Taylor expansions in chemical potential

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Properties of QCD at finite chemical potential (μ) are extracted using Taylor series expansions. The continuum limits of lattice results are presented. The result of expanding the free energy density, i.e., the pressure, to 6th order in the expansion is shown. The Taylor coefficients of the chiral condensate are also shown. Relations between various Taylor coefficients are demonstrated. All this information is utilized to remove various lattice artifacts from the determination of the Wroblewski parameter in strangeness production.

§1. Introduction

Lattice simulations of QCD are possible whenever the determinant of the Dirac operator, M, is positive. The proof of positivity amounts to constructing an operator Q such that QMQ⁻¹ = M†. Once such a Q has been obtained, the result that Det M is real follows trivially. For QCD at zero chemical potential (μ = 0), Q = γ₅. In the limit when isospin symmetry is exact, and an isovector chemical potential μ₃ is switched on, an isospin flip is the appropriate Q, thus showing that QCD at finite μ₃ is amenable to direct lattice simulation. A chiral model analysis found the phase diagram in the T–μ₃ plane and lattice simulations verified these results soon thereafter. At finite baryon chemical potential (μ) there is no such operator, and direct simulations are impossible. CP symmetry nevertheless dictates that the free energy remains real, and that normal thermodynamics is obtained.

Many methods have been developed to explore the interesting physics in the T–μ plane. Here I discuss high-order Taylor expansions of the pressure and first results of systematic Taylor expansions of many other quantities. The first results on the Taylor expansion of the free energy (pressure) were presented in and that of meson correlators in. This report is in two sections—the first deals with the Taylor expansion of the pressure and the second with that of the quark condensate and related quantities. Following these two sections is a brief summary.

§2. The pressure

In the following series expansion is utilized for the pressure,

\[ P(T, \mu) = P(T, 0) + \chi_{uu}(T)\mu^2 + \frac{1}{12}\chi_{uuuu}(T)\mu^4 + \frac{1}{360}\chi_{uuuuuu}(T)\mu^6 + \cdots \]  \hspace{1cm} (2.1)

where the pressure, P, of a system at temperature T is given in terms of the free energy, F, by \( P = -F/V \), where V is the volume. A similar expansion is used by

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the Bielefeld-Swansea group. CP symmetry forces the odd terms in the expansion to vanish. The neglected terms are meant to be of higher order in $\mu$. The Taylor coefficients are the generalised susceptibilities, which are best defined by introducing one chemical potential for each flavour of quarks. This is allowed since flavour is a conserved quantum number in QCD. Then the susceptibilities of order $n$ are defined as the partial derivatives

$$\chi_{f_1 \cdots f_n} = -\frac{1}{V} \frac{\partial^n F}{\partial \mu_{f_1} \cdots \partial \mu_{f_n}} \bigg|_{\mu_{f_i} = 0}, \quad (2.2)$$

where $\{f_1, \cdots, f_n\}$ are flavour labels. It is then clear that two assumptions have been made in writing eq. (2.1), first that we consider the isospin symmetric case with 2 flavours of quarks, and second that only the diagonal susceptibilities ($f_1 = f_2 = \cdots = f_n$) need to be retained. Both these restrictions are non-essential, but they are justified by the respective observations that flavour asymmetry plays a negligible role in the problem and that the off-diagonal susceptibilities are negligibly small.

We note here that the susceptibilities are not merely of formal interest as expansion coefficients of the pressure, but also form observables in their own right. They control fluctuations and the strangeness production rate in heavy-ion collisions.

The Taylor expansion can be cast into a form which makes clear how good the approximation is, and when it breaks down. Define $\mu^*_i$ to be that value of $\mu$ at which the $i$-th term is equal to the $i+2$-nd (for example, $\mu^*_2 = \sqrt{12\chi_{uu}/\chi_{uuuu}}$). Then the expansion in eq. (2.1) can be written as

$$\Delta P(T, \mu) = \chi_{uu}(T)\mu^2 \left[ 1 + \left( \frac{\mu}{\mu^*_2} \right)^2 \left[ 1 + \left( \frac{\mu}{\mu^*_4} \right)^2 \left[ 1 + \cdots \right] \right] \right], \quad (2.3)$$

where $\Delta P(T, \mu) = P(T, \mu) - P(T, 0)$. This is manifestly well-behaved if we have $\mu^*_2 > \mu^*_4 > \cdots$, and equally well-behaved series of approximations arise by neglecting terms of order $i$ and above when $\mu \ll \mu^*_i$. Thus term by term improvement of the series is possible. Another advantage is that each susceptibility (and hence $\mu^*_i$) is computed at zero chemical potential, whereby the continuum limit can be (and has been) obtained by the usual techniques of lattice gauge theory.

The other nice point about the Taylor series expansion emerges when one examines its failure. If the sequence $\mu^*_i$ tends to a limit $\mu_s$, then clearly the series fails to converge for $\mu = \mu_s$. Therefore any finite $\mu_s$ is an estimate of the nearest phase boundary. Other series extrapolation methods can also be used—for example, Padé analysis. Results using susceptibilities up to 8th order for QCD with 2 flavours of light dynamical quarks in the continuum limit will be presented elsewhere.

Like all other lattice methods in current use for this problem, the Taylor series expansion is limited up to the transition point (or line) nearest to $\mu = 0$. I believe that it has some advantage over other methods. The primary problem with direct lattice computations at finite chemical potential is to gain control over phase fluctuations of the determinant. In the reweighting methods this is achieved by simultaneous movement in both $T$ and $\mu$. If one could develop a method to sum over CP orbits in configuration space, then the sign problem would be automatically
In the Taylor series expansion, one starts from the free energy, where the sum over CP orbits has already been performed to yield a real quantity. Thus, an expansion in the single variable \( \mu \) completely captures the physics. The mechanics of the proof involves taking the double Taylor series expansion of \( P \) and checking that it gives no advantage.

In Figure 1 we display the continuum limits of the diagonal susceptibilities and the EOS. The latter is compared with the Taylor series truncated at the second order, and with results obtained through reweighting on lattices with \( N_t = 4 \) which were extrapolated to the continuum using the known ratio \( \chi_{uu}(\text{cont})/\chi_{uu}(N_t = 4) \). These comparisons show the interesting fact that in the high temperature phase of the QCD plasma the computation of the linear susceptibility \( \chi_{uu} \) is sufficient to determine the continuum value of the pressure at \( \mu \) of interest to heavy-ion experiments. This is also evidence that extrapolation in one variable of \( P \) is equivalent to reweighting in two variables.

Not all observable physics in the continuum limit can be extracted by a simple rescaling by the factor \( \chi_{uu}(\text{cont})/\chi_{uu}(N_t = 4) \). At finite chemical potential lattice artifacts are large and connected to the fact that there is an infinity of equivalent prescriptions for putting chemical potential on the lattice. This results in an
ambiguity in the definition of susceptibilities, and in the critical end point, which vanishes only in the continuum limit. We have estimated that this ambiguity may move estimates of the critical end point by an amount much larger than the present statistical errors.\(^5\) Hence, taking the continuum limit becomes crucial to obtaining this unique signature of QCD dynamics.

The diagonal linear susceptibilities are in good agreement with perturbative computations.\(^19\), \(^20\) Consequently, \(\Delta P(T, \mu)\) is also in good agreement with perturbative results.\(^21\) This is interesting since \(P(T, 0)\) is badly reproduced by perturbation theory. Perturbative computations of the fourth order susceptibility are not as good, and the off-diagonal susceptibilities fare poorly. It has been suggested that the large \(N_f\) behaviour of perturbation theory can be tested to throw more light on this.

§3. The quark condensate and meson correlators

The success of the Taylor expansion of the pressure leads us to believe that other quantities of interest can also be successfully investigated at finite chemical potential through Taylor expansions. We use the quark condensate as an example. This is defined to be

\[
C(T, \mu) \equiv \langle \bar{\psi} \psi \rangle_{T, \mu} = \frac{1}{Z} \frac{\partial Z(T, \mu)}{\partial m} = -\frac{1}{TV} \frac{\partial F(T, \mu)}{\partial m}, \tag{3.1}
\]

where \(Z\) is the partition function, and we have introduced a non-standard notation, \(C\), for the quark condensate which is usually denoted by \(\langle \bar{\psi} \psi \rangle\). We develop this in a Taylor series expansion around \(\mu = 0\),

\[
C(T, \mu) = C(T, 0) + c_1(T)\mu + \frac{1}{2} c_2(T)\mu^2 + \cdots \tag{3.2}
\]

Interesting results follow immediately.

The first derivative at a general value of \(\mu\) is

\[
c_1(T, \mu) = \frac{\partial C(T, \mu)}{\partial \mu} = \frac{1}{T} \frac{\partial n(T, \mu)}{\partial m}, \tag{3.3}
\]

where \(n(T, \mu)\) is the quark number density, obtained by taking the first derivative of the pressure with respect to \(\mu\). We have related two seemingly different physical objects by interchanging orders of derivatives; this is a prototype of a Maxwell relation in thermodynamics. Further, the Taylor expansion of the pressure shows that \(n(T, \mu) \approx 2\chi_{uu}(T)\mu\), and hence

\[
c_1(T, \mu) = \frac{2\mu}{T} \frac{\partial \chi_{uu}(T)}{\partial m} + \cdots \tag{3.4}
\]

where the neglected terms start at order \(\mu^3\). From this it immediately follows that \(c_1\) in eq. \(^{19}\) vanishes. The outline of a proof that the Taylor expansion of \(C\) in eq. \(^{19}\) is even is clear from this. Furthermore, it also follows that the limiting value of \(c_1/\mu\) is proportional to the slope of \(\chi_{uu}\) with mass.
A Maxwell relation for the second Taylor coefficient $c_2$ follows in a very similar manner,

$$c_2(T) = \frac{1}{T} \frac{\partial \chi_{uu}(T)}{\partial m}.$$  

This is of great use in lattice computations of strangeness production. It has been argued that the Wroblewski parameter which can be extracted from heavy-ion collision experiments on strangeness production can be written as

$$\lambda_s(T) = \frac{\chi_{ss}(T)}{\chi_{uu}(T)}.$$ 

The strange and light quark masses are not direct physical observables, but are free parameters of QCD which are obtained by fitting the spectrum of mesons at $T = 0$. At present it is hard to perform a lattice computation at realistic values of the light quark masses. One can then compute $\lambda_s$ at a value of the light quark mass for which the computation is feasible and use a Taylor expansion in the quark mass to extrapolate to the physical quark mass value. The leading term in this Taylor expansion is then $-Tc_2/\chi_{uu}$.

![Fig. 2. The renormalised second derivative of the quark condensate, $c_2^r$ for $T = 1.5T_c$ (circles), $2T_c$ (boxes) and $3T_c$ (pentagons). The continuum limit ($1/N_t^2 = 0$) is consistent with zero at the 99% confidence level at all $T$.](image)

One subtlety in these arguments is the effect of renormalisation. Since $\mu$ appears as a coupling to a conserved charge, it is not renormalised, and hence renormalisation affects the computations of the susceptibilities only in so far as they need to be extrapolated to the continuum limit. The situation is different for the quark condensate and its Taylor coefficients. The mass is renormalised, by a multiplicative factor for staggered quarks. This requires a multiplicative renormalisation of every term in
the series in eq. (3.2). This is straightforward. Since the renormalisation constant depends only on the ultraviolet cutoff, i.e., the lattice spacing $a$, and not on $T$ and $\mu$, renormalisation can be accounted for simply by making a Taylor series expansion of $C(T, \mu)/C(0, 0)$. The series remains even, and results for $c_2(T)$ are shown in Figure 2. The renormalised value of $c_2$ is consistent with zero at the 99% confidence level.

The Taylor expansion can also be performed in the isovector chemical potential, $\mu_3$. A comparison of the corresponding Taylor coefficients reveals that numerically $c_2$ is very nearly equal to the corresponding coefficient in the series in $\mu_3$ (in contrast, exact equality is obtained in a random matrix model). This turns out to be a fairly general feature, being reproduced also in the Taylor expansions of the meson correlators. It is due to the observed fact that off-diagonal susceptibilities like $\chi_{ud}$ are small.

We turn now to correlators of quark bilinears, which are called meson correlators in extension of their zero-temperature meaning. Taylor expansions of the correlation lengths have been computed earlier using an expression in which each correlator is saturated by a single mass. We make instead a Taylor expansion of the meson susceptibilities. In the thermodynamic limit of the low-temperature phase of QCD where mesons are physical degrees of freedom, these susceptibilities are proportional to the inverse square of the mass.

An interesting point is the fact that these meson susceptibilities can be considered either as a sum over the temporal correlator at all temporal separation, or as a screening correlator summed over all spatial separation. Above $T_c$ the effective representations of these two correlators are different. As a result, the meson susceptibilities can also be used to extract the dependence on $\mu$ of both masses and screening lengths without any need to use a spectral function in intermediate steps.

Further relations between coefficients of different Taylor series are given by chiral Ward identities such as

$$C(T, \mu) = m \chi_{PS}(T, \mu),$$

where $\chi_{PS}(T, \mu)$ is the pseudo-scalar susceptibility. This particular identity is quite interesting, as can be seen by writing out the Taylor expansion of $\chi_{PS}$—

$$\chi_{PS}(T, \mu) = \chi_{PS}(T, 0) + \chi^\prime_{PS}(T)\mu + \frac{1}{2}\chi^\prime\prime_{PS}(T)\mu^2 + \cdots. \quad (3.6)$$

The chiral Ward identity then allows us to use the arguments already given for the series expansion of $C(T, \mu)$ to argue that the series for $\chi_{PS}$ is even.

Furthermore, we obtain the interesting relations

$$\chi''_{PS}(T) = \frac{1}{m} c_2(T) = \frac{1}{mT} \frac{\partial \chi_{uu}(T)}{\partial m}. \quad (3.7)$$

Recall that for $T > T_c$, the infrared cutoff is the Matsubara frequency, $\Omega = \pi T$, whenever $m < \Omega$. As a result, the meson screening masses are given by $2\Omega$ (or its lattice equivalent) and is independent of $m$. The susceptibility $\chi_{uu}$ is equal to the vector meson susceptibility (for staggered quarks, the identity is with a one-link separated meson). By the previous argument, this must be independent of $m$ for $m < \Omega$. This is also seen through explicit computation. This explains the observation that both the quark condensate and the PS susceptibility are independent of $\mu$. [29]
at least to quadratic order in $\mu$. By the connection established earlier between the variation of $\lambda_s$ and $c_2$, we therefore conclude that the Wroblewski parameter is insensitive to the light quark mass, provided that $m < \Omega$. At the same time, if the dependence of $\lambda_s$ on the strange quark mass, $m_s$, is considered, then, since $m_s \approx T_c$, there should be strong dependence of $\lambda_s$ on $m_s$.

§4. Summary

We have explored the physics of QCD at finite chemical potential through systematic Taylor expansions of various quantities. This allows us to use standard lattice techniques to tackle this problem, and obtain the continuum limit of every observable. The Taylor coefficients themselves contain interesting physics, and we have given some examples. There are numerous relations between them—we have used a chiral Ward identity and a Maxwell relation as illustrations. In this report we have shown how the quark mass dependence of the Wroblewski parameter is related to physics at finite chemical potential through such relations.

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