one can generalize from the continuum prescription where a term  $\mu N$  is introduced to the Lagrangian,  $N$  being the number density of particles.

## 1.2 Chemical Potential in continuum

To define a system at a finite density means to define it at a finite number of particles. The change in such number of particles, i.e. its density, can affect the total energy of the system. In general when we think of chemical potential, it is basically the energy cost associated with adding or removing a particle (of one kind) to the system. Hence it is multiplied with the number of such particles  $N$  to give the total energy addition to the system.

$$L = L_s + \mu N \quad (1.1)$$

where  $L_s$  is the Lagrangian free of chemical potential. In field theoretic notions, where instead of Lagrangian we have a Lagrangian density, the number density charge is only the zeroth component of a conserved vector current arising as a result of a global gauge symmetry. Since we already are going to work on the lattice, we shall no longer work in the Minkowski formalism and from here on define everything in the Euclidean formalism, where imaginary time (by doing a wick rotation) it is equated with the inverse temperature  $\beta = \frac{1}{T}$ . The action with chemical potential  $\mu$  can be written as

$$S = \int dx^4 \left[ \frac{1}{4} G^{\mu\nu} G_{\mu\nu} + \bar{\psi}_i (\gamma_\mu (D_\mu)_{ij} + m) \psi_i + \mu \bar{\psi}(x) \gamma_4 \psi(x) \right] \quad (1.2)$$

where  $\psi(x, x_4) = -\psi(x, x_4 + \beta)$  describes the fermionic wavefunction that is anti-periodic along the imaginary temporal axis with a periodicity of inverse temperature  $\beta$ . The  $\bar{\psi}(x) \gamma_4 \psi(x)$  term appears to be the temporal component ( $x_4$ ) of the conserved vector current  $\bar{\psi}(x) \gamma_4 \psi(x)$ . This is similar to how in continuum QED, the vector potential is introduced exactly as a photon field [1].

One must keep in mind however that the gamma matrices are all defined in Euclidean space and  $\gamma_4$  is just  $\gamma_0$  in said space. It is not  $\gamma_5$  matrix which is just the product  $\gamma_3 \gamma_2 \gamma_1 \gamma_0$ .

## 1.3 A brief primer to the Lattice

Before we proceed any further, we must first understand how discretization happens on the lattice and how quantities that we are familiar with in the continuum are defined on the lattice. A lattice is basically a grid in 4 dimensional space time with  $N_T$  steps in the time direction and  $N_\sigma$  steps in each of the 3 space dimensions.

The 4 dimensional Euclidean action consists of a gauge part

$$S_g = \frac{1}{4} \int dx^4 G^{\mu\nu} G_{\mu\nu} \quad (1.3)$$

and a fermionic part

$$S_f = \int d^4x \bar{\psi}(x) (\gamma_\nu D_\nu + m + \mu \gamma_4) \psi(x) \quad (1.4)$$

Notice that the chemical potential term is added only to the fermionic part of the action. Obviously the system can be defined by a path integral (which we'll later use as the grand canonical partition function once we define temperature)

$$Z = \int D A D \bar{\psi} D \psi e^{-(S_g + S_f)} \quad (1.5)$$

where one integrates over all gauge configurations, and fermion fields  $\psi(x)$  and  $\bar{\psi}(x)$ . Since the latter two are Grassman numbers they have the property

$$\int D \bar{\psi} D \psi e^{\bar{\psi} M \psi} = \det M \quad (1.6)$$

we can rewrite the path integral as

$$Z = \int D A e^{-S_g} \det M \quad (1.7)$$

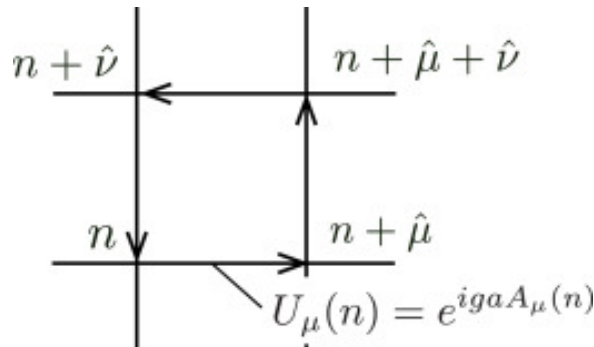
Thus only the  $\det M$  part has any dependence on the chemical potential. This fact is crucial and will come in handy later on.

### 1.3.1 Discretizing gauge action

Since we are concerned with the fermionic part of the action, we shall be brief with this part and push forward a more intuitive understanding of results without any derivations.

To discretize the action we must first visualize the lattice as a grid where each vertex point, separated by a distance  $a$ , is a quark which is connected to its neighboring quarks by gauge links. Since space is discretized, the position  $x$  is defined a discrete point  $n$  which is a set of four integer coordinates. Each gauge link at a point  $n$  in a direction  $\nu$  can be given by  $U_\nu(n)$ . A plaquette  $U_{\nu\mu}$  is a gauge variable that is defined on the square that connects the points  $n$  and  $n + \hat{\nu} + \hat{\mu}$ . It is the product of all the gauge links that connects all points  $n$ ,  $n + \hat{\nu}$ ,  $n + \hat{\nu} + \hat{\mu}$ ,  $n + \hat{\mu}$  in that order, i.e.

$$U_{\nu\mu}(n) = U_{n,\hat{\nu}} U_{n+\hat{\nu},\hat{\mu}} U_{n+\hat{\nu}+\hat{\mu},-\hat{\nu}}^\dagger U_{n+\hat{\mu},-\hat{\mu}}^\dagger \quad (1.8)$$



**Fig. 1.2:** Schematic view of a plaquette

The daggers are from the links that move towards the original point  $n$  in contrast to the first

two links that moved away from it. It is related to the familiar  $G_{\mu\nu}$  by

$$U_{\mu\nu}(n) = e^{iga^2 G_{\mu\nu}} \quad (1.9)$$

where  $g$  is the coupling constant. By imposing the constraints of gauge invariance and reproduction of QCD in continuum limit  $a \rightarrow 0$ , our discretized gauge action looks something like this

$$S_g = \frac{2}{g^2} \sum_n \sum_{\mu \neq \nu} \text{Re tr}[U_{\mu\nu}(n)] \quad (1.10)$$

where we have replaced continuous integration with summation over all points.

### 1.3.2 Discretizing the fermion action

Since the fermion action consists of a covariant derivative  $D$  and on the lattice the derivative is just the difference between two functions at points differing by the smallest possible distance, i.e.  $a$  divided by that distance, our naively discretized fermionic action for fields looks like this

$$M = a^4 \sum_{n,m \in \Lambda} \left( \sum_{\mu=1}^4 \frac{U_{\mu}(n) \delta_{n+\hat{\mu},m} - U_{-\mu}(n) \delta_{n-\hat{\mu},m}}{2a} + \delta_{n,m} \right) \quad (1.11)$$

where  $M$  is the argument of  $\det M$ , i.e. the form that is squeezed between the fermionic fields  $\bar{\psi}(n)$  and  $\psi(m)$ . This naive discretization can lead to a problem called Fermion doubling problem that defines sixteen identical fermion states with different tastes instead of one. There are many modifications to the action to deal with said problem such as Wilson action, Kogut-Susskind action but that is beyond the scope of this report.

### 1.3.3 Temperature on the Lattice

As is done in the continuum, while defining the Euclidean path integral at a finite temperature actually equate it with the grand canonical partition function. The temperature

$$T = \frac{1}{t} = \frac{1}{aN_t} \quad (1.12)$$

This can be intuitively thought of in the following way. The path integral is essentially a transition amplitude between states  $f$  and  $i$ . Since inverse temperature becomes time

$$Z = \langle f | e^{-S} | i \rangle = \langle f | e^{Ht} | i \rangle = \langle f | e^{H/T} | i \rangle = \text{tr}(e^{H/T}) \quad (1.13)$$

## 1.4 Chemical Potential on the Lattice

To implement the chemical potential on the lattice, a rather intuitive form of the action appears to be adding the  $\mu \bar{\psi}(x) \gamma_4 \psi(x)$  to the naive fermion action. As we shall see this ansatz is problematic. Of course we can manage the doubling problem by using Wilson fermions or Staggered fermions instead of the naive fermionic action but problem with the chemical potential term would still be there. To understand why, let us define the energy density

$$\epsilon = -\frac{1}{V} \frac{\partial \ln Z}{\partial \beta} \quad (1.14)$$

where  $V$  is the spatial volume  $= (aN)^3$  for a lattice with space discretized into  $N$  parts of spacing  $a$  in each space direction and  $Z$  is the partition function  $= \int [DU] e^{-S_G} \det D$ , where  $S_G$  is the gauge action,  $[DU]$  is the Haar measure of gauge configurations, and  $D$  is the fermionic part of the action defined by

$$D(n|m) = \sum_{j=1}^3 \gamma_j \frac{\delta_{n+\hat{j},m} - \delta_{n-\hat{j},m}}{2a} + \gamma_4 \frac{\delta_{n+\hat{4},m} - \delta_{n-\hat{4},m}}{2a} + m\delta_{nm} + \mu\gamma_4\delta_{nm} \quad (1.15)$$

Consider the time direction to be divided into  $N_t$  parts of spacing  $a$ , we have  $\beta = aN_t$  and can write the energy density as

$$\epsilon = -\frac{1}{(aN)^3 N_t} \frac{\partial \ln[\det D]}{\partial a} \quad (1.16)$$

To see where the problem lies let us go to the momentum space using Fourier transform

$$D(p|q) = \frac{1}{\Lambda} \sum_{n,m \in \Lambda} e^{-ipn} D(n|m) e^{iqm} = \delta(p-q) \frac{1}{a} \left( i \sum_{j=1}^3 \gamma_j \sin(p_j a) + i\gamma_4 \sin(p_4 a) + m\delta_{nm} + \mu\gamma_4\delta_{nm} \right) \quad (1.17)$$

Using

$$\ln(\det D) = \ln\left(\prod_p \det D(p)\right) = \sum_p \text{tr}[\ln(D(p))] \quad (1.18)$$

we can rewrite the energy density as [2]

$$\epsilon = -\frac{4N_T N^3}{a} + \sum_p \text{tr}[(aD(q))^{-1} \left( \frac{i}{a} \sum_{j=1}^3 \gamma_j \sin(p_j a) + m \right)] \quad (1.19)$$

$$-\frac{4N_T N^3}{a} + \sum_p \frac{\sum_{j=1}^3 \sin^2(p_j a) + (am)^2}{\sum_{j=1}^3 \sin^2(p_j a) + (am)^2 + (\sin(ap_4) - iam)^2} \quad (1.20)$$

In the continuum limit, the leading term maybe extracted in  $p_4$  plane, which for  $p_4 \rightarrow 0$  limit goes as  $(\frac{\mu}{a})^2$ . Clearly the energy density is divergent in the continuum limit  $a \rightarrow 0$ .

We therefore need a different approach to defining the chemical potential term on the lattice. Since the  $\bar{\psi}\gamma_4\psi$  is a Noether current, we can take into account the contributions of the nearest neighbouring terms and therefore use a term of the form [2]

$$\frac{1}{2a} \sum (f(a\mu)(1 - \gamma_4)U_4(n)\delta_{n+\hat{4},m} + f(a\mu)(1 + \gamma_4)U_4(n - \hat{4})\delta_{n-\hat{4},m}).$$

To determine the form  $f(a\mu)$ , we perform a series expansion in  $a\mu$ , i.e. we take  $f(a\mu) = c_0 + c_1(a\mu) + O((a\mu)^2)$ . Now we know that  $f(0) = 1$  for  $\mu = 0$  to recover the original action, so that  $c_0 = 1$ . By the time reflection symmetry we have

$$f(a, \mu) = \frac{1}{f(-a\mu)} \quad (1.21)$$

Then the simplest form of the function we can have is the exponential form, i.e.

$$f(a, \mu) = e^{a\mu} \quad (1.22)$$

On the lattice, we can implement an action having  $e^{a\mu}$  in the lattice using the staggered fermion, a.k.a Kogut-Susskind Fermion.

From now on we will use  $M$  as the staggered fermionic action, instead of naive action  $D$  used

earlier.  $M$  is defined as  $M = \bar{\psi} M_{nm} \psi$  where [3]

$$M_{nm} = m\delta_{nm} + \sum_{\nu} \frac{\eta_{\nu}(n)}{2a} [e^{\delta_{\nu,4}a\mu} U_{n+\hat{\nu}} \delta_{n+\hat{\nu}m} - e^{\delta_{-\nu,4}a\mu} U_{n-\hat{\nu}}^{\dagger} \delta_{n-\hat{\nu}m}] \quad (1.23)$$

Here  $\eta_{\nu}(x)$  is the Kawamoto-Smit phase given by  $n_i (-1)^{\sum_{j<i} n_j}$ . We'll be using the notation  $Z = \int [DU] e^{-S_G} (det M)^{N_f}$  from now on.  $N_f$  is the number of flavors.

We can see that the only part of the action containing the chemical potential is the temporal part which we can write as

$$\frac{(-1)^{n_1+n_2+n_3}}{2a} [e^{a\mu} U_{n+\hat{4}} \delta_{n+\hat{4}m} - e^{a\mu} U_{n-\hat{4}}^{\dagger} \delta_{n-\hat{4}m}] \quad (1.24)$$

One ponders over the question of what  $e^{a\mu}$  could signify in a lattice. Consider a loop of over link variables. Diagrammatically one can visualize this in Fig.1.1. When the term  $\bar{\psi} M_{xy} \psi$  is integrated out in the Lagrangian, physically it can be interpreted as a quark being created at space-time point  $x$  and annihilated at  $y$ . In our action, for the chemical potential term the quark moves only in the imaginary time direction, hopping from site to site and each time it moves across one lattice spacing  $a$ , it gains a factor of  $e^{a\mu}$  moving in the forward direction or a factor of  $e^{-a\mu}$  in the backward direction. We can think of it as the link variables having a factor of  $e^{a\mu}$  associated with them, or rather an  $i\mu$  being added to the fourth component  $A_4$  of the gauge potential.

As shown in Fig. 1, if we loop around only space directions, there are an equal number of upward and downward links so all the forward  $e^{a\mu}$  and backward  $e^{-a\mu}$  factors cancel out. But in part C, as there are only upward links in the time direction,  $e^{a\mu}$   $N_t$  times. The factor

$$(e^{a\mu})^{N_t} = e^{\beta\mu} = e^{\mu/T} \quad (1.25)$$

is known as the fugacity.

## 1.5 Sign Problem

In the lattice, we calculate several observables from the path integral, some of which are

- Pressure

$$P = \frac{T}{V} \ln Z(\mu, T) \quad (1.26)$$

- Quark number density

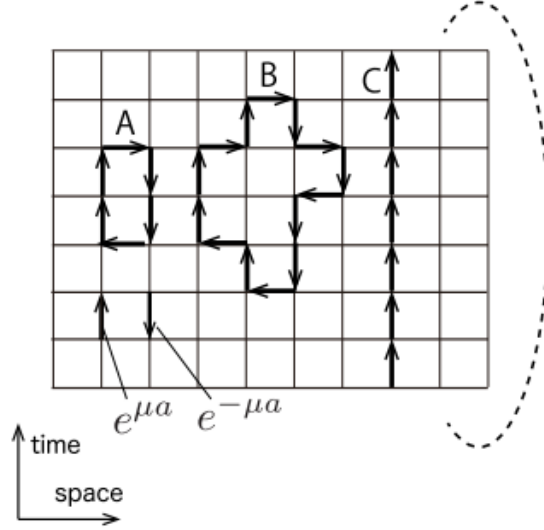
$$n_q = \frac{1}{V} \frac{\partial \ln Z}{\partial (\mu/T)} = \frac{1}{V} \langle N_f \text{tr}[M^{-1} M'] \rangle \quad (1.27)$$

- Quark number susceptibility

$$\chi_q = \frac{\partial n_q}{\partial \mu} = \frac{1}{VT} \left( \frac{\partial}{\partial (\mu/T)} \right)^2 \ln Z \quad (1.28)$$

To make the RHS dimensionless we can divide both sides by  $T^2$  to get

$$\frac{\chi_q}{T^2} = \left( \frac{N_t}{N_s} \right)^3 [-N_f \langle \text{tr}[M^{-1} M' M^{-1} M'] \rangle + N_f \langle \text{tr}[M^{-1} M''] \rangle + N_f^2 \langle \text{tr}[M^{-1} M']^2 \rangle] \quad (1.29)$$



**Fig. 1.3:** (A) and (B) show loops in the space directions. Even though they have different configurations, but after returning to the same point, the forward and backward  $e^{i\mu a}$  factors cancel out due to an equal number of upward and downward links. (C) shows a loop in the temporal direction. As the links are all upwards, only the forward  $e^{i\mu a}$  factors remain

where  $M'$  and  $M''$  are first and second derivatives of  $M$  respectively w.r.t  $\mu/T$ .

To calculate the path integral we perform using Monte Carlo importance sampling. Basically we select points for integration are not chosen at random but rather there is a bias towards sampling those points which contribute more to the integral, i.e. while integrating  $f(x)$  over  $x$ , we prefer those  $x$  for which  $f(x)$  is larger.

For a given quantity and a configuration of sampled  $K$  points  $\{x_i\}$  in phase space, the expectation value of that quantity is:

$$\langle O \rangle = \frac{1}{n} \sum_{i=1}^K O(x_i) \quad (1.30)$$

In Lattice QCD, our integration variables are the gauge links on which our observable will depend and we integrate over different gauge configurations. Several Markov Chain Monte algorithms exist to select these configurations and perform integrations over them such as the Metropolis algorithm, the Hybrid Monte Carlo algorithm, etc. All of these rely on moving from one gauge configuration to the next by changing one gauge link at a time.

A key feature of the metropolis algorithm is that given two configurations A and B, the likelihood of moving from one configuration to the other depends upon  $e^{-\Delta S}$  where  $\Delta S = S(A) - S(B)$  is the difference between their full actions (gauge and fermion part).

Configurations with smaller actions are more likely to be targeted. But all this works only because the action is real and positive for  $\mu=0$ .

If  $\mu \neq 0$ , then our action has a non-zero imaginary part and hence can become complex (A1). In that case importance sampling becomes impossible. If the full action  $S = S_R + iS_I$ , then there is no way to tell which action is smaller for which configuration. If say  $S_I = \pi$ ,  $e^{-S(A)} = -e^{-S(B)}$ , the configurations cancel each other. At the same time the configurations which with small  $e^{-S}$  which would have contributed less to the partition function for real action can no longer be ignored and have to be taken into consideration due to the cancellation of configuration with bigger absolute value of  $e^{-S(A)}$ . This is known as the sign problem. Until we can devise algorithms to work properly with complex actions, we use several already

existing methods to circumvent the sign problem. Some of these include reweighting, imaginary chemical potential and Taylor expansion, the last of which we will study in the next section.

# Chapter 2

## Taylor Expansion

For a function  $f(x)$ , we define its Taylor series at a point  $x_0$  as

$$f(x) = f(x_0) + f_1(x_0)(x - x_0) + f_2(x_0)(x - x_0)^2 + \sum_{n=0}^{\infty} f_n(x_0)(x - x_0)^n \quad (2.1)$$

where  $f_n$  is the  $n$ th derivative of the function  $f$ . Say we wanted to calculate a quantity which just happens to be function of the partition function which in turn is a function of the chemical potential. If we can Taylor expand the observable around zero chemical potential, removing all  $\mu$  dependence from the action, we can conveniently avoid the sign problem. For a given thermodynamic observable  $O$ , we can expand it in terms of the ratio of chemical potential to temperature ( $\mu/T$ ) in the form of a Taylor series.

$$O(T, \mu) = \sum_n c_n(T) \left(\frac{\mu}{T}\right)^n \quad (2.2)$$

where the coefficients

$$c_n = \frac{1}{n!} \left( \frac{\partial^n O}{\partial \left(\frac{\mu}{T}\right)^n} \right) \Big|_{\mu=0} \quad (2.3)$$

As the expansion coefficients are defined at  $\mu = 0$ , in accordance with a typical Taylor expansion, the action remains real and hence they can be computationally obtained from importance sampling.

### 2.1 Pressure

For the thermodynamic observable pressure, to make the 1.14 dimensionless, we divide both sides by  $T^4$  and this gives us

$$\frac{P(\mu, T)}{T^4} = \left(\frac{N_t}{N}\right)^3 \ln Z = \frac{P(0, T)}{T^4} + \sum_n c_n(T) \left(\frac{\mu}{T}\right)^n \quad (2.4)$$

where obviously

$$c_n = \frac{1}{n!} \frac{\partial^n P}{\partial \left(\frac{\mu}{T}\right)^n} \Big|_{\mu=0} \quad (2.5)$$



Due to CP symmetry, the only terms which are non-zero are the ones having even  $n$ . For odd  $n$ , the coefficient  $c_n$  is purely imaginary and when acted upon by the charge conjugation operator must be equal to its complex conjugate, i.e. it must be equal to its negative and so it must be zero.

We can further express other thermodynamic quantities in a similar fashion

Quark number density

$$\frac{n_q}{T^3} = \sum_{n=2,4,\dots}^{\infty} n c_n \left(\frac{\mu}{T}\right)^{n-1} \quad (2.6)$$

and Quark number Susceptibility

$$\frac{\chi_q}{T^2} = \sum_{n=2,4,\dots}^{\infty} n(n-1) c_n \left(\frac{\mu}{T}\right)^{n-2} \quad (2.7)$$

Currently people studying Taylor expansion work on truncating up to a finite number of orders in  $\frac{\mu}{T}$  and analyze the results to obtain whatever useful physical interpretations they can get. In the next section we shall see how the Taylor expansion can be used to obtain results in extensively researched subjects such as the QCD phase diagram.

## 2.2 Radius of Convergence and Critical Endpoint

### 2.2.1 Radius of Convergence

We can compare the Taylor expansion of the pressure and the quark number susceptibility (QNS) at non-zero chemical potential. If a critical endpoint exists in the QCD phase diagram, then we expect that the QNS diverges at that point while the pressure is finite.

To check for the divergence we define the radius of convergence as  $r$  [5]

$$r = \lim_{n \rightarrow \infty} r_{2n} = \lim_{n \rightarrow \infty} \left| \frac{c_{2n}}{c_{2n+1}} \right|^{1/2} \quad (2.8)$$

The location of the singularity in the complex  $\mu$ -plane corresponds to the breakdown of the Taylor expansion. Should the singularity lie on the real axis (i.e. for real  $\mu$ ) then the radius of convergence corresponds to the location of the critical endpoint in the  $(T, \mu)$  plane.

Since we only have finite number of terms, we cannot take the  $n \rightarrow \infty$  limit, although it might be possible to extrapolate to the  $\infty$  limit. Else we can assume that the radius of convergence  $r$  has been reached when certain estimators  $r_{2n}$  don't change much (within some small but acceptable error) with increasing  $n$ . For QNS  $\chi_q$

$$r_{2n}^{\chi} = \left| \frac{c_{2n}^{\chi}}{c_{2n+2}^{\chi}} \right|^{1/2} = \sqrt{\frac{(2n+2)(2n+1)}{(2n+3)(2n+4)}} r_{2n+2} \quad (2.9)$$

As we can see the estimator for QNS, i.e. the factor before  $r_{2n+2}$  is smaller than that for  $P$ . For  $n \rightarrow \infty$ , both  $r_{2n}$  for pressure and  $r_{2n}^{\chi}$  for QNS will converge to the same limit  $r$  but at a finite  $n$ , they will differ and will approach the limit  $r$  at different rates.

### 2.2.2 Critical endpoint

In the QCD phase diagram, the Critical Endpoint is defined as the point in the  $T$ - $\mu$  plane where the transition from the Hadronic phase to the Quark Gluon Plasma stops being a crossover and starts being a phase transition.

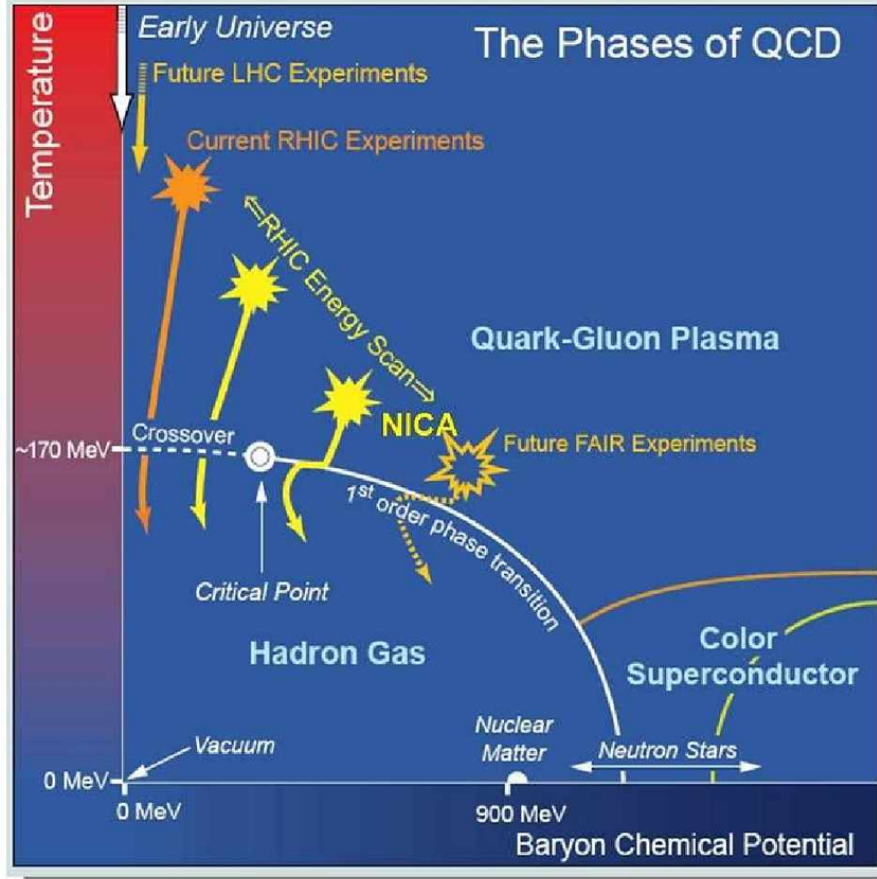


Fig. 2.1: The Critical Endpoint in the  $T$ - $\mu$  plane

If the Critical endpoint (CEP) exists there will be divergences in thermodynamic observables with a power law behavior. Therefore to locate the critical endpoint, we must find out where the Taylor expansion has a singularity on the real  $\mu$ -axis. This can happen only if, for some real  $\mu$ , there is  $n_s$  such that for all  $n > n_s$  the expansion coefficients are positive so the series must diverge.

In phase transition, near the  $\mu \rightarrow 0$  limit, due to the survival of even terms we see a quadratic dependence on  $\mu$  as compared to a linear dependence [5] on the reduced temperature  $(T-T_c)$ ,  $T_c$  here being the critical temperature.

To have an idea of the form of  $c_{2n+2}$  we look to the temperature dependence of the preceding term  $c_{2n}$ . If we can find that for some temperature the  $c_{2n}$  term has its first minimum, then  $c_{2n+2}$  will be positive. Estimating such a temperature for an order  $n$ , the higher possible the better, for which we have such a first minimum, such that all the subsequent terms will be positive will give us the critical temperature  $T_c$ . From this we can estimate the critical chemical potential  $\mu_c$  from the radius of convergence  $r(T_c)$  as a function of  $T_c$ .

It should be noted that this is a rather simplistic view of obtaining the CEP or rather the pseudo-critical endpoint since the lattice only has a finite volume.

# Chapter 3

## Exponential Resummation

As it turns out the Taylor series expansion has a number of inconveniences. First of all the series has to be truncated at a finite order as it becomes more and more computationally expensive to calculate higher order coefficients. One could ask the question if it is possible to capture the behaviour of the series after calculating upto a certain order. Unfortunately the series has a very slow rate of convergence due to which the successive coefficients are not insignificant compared to the previous coefficients which makes it impossible to ignore higher order terms. Therefore a truncated version of the series cannot be considered as a useful approximation.

We look to new analytical methods to evaluate the Taylor series upto all orders in chemical potential  $\mu$  using the computationally calculated quantities of upto a finite order  $N$ .

Resummation is a technique by which we can capture the contribution (fully or partially) upto all orders. There are many resummation methods such as Pade approximation. Here we use the exponential resummation method.

First we give a brief review of the Taylor expansion formalism. The excess pressure can be given in terms of chemical potential  $\mu$  and

$$\frac{\Delta P_N}{T^4} = \sum_{n=1}^N \frac{c_n}{n!} \left(\frac{\mu}{T}\right)^n \quad (3.1)$$

Where

$$c_n(T) = \frac{1}{VT^3} \sum_{n=1}^N \frac{\partial^n \ln Z}{\partial (\mu/T)^n} \Big|_{\mu=0} \quad (3.2)$$

The partition function

$$Z(\mu T) = \int DU e^{-S_G(U,T)} \det M(\mu, T, U) \quad (3.3)$$

where  $S_G$  is the purely gauge dependent part of the action and  $\det M$  is the fermionic part of the action, i.e. the only part which depends upon the chemical potential.

We define:

$$\hat{\mu} = \left(\frac{\mu}{T}\right) \quad (3.4)$$

Define  $D_n$  as the  $n$ th derivative of the partition function  $Z$  with respect to  $\hat{\mu}$  [A1]

$$D_n = \frac{\partial^n Z}{\partial \hat{\mu}^n} \quad (3.5)$$

Define  $A_n$  as

$$A_n = \langle e^{-D_0} \frac{\partial^n e^{D_0}}{\partial \hat{\mu}^n} \rangle \quad (3.6)$$

We shall use this to generate higher order derivatives using the rule

$$\frac{\delta^{n+1} \ln Z}{\partial \hat{\mu}^{n+1}} = \frac{\partial^n A_1}{\delta \hat{\mu}^n} \quad (3.7)$$

Then the first few terms would be

$$A_1 = \langle D_1 \rangle \quad (3.8)$$

$$A_2 = \langle D_2 \rangle + \langle D_1^2 \rangle \quad (3.9)$$

$$A_3 = \langle D_3 \rangle + 3 \langle D_1 D_2 \rangle + \langle D_1^3 \rangle \quad (3.10)$$

$$A_4 = \langle D_4 \rangle + 4 \langle D_3 D_1 \rangle + 3 \langle D_2^2 \rangle + 6 \langle D_2 D_1^2 \rangle + \langle D_1^4 \rangle \quad (3.11)$$

And finally using the the  $A_n$ s we can define the coefficients as

$$c_1 = \frac{\partial \ln Z}{\partial \mu} = A_1 \quad (3.12)$$

$$c_2 = \frac{\partial^2 \ln Z}{\partial \mu^2} = A_2 - A_1^2 \quad (3.13)$$

$$c_3 = \frac{\partial^3 \ln Z}{\partial \mu^3} = A_3 - 3A_2 A_1 + 2A_1^3 \quad (3.14)$$

$$c_4 = \frac{\partial^4 \ln Z}{\partial \mu^4} = A_4 - 4A_3 A_1 - 3A_2^2 + 12A_2 A_1^2 - 6A_1^4 \quad (3.15)$$

and so on.

To understand our exponential scheme let us draw the  $A_n$ s in a schematic form

In Fig. 1.1, we use mnemonics to present the derivatives  $D_n$ [9]. If we look at the terms along the solid lines and imagine them extending upto all orders in  $\hat{\mu}$  then we can see that adding them after multiplying with appropriate powers of  $\frac{\mu}{T}$  and dividing by the proper factorials we shall get a series of the form

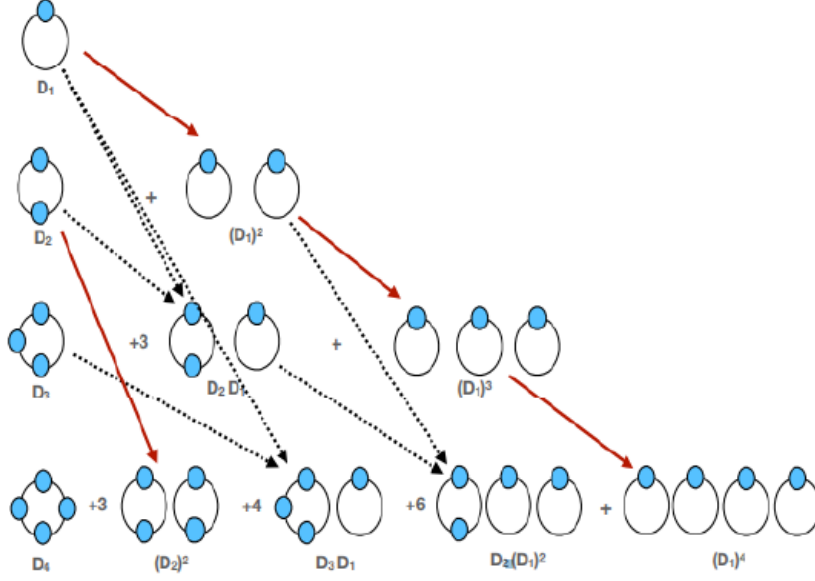
$$1 + D_1 \left( \frac{\mu}{T} \right) + \frac{D_1^2}{2!} \left( \frac{\mu}{T} \right)^2 + \frac{D_1^3}{3!} \left( \frac{\mu}{T} \right)^3 + \dots \quad (3.16)$$

which is indeed the exponential series expansion of  $D_1(\frac{\mu}{T})$ . So going along the first solid line can give us  $\exp(D_1(\frac{\mu}{T}))$ . In fact we can do the same for  $D_2(\frac{\mu}{T})^2$  and  $D_n(\frac{\mu}{T})^n$  can give us their respective exponentials.

Next we move on to the dashed lines which contain mixed terms of the form  $\frac{D_i D_j}{i! j!} (\frac{\mu}{T})^{i+j}$ . If we carefully analyze the first dashed line containing  $D_1$  and  $D_2$  and add all the terms along the  $D_1$  and  $D_2$  solid lines (with their respective multiplicative coefficients as pointed out earlier) we shall get a series of the form [4]

$$1 + D_1 \left( \frac{\mu}{T} \right) + D_2 \left( \frac{\mu}{T} \right)^2 + \frac{1}{2!} (D_1^2 \left( \frac{\mu}{T} \right)^2 + D_2^2 \left( \frac{\mu}{T} \right)^4 + 2D_1 D_2 \left( \frac{\mu}{T} \right)^3) + \dots \quad (3.17)$$

$$= 1 + \left( D_1 \left( \frac{\mu}{T} \right) + D_2 \left( \frac{\mu}{T} \right)^2 \right) + \frac{1}{2!} \left( D_1 \left( \frac{\mu}{T} \right)^2 + \dots D_2 \left( \frac{\mu}{T} \right)^2 \right) \quad (3.18)$$



**Fig. 3.1:** The  $D_n$  in graphical representation. Each term along a solid line corresponds to the pure exponential of a single derivative  $D_i$  whereas each dashed line corresponds to mixed exponential of two or more derivatives.

$$= \exp(D_1(\frac{\mu}{T}) + D_2(\frac{\mu}{T})^2) \quad (3.19)$$

So basically adding all the terms along both kinds of lines (dashed and solid) for a given  $D_i$  and  $D_j$  should give us the exponential of  $D_i(\frac{\mu}{T})^j + D_j(\frac{\mu}{T})^j$ .

Say instead of just  $D_1$  and  $D_2$  we repeat this scheme for all the solid and dashed lines from  $D_1$  upto  $D_N$ . Then we should get something of the form

$$1 + \left( \sum_{n=1}^N D_n \left( \frac{\mu}{T} \right)^n \right) + \frac{1}{2!} \left( \sum_{n=1}^N D_n \left( \frac{\mu}{T} \right)^n \right)^2 + \dots = \exp \left( \sum_{n=1}^N D_n \left( \frac{\mu}{T} \right)^n \right) \quad (3.20)$$

This puts us at one advantage. If we have exponential form, then expanding it will give us contributions from all orders in  $(\frac{\mu}{T})$  even though we only need calculate derivatives  $D_n$  upto some finite order  $N$ . But doing this is possible if we exactly equate the coefficients  $c_n$  to  $A_n$  even though as we have seen in Eqns 1.13 to 1.15 that there are more terms of  $A_m$  (m≠n) involved to calculate  $c_n$ . So we'll have to ignore those terms to get the exponential form. This implies that we don't get the full contributions from the coefficients. So this is the trade off we have to deal with. In order to get all orders of  $\frac{\mu}{T}$  we must take partial contributions of the derivatives of partition function in each order.

So we can write the partition function as

$$Z_N^R = 1 + c_1 \left( \frac{\mu}{T} \right) + c_2 \left( \frac{\mu}{T} \right)^2 + \dots = 1 + A_1 \left( \frac{\mu}{T} \right) + A_2 \left( \frac{\mu}{T} \right)^2 + \dots = \langle \exp \left( \sum_{n=1}^N D_n \left( \frac{\mu}{T} \right)^n \right) \rangle \quad (3.21)$$

from which we can write the resummed pressure as [4]

$$\frac{\Delta P_N}{T^4} = \frac{1}{VT^3} \ln \langle \exp \left( \sum_{n=1}^N D_n \left( \frac{\mu}{T} \right)^n \right) \rangle \quad (3.22)$$

# Chapter 4

## Phase Angle

One of the most important fields of study in which finite density QCD has an application is the QCD phase diagram. During a phase transition the free energy diverges and the partition function becomes zero. As a result the sign problem becomes very severe. So how do we measure this severity.

Here is where exponential resummation comes in handy. We define an entity known as the phase angle which can be used to capture the aforementioned sign problem. We know that the partition function is real as it must preserve CP symmetry. Then [4],[8]

$$Z_N^R = \langle \exp(\sum_{n=1}^N D_n (\frac{\mu}{T})^n) \rangle \quad (4.1)$$

As the argument inside the bracket can be complex, we may write it as [6]

$$\exp(\sum_{n=1}^N D_n (\frac{\mu}{T})^n) = R e^{i\theta} \quad (4.2)$$

where R is real.  $\theta$  is the phase angle. We can write

$$\theta = \sum_{n=1}^{N/2} \text{Im}(D_{2n-1}) (\frac{\mu}{T})^{2n-1} \quad (4.3)$$

since the even derivatives are purely real and odd derivatives are purely imaginary.

Now coming to the QCD phase diagram. For a system with m energy states the partition function is of the form

$$\sum_{n=1}^m e^{-\beta E_n} \quad (4.4)$$

In some systems such as a simple harmonic oscillator the energies are all linear functions of  $\frac{\hbar\omega}{2}$  so the partition function becomes a polynomial of degree m. But one cannot analytically find out the roots of such a polynomial for  $m \geq 4$ . For other systems with different kinds of energy states, the it becomes even more complicated to locate the zeros of the partition function. Therefore we must numerically locate the roots of the partition function. One can use root finding computational methods such as Newton-Raphson. But given our scheme this is where the phase angle becomes useful. Since the partition function is only the real part of

$\exp(\sum_{n=1}^N D_n(\frac{\mu}{T})^n)$  and

$$Re(Re^{i\theta}) = R \cos \theta \quad (4.5)$$

then

$$Z = \langle R \cos \theta \rangle \quad (4.6)$$

From this we can conclude that the region when  $\langle \cos \theta \rangle \approx 0$  gives the region where the partition function is zero. The phase angle can only be defined for the exponential resummation scheme due to its exponential form which can be equated with a real part times a complex phase. No such analog exists for the original Taylor series as we must truncate the series at some finite order of  $\frac{\mu}{T}$ .

To understand qualitatively why this is indicative of the sign problem we must first remember that the sign problem in QCD arises due to the fermion determinant becoming complex when we add a chemical potential term to it, which in turn makes it difficult to jump from one gauge ensemble to the next based on the metropolis accept reject algorithm.

As the fermionic action acquires a complex phase dependent on  $\mu$  (at a single gauge configuration), the increasing sign problem causes it to oscillate more and more, making the action more unpredictable. There the phase angle  $\theta$  averaged over all gauge configurations is an indicator of the oscillations of  $\det M$ .

When the partition function becomes 0, calculations breakdown and thus the gauge-ensemble averaged phase angle can be used as an estimate of the commencement of breakdown.

# Chapter 5

## Biasedness, Unbiasedness and Cumulant expansion

### 5.1 Biasedness and Unbiasedness

When the  $\mu$ -derivatives of  $Z$ ,  $D_n$  were obtained after stochastic averaging of the random volume estimates, to find the coefficients each of them is raised to some integral positive power, that introduces some biasedness into the estimate. Let  $\bar{D}_n^m$  the mth power of the  $D_n$  averaged over  $R$  gauge ensembles. Then it can be expanded as [7]

$$\bar{D}_n^m = \left[ \frac{1}{R} \sum_{n=1}^R D_n \right]^m = \left( \frac{1}{R} \right)^m \sum_{C(r_1 \neq r_2 \neq \dots \dots \neq r_m)}^R \dots \sum_{\dots \neq r_m}^R D_n^{r_1} \dots D_n^{r_m} + \left( \frac{1}{R} \right)^m \sum_{r_1 \neq r_2 \neq \dots \dots \neq r_m}^R \sum_{\dots \neq r_m}^R D_n^{r_1} \dots D_n^{r_m} \quad (5.1)$$

Here  $C(r_1 \neq r_2 \neq \dots r_m)$  indicates the complement of the condition  $r_1 \neq r_2 \neq \dots r_m$ , i.e. atleast one of the powers of  $D_n$  is repeated more than once while on the other hand  $r_1 \neq r_2 \neq \dots r_m$  means that every integral power of  $D_n$  appears atmost once in a given term of the sum. Before commenting on the nature of the terms on LHS pertaining to these respective conditions one must first understand that biasedness. For  $M$  independent random estimates  $K_1 \dots K_M$ , the unbiased estimate  $K^n$  of at an integral power  $n$  is given by

$$UE[K^n] = \sum_{i_1 \neq i_2 \neq \dots i_n} \frac{K_{i_1} \dots K_{i_n}}{N(N-1) \dots (N-n+1)} \quad (5.2)$$

So that no single  $K_{i_r}$  is repeated more than once in a term meaning there is no bias towards any particular random volume estimate  $K_{i_r}$ . But when the same estimate appears more than once in a term of the sum, then it contributes more than all those terms which appear atmost once which means there is a bias introduced towards that estimate.

This would imply that the first term in the far LHS of 3.1 is biased and the second term is unbiased. Consequently stochastic bias is introduced into the exponential form .1

$\exp \left( \sum_{n=1}^N D_n \left( \frac{\mu}{T} \right)^n \right)$ . It becomes necessary to eliminate and at least minimize this bias because if we don't do that then it could cause problems in calculations at large values of  $\mu$  where even a small bias at small  $\mu$  may become amplified.

One way to minimize the bias in  $(D_n)^m$  itself is to take a large number of Random value sources such that  $m \leq N_R$  therefore not single  $r_i$  in 3.1 has to be repeated and there won't be any bias in favour of a specific random source.

In the original Taylor expansion since we have efficient formulas to evaluate the unbiased



product of  $n$  operators in order  $O(N)$  instead of  $O(N^n)$  time. That makes it easier to deal with stochastic bias in the Taylor series. However, as mentioned before, the Taylor series itself has drawbacks. To go beyond it one might use the cumulant expansion formula which corrects for bias but we still have to truncate at a finite order. Also there is no well defined phase factor for the cumulant expansion.

Currently there is no known way to getting a fully unbiased estimate of an exponential series (because it is transcendental). Therefore we try a different approach: if we can replicate the Taylor series or the cumulant series using our exponential resummation as much as possible while still maintaining the all orders in  $\frac{\mu}{T}$  resummation we can get a more unbiased estimate. Eventhough it is not a full solution to the problem it can yield results depending on the value of  $\mu$  and the maximum order of  $D_n$  calculated.

In the upcoming chapters we explore 2 new formalisms which remove bias from exponential resummation upto some extent. For the second formalism we need to know about the cumulant expansion.

## 5.2 Cumulant Expansion

The cumulant expansion formula [6]

$$\ln \langle e^{tX} \rangle = \sum_{j=1}^{\infty} \frac{t^j}{j!} C_j(X) \quad (5.3)$$

where

$$C_1(X) = \langle X \rangle \quad (5.4)$$

$$C_2(X) = \langle X \rangle^2 - \langle X^2 \rangle \quad (5.5)$$

$$C_3(X) = \langle X^3 \rangle - 3 \langle X^2 \rangle \langle X \rangle + 2 \langle X \rangle^3 \quad (5.6)$$

$$C_4(X) = \langle X^4 \rangle - 4 \langle X^3 \rangle \langle X \rangle - 3 \langle X^2 \rangle^2 + 12 \langle X^2 \rangle \langle X \rangle^2 - 6 \langle X \rangle^4 \quad (5.7)$$

For our case  $t=1$ . and  $X$  is given by

$$X_N = \sum_{n=1}^N \frac{D_n}{n!} \left( \frac{\mu}{T} \right)^n \quad (5.8)$$

This may look similar to the argument of the resummed exponential but notice there is extra  $n!$  dividing each order. The cumulant expanded pressure can then be given by

$$\frac{\Delta P_N^C}{T^4} = \sum_{j=1}^{M>N} \frac{1}{j!} C_j(X_N) \quad (5.9)$$

By doing so the Taylor and Cumulant expansion are identical upto order  $N$  in  $\frac{\mu}{T}$  after which the Cumulant expansion manages to capture the contribution of some higher order terms which the Taylor expansion does not. However the Cumulant expansion is unbiased unlike the exponential resummation, due to having a finite number of terms in the entire expansion, each of which is a finite product of powers of different  $D_n$ s. But alas this too cannot be used for applications in determining the sign problem due to unavailability of higher orders of  $\mu$  and lack of well defined phase factor.

# Chapter 6

## Unbiased estimates

Finally we arrive at defining the two formalisms of unbiased exponential resummation. The first one, known as the chemical potential basis formalism is an attempt to make the resummed exponential agree with the Taylor series upto some finite order  $N$  followed by partial contributions from coefficients of all higher orders. The second one, the Cumulant expansion basis attempts to do the same with resummed exponential except this time its to replicate the Cumulant expansion series upto some order followed by contributions from higher order.

### 6.1 Chemical potential Basis

In the chemical potential basis, we redesign the argument of the exponential. Define [7],[6]

$$W_N(\mu) = \sum_{n=1}^N \left(\frac{\mu}{T}\right)^n \frac{C_n}{n!} \quad (6.1)$$

Where the  $C_n$  upto  $n=4$  can be given by

$$C_1(X) = \bar{D}_1 \quad (6.2)$$

$$C_2(X) = \bar{D}_2 + \bar{D}_1^2 - \bar{D}_1^2 \quad (6.3)$$

$$C_3(X) = \bar{D}_3 + 3(\bar{D}_2\bar{D}_1 - \bar{D}_2\bar{D}_1) + (\bar{D}_1^3 - 3\bar{D}_1^2\bar{D}_2 + 2\bar{D}_1^3) \quad (6.4)$$

$$C_4(X) = \bar{D}_4 + 2(\bar{D}_2^2 - \bar{D}_2^2) + 4(\bar{D}_3\bar{D}_1 - \bar{D}_3\bar{D}_1) + 6(\bar{D}_2\bar{D}_1^2 - \bar{D}_2\bar{D}_1^2) - \quad (6.5)$$

$$12(\bar{D}_2\bar{D}_1\bar{D}_1 - \bar{D}_2\bar{D}_1^2) + (\bar{D}_1^4 - 4\bar{D}_3\bar{D}_1 + 12\bar{D}_2\bar{D}_1^2 - 6\bar{D}_1^4 - 33(\bar{D}_2^2)) \quad (6.6)$$

The we define the unbiased partition function in the chemical potential basis

$$Z_{cp}^N = \langle Re(\exp(W_N)) \rangle \quad (6.7)$$

and consequently the pressure in chemical potential basis can be given by

$$\frac{\Delta P_{cp}^N}{T^4} = \frac{1}{VT^3} \ln Z_{cp}^N = \frac{1}{VT^3} \ln \langle Re(\exp(W_N)) \rangle \quad (6.8)$$

We can demonstrate how the chemical potential basis is unbiased by using some finite number of  $C_n$ s. Since in Eqns 4.2 to 4.6 we have the first four of them, we shall use them only. Our

$W_4$  given by

$$W_4 = \bar{C}_1 \left( \frac{\mu}{T} \right) + \frac{\bar{C}_2}{2!} \left( \frac{\mu}{T} \right)^2 + \frac{\bar{C}_3}{3!} \left( \frac{\mu}{T} \right)^3 + \frac{\bar{C}_4}{4!} \left( \frac{\mu}{T} \right)^4 \quad (6.9)$$

If we find the exponential series of  $A_4$  we get

$$\exp(W_4) = 1 + W_4 + \frac{W_4^2}{2!} + \frac{W_4^3}{3!} + \frac{W_4^4}{4!} + O(W_4^5) \quad (6.10)$$

which when we expand using Eqn 4.9 and 4.2 to 4.6 gives us

$$\begin{aligned} \exp(W_4) = 1 + \bar{D}_1 \left( \frac{\mu}{T} \right) + \frac{\bar{D}_2 + \bar{D}_1^2}{2!} \left( \frac{\mu}{T} \right)^2 + \frac{\bar{D}_3 + 3\bar{D}_2\bar{D}_1 + \bar{D}_1^3}{3!} \left( \frac{\mu}{T} \right)^3 + \\ \frac{\bar{D}_4 + 3\bar{D}_2^2 + 4\bar{D}_3\bar{D}_1 + 6\bar{D}_2\bar{D}_1^2 + \bar{D}_1^4}{4!} \left( \frac{\mu}{T} \right)^4 + O\left(\left(\frac{\mu}{T}\right)^5\right) \end{aligned} \quad (6.11)$$

On examining closely the coefficients of each order of  $\frac{\mu}{T}$ , these sums are exactly the  $A_n$ s we had shown earlier from 1.8 to 1.11. That is

$$\exp(W_4) = 1 + \sum_{n=1}^4 \frac{A_n}{n!} \left( \frac{\mu}{T} \right)^n + O\left(\left(\frac{\mu}{T}\right)^5\right) \quad (6.12)$$

When we find the resummed pressure in this scheme using

$$\frac{\Delta P_{cp}}{T^4} = \frac{1}{VT^3} \ln \langle \text{Re}(e^{W_4}) \rangle \quad (6.13)$$

Using the expansion for natural log

$$\ln(1+x) = x - \frac{x^2}{2} + \dots \quad (6.14)$$

We get (Keeping in mind that the odd terms vanish as they are purely imaginary)

$$\frac{\Delta P_{cp}}{T^4} = \frac{1}{VT^3} \ln\left(1 + \frac{A_2}{2!} \left( \frac{\mu}{T} \right)^2 + \frac{(A_4 - 3A_2^2)}{4!} \left( \frac{\mu}{T} \right)^4 + O\left(\left(\frac{\mu}{T}\right)^6\right)\right) \quad (6.15)$$

As we can see in the  $\ln$  expansion the coefficients of  $\frac{\mu}{T}$  are exactly equal to the even coefficients  $c_2$  and  $c_4$  given Eqn. 1.13 and 1.15 provided that the odd  $A_n$ s vanish. Therefore they reproduce the Taylor series term by term upto order 4 and then add some contributions from each of the higher orders.

## 6.2 Cumulant Basis

Similar to how we reproduced the Taylor series upto an order from the resummed exponential using the chemical potential basis here we shall attempt to reproduce the Cumulant

expansion series. Here we shall again modify the exponent and define a variable  $X_N$  [7], [6]

$$X_N = \sum_{n=1}^N \frac{D_n}{n!} \left(\frac{\mu}{T}\right)^n \quad (6.16)$$

This looks just like the exponent of the original resummed exponential. However this time each  $D_n$  belongs to a single gauge ensemble. Now we know that the average of a function is more unbiased compared to the function of an average. If we think of  $X_N$  as a function of  $N$  then instead of taking a sum over gauge ensembles of different  $D_n$ s and then finding  $X_N$ , here we take  $X_N$  over a single gauge ensemble and then find an average  $\bar{X}_N$  over a number of gauge ensembles. The scheme is as follows. For an order  $M$ ,

$$Z_{cm}^M = \langle \text{Re}[\exp(\sum_{n=1}^M \frac{L_n(X_N)}{n!})] \rangle \quad (6.17)$$

where

$$L_1(X_N) = \bar{X}_N \quad (6.18)$$

$$L_2(X_N) = \bar{X}_N^2 - \bar{X}_N^2 \quad (6.19)$$

$$L_3(X_N) = \bar{X}_N^3 - 3(\bar{X}_N^2 \bar{X}_N) + 2\bar{X}_N^3 \quad (6.20)$$

$$L_4(X_N) = \bar{X}_N^4 - 4(\bar{X}_N^3 \bar{X}_N) + 12\bar{X}_N^2 (\bar{X}_N)^2 - 6(\bar{X}_N)^4 - 3(\bar{X}_N^2)^2 \quad (6.21)$$

Clearly this looks similar to form of Cumulant expansion we saw in Eqn 3.4 to 3.7. Following the procedure of expanding the exponential of  $\bar{X}_N$  as we had done for  $W_N$  in the last section, we can find out that the resummed pressure in Cumulant basis will indeed reproduce term by term upto order  $M$  the Cumulant series we had seen in 3.2 followed by additional contributions from all higher orders. The resummed pressure in cumulant basis can be written as

$$\frac{\Delta P_{cm}}{T^4} = \frac{1}{VT^3} \ln \langle \text{Re}[\exp(\sum_{n=1}^M \frac{L_n(X_N)}{n!})] \rangle \quad (6.22)$$

### 6.3 Unbiased phase angles

Since we redefined the argument of the exponential to make it more unbiased and obtained forms for partition function and pressure for the both schemes we shall do the same for the phase angle [7].

For the chemical potential basis we define

$$\theta_N^{cp}(\mu, T) = \text{Im}[\sum_{n=1}^N \frac{C_n}{n!} \left(\frac{\mu}{T}\right)] \quad (6.23)$$

And for the cumulant basis we define

$$\theta_{N,M}^{cm}(\mu, T) = \text{Im}[\sum_{n=1}^M \frac{L_n(X_N(\mu, T))}{n!}] \quad (6.24)$$

## 6.4 Comments and Comparative Analysis

Few things one must keep in mind about the Cumulant expansion [7]

- The random estimates all belong to a single gauge configuration rather than being averaged in the space of all gauge configurations.
- Instead of using  $\left(\sum_{n=1}^N \frac{\bar{D}_n}{n!} \left(\frac{\mu}{T}\right)^n\right)^p$  we use  $(\bar{X}_N)^p$ , where  $X_N^p = \left(\sum_{n=1}^N \frac{D_n}{n!} \left(\frac{\mu}{T}\right)^n\right)^p$ , which is the unbiased estimate of the pth power of  $\bar{X}_N$
- In the condition that the number of random estimate sources  $R \rightarrow \infty$  then the estimate itself becomes fully unbiased as no random source needs to be repeated in a given term to satisfy the condition that sum of the exponents of the products must equal the order of the term (i.e. at given order  $x$ ,  $r_1 + \dots + r_m = x$ ). Therefore there will not be bias in favor of an one particular random source.
- Also in the limit  $M \rightarrow \infty$ , the  $\sum_{m=1}^M \frac{L_m(X_N)}{m!}$  becomes identical to the cumulant expansion of  $\exp(\bar{X}_N)$ .

As was discussed earlier, the chemical potential basis reproduces the Taylor series upto some order  $N$  followed by contributions from each higher order which are not the exact form of the full Taylor series. The cumulant basis reproduces the cumulant expansion series upto some finite order  $N$  followed by contributions from higher order terms upto all orders.

As the cumulant expansion itself manages to include some terms beyond agreeing term by term with Taylor series upto some order, the cumulant basis therefore does a better job of capturing the larger spectrum of the infinite Taylor series than the chemical basis [6].

Say the argument of the exponential contains terms upto  $\left(\frac{\mu}{T}\right)^k$  in the chemical potential basis. But in the cumulant basis, due to terms of the form in the second and third terms of the expansion itself (in fact upto the  $k$ th term of the cumulant expansion), contributions from  $\left(\frac{\mu}{T}\right)^l$  ( $l \geq k$ ) are also included. The largest value of such  $l$  which can be obtained from the cumulant expansion and the difference between  $l$  and  $m$  becomes larger and larger with increasing number of coefficients calculated for the both the bases. So basically the higher the value of  $n$  for  $c_n$  one can go upto, the more the gap between the two bases increases in encapsulating the essence of higher order terms.

# Chapter 7

## Summary

In this report we have motivated the necessity of studying QCD at a finite density. We first defining our formal theory in continuum and transition to the Lattice. In doing so we encounter the sign problem, which we hinders us from calculating observables as long as there is finite chemical potential which makes the action complex. To bypass it we present the Taylor expansion of observables around zero chemical potential. Realizing the problems associated with the Taylor expansion such as calculation of higher order coefficients being too computationally expensive and a slow rate of convergence motivated us to find alternate schemes that can resum the Taylor series upto all orders.

We presented the exponential resummation scheme as an attempt at finding contributions of the Taylor expansion of the partition function upto all orders in chemical potential. We have discussed why it is biased and proposed resummation methods to remove biasedness to some extent. In the process we introduce two new resummation methods, the chemical potential basis which reproduces the original Taylor series exactly upto a certain order followed by contributions from higher orders and the cumulant basis which reproduces the cumulant expansion of the Taylor series upto some order followed by higher order terms. We also present analytical forms for the resummed partition function, pressure and phase angles respectively for each of the two methods and discuss at lengths the difference between them.

# Bibliography

- [1] P. Hasenfratz, F. Karsch. Chemical potential on the Lattice. *Ref.TH.3530-CERN* (February 1982)  
<https://www.sciencedirect.com/science/article/abs/pii/037026938391290X>
- [2] C. Gattringer, C. B. Lang. Quantum Chromodynamics on the Lattice.
- [3] Keitaro Nagata. Finite-density lattice QCD and sign problem: Current status and open problems. *Progress in Particle and Nuclear Physics 127 (2022) 103991*  
<https://www.sciencedirect.com/science/article/pii/S0146641022000497>
- [4] Prasad Hegde, Swagato Mukherjee, Sourav Mondal. Lattice QCD Equation of State for Nonvanishing Chemical Potential by Resumming Taylor Expansion (January 24, 2022) <https://arxiv.org/pdf/2106.03165.pdf>
- [5] F. Karsch, B.J. Schaefer, M. Wagner, J. Wambach. Towards finite density QCD with Taylor expansions. (9 March, 2011) <https://arxiv.org/pdf/1009.5211.pdf>
- [6] Sabarnya Mitra. Exponential Resummation of QCD at finite chemical potential. (2023) PhD thesis. <https://arxiv.org/pdf/2307.05751.pdf>
- [7] Sabarnya Mitra, Prasad Hegde. QCD equation of state at finite chemical potential from unbiased exponential resummation of the lattice QCD Taylor series.  
<https://arxiv.org/pdf/2302.06460.pdf>
- [8] Sabarnya Mitra. A Comparative Analysis between Unbiased Exponential Resummation and Taylor Expansion in Finite-Density QCD with a new phasefactor for Isospin. <https://arxiv.org/pdf/2303.12063.pdf>
- [9] Rajiv Gavai, Sourendu Gupta. Pressure and non-linear susceptibilities in QCD at finite chemical potentials. <https://arxiv.org/pdf/hep-lat/0303013v2.pdf>

## .1 Proof that chemical potential term makes fermion determinant complex

The gauge action  $S_G$  is always real as is the fermion determinant  $\det M$  when  $\mu=0$ . Let's see what happens when  $\mu \neq 0$ .

In the imaginary time formalism (Euclidean), the gauge-covariant derivative  $D_\nu$  is anti-Hermitian, i.e.

$$(D_\nu)^\dagger = -D_\nu \tag{1}$$

therefore it only has purely imaginary eigenvalues  $ix_n$ , where  $x_n$  is real.

The fermion determinant  $\det M$  can be expressed as product of it's  $N$  eigenvalues of the form  $\pm ix_n + m$

$$\det M = \det(D + m) = \prod_{n=1}^N (-ix_n + m)(ix_n + m) = \prod_{n=1}^N (x_n^2 + m^2) \quad (2)$$

Therefore  $\det M$  is always real in the Naive action. The same proof holds for Staggered fermion action as well but not Wilson fermions as they are not anti-hermitian due to the Wilson term  $D_\mu D_\nu$ . Nevertheless, using their  $\gamma_5$  hermiticity property, i.e. for  $M_{Wilson} = D_\nu \gamma_{nu} + m + ra + D_\mu D_\nu$

$$\gamma_5 M_{Wilson}^\dagger \gamma_5 = M_{Wilson} \quad (3)$$

and using  $\det(CD) = (\det C)(\det D)$ , for  $(\det M_{Wilson})^\dagger = \det M_{Wilson}$  and there the determinant must be real.

For a non-zero chemical potential  $\mu$ , we have the gauge-covariant derivative becomes  $D = D_\nu \gamma_\nu + \mu \gamma_4$ . Due to the  $\mu \gamma_4$  term it is no longer anti-Hermitian nor  $\gamma_5$  Hermitian. In consequence,  $\det M = \det (D_\nu \gamma_\nu + \mu \gamma_4 + m)$  may aquire an imaginary part and hence become complex.

## .2 Derivatives of Z

A quantity that is extensively used throughout the report is  $D_n$  which are the derivatives of the partition function  $Z$ , specifically the fermion determinant  $\det M$  as it is the only  $\mu$  dependent part.

$$D_n = \frac{\partial^n Z}{\partial \hat{\mu}^n} \quad (4)$$

where  $\hat{\mu} = \frac{\mu}{T}$ .

In the continuum the chemical potential term is of the form

$$\mu \bar{\psi} \gamma^4 \psi \quad (5)$$

where  $\bar{\psi} \gamma^\nu \psi$  can be thought of as the wick rotated zeroth component of the conserved current density, i.e. the number density of particles of the system. In thermodynamics it is akin to multiplying the number of particles with the associated energy cost of adding a single particle to the system.

Therefore in the lattice, eventhough the form of the chemical potential term differs, the coefficient of the chemical potential is akin to the zeroth component of the conserved current. Let's call it  $J_0(x)$ .

Then the  $n$ th derivative of the partition function  $D_n$  can be physically interpreted of as the  $n$ -point correlation function of  $J_0(x)$

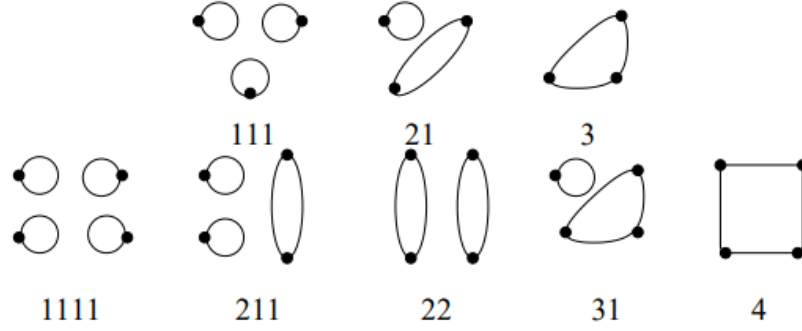
$$D_n = \int dx_1 dx_2 \dots dx_n J_0(x_1) \dots J_0(x_n) \quad (6)$$

We can graphically represent by using the diagrams by following these rules [9]

1. Draw  $n$  vertices, each corresponding to a derivative of  $Z$  with respect to  $\mu$ .
2. Join the vertices by lines (each representing a quark) into collection of closed loops.  $D_i$  is represented by a single loop going around a  $i$  vertices.



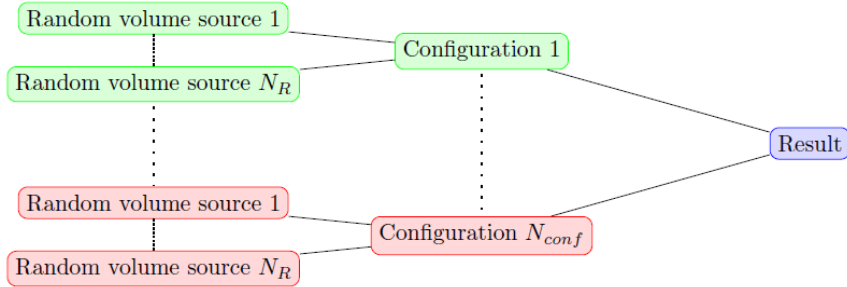
3. For each n-th order, add all the operator topologies for such that the total number of vertices adds upto n.



**Fig. 1:** Contribution of different random volume sources inside each of the available gauge field configuration to the n-point correlation function

### .3 Random volume Sources and Stochastic Bias

To calculate the  $D_n$ , we have a total of  $N_G$  gauge configurations each of which has  $N_R$  random volume sources that give an estimate of  $D_n$  for each n. [9].



**Fig. 2:** Random Volume Sources

Since the free energy  $F = -T \ln Z$ , each coefficient of the Taylor series is given by

$$c_n = \frac{\partial^n \ln Z}{\partial \hat{m} u^n} \quad (7)$$

and as

$$\frac{\partial^n \ln Z}{\partial \hat{m} u^n} = (\det M)^{-1} \frac{\partial^n \det M}{\partial \hat{m} u^n} \quad (8)$$

, where  $\det M$  is the only  $\mu$  dependent part so all the other factors in  $Z$  and  $Z^{-1}$  cancel out. Each of these random volume estimates of  $D_n$  are stochastically generated using conjugate gradient algorithm of numerically approximating the inverse of the fermion determinant  $\det M$ . All these random volume estimates for a given gauge configuration are averaged out to obtain an estimate of  $D_n$  at the level of individual gauge field configurations. The stochastic averaging at the level of random sources is given by

$$\bar{D}_n = \frac{1}{N_R} \sum_{r=1}^{N_R} D_n(r) \quad (9)$$

This gives rise to stochastic bias of two kinds namely

1. Estimate bias
2. Formalism Bias

Estimate bias can arise from the use of finite number of random volume sources used per configuration to estimate  $D_n$  for each n. The bias decreases with increasing number of random volume sources and increases with decreasing number of sources.

On the other hand, the formalism bias is the main theme of the latter half of this report and what we focus on minimizing. It is, as the name suggests, formalism dependent and originates when the resummation scheme deviates from the Taylor series which itself is unbiased.