Chemical potential on the lattice: Universal or Unique?

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Abstract

Lattice techniques are the most reliable ones to investigate non-perturbative aspects of quantum chromodynamics (QCD) such as its phase diagram in the temperature-baryon density plane. They are, however, well-known to be beset with a variety of problems as one increases the density. We address here the old question of placing the baryonic (quark) chemical potential on the lattice. We point out that it may have important consequences for the current and future experimental searches of QCD critical point.
1. Introduction

The behaviour of strongly interacting matter, described by Quantum Chromodynamics (QCD), at nonzero temperatures or baryon densities has continued attracting attention both theoretically and experimentally for more than three decades \[1, 2, 3\]. Since QCD coupling is known to be large at or near the scale of QCD, $\Lambda_{QCD}$, investigating the QCD phase diagram necessitates strong coupling techniques. Lattice QCD is the most successful non-perturbative technique which has provided us with key interesting results pertaining to the phase diagram. For instance, it is known from independent lattice studies that the transition from the hadron phase to the quark gluon plasma phase at zero baryon density is a crossover \[4, 5, 6\]. Extending these results to non-zero baryon density, or equivalently nonzero quark chemical potential $\mu$, one encounters the famous sign problem: the quark determinant becomes a complex number, inhibiting the use of the trusted importance sampling based Monte Carlo methods.

Several ways have been proposed to confront the sign problem in QCD \[7, 8, 9, 10\]. Based on an analysis of model quantum field theories with the same symmetries as two light flavour QCD \[11, 12\], a critical end-point is expected to exist in the QCD phase diagram. One expects the baryon number susceptibility to diverge \[13\] there. Consequently, its Taylor series expansion at finite baryon density would have a finite radius of convergence, leading to an estimate of the location of the critical end-point \[13, 14\].

First such estimates of the radius of convergence of the Taylor series suggested the critical end-point to be at $T_E/T_c = 0.94$ and $\mu_B/T_E = 1.8(1)$ \[14\]. A study on a finer lattice refined the continuum limit to be around $T_E/T_c = 0.94(1)$, $\mu_B/T_E = 1.68(5)$ \[15\]. On the other hand, other approaches, such as employing imaginary chemical potential and/or 'improved' actions, have reported only bounds on the location of critical point which at 1-$\sigma$ level disagree \[16\] with the results of \[15\]. In heavy-ion experiments at RHIC, the fluctuations of the net proton number are employed as a proxy for the net baryon number. The STAR experiment at Brookhaven National Laboratory has measured the fluctuations of the net proton number up to the fourth order for a wide range of center of mass energy $\sqrt{s}$. At $\sqrt{s} = 19.6$ GeV the experimental data are seen \[17, 18\] to deviate maximally from the predictions of the proton fluctuations for models which do not have a critical end-point, and are similar to the lattice QCD-based predictions \[19\] for a critical point. While these above mentioned results employ kurtosis of
baryon/proton number, it has been proposed that the 6th-order fluctuations may shed light on whether the crossover at zero baryon density is a shadow of the $O(4)$ criticality in the chiral limit \cite{20}. Clearly, still higher orders will eventually need to be computed for better control over the radius of convergence. Thus higher order susceptibilities are, and will continue to remain, of immense interest.

In this paper, we compare and contrast the different ways of introducing the chemical potential on the lattice, and assess their impact on these higher order susceptibilities which also govern the coefficients of the Taylor series. Astonishingly, we find that the results depend on the way chemical potential is introduced. The differences appear to persist in the continuum limit. This observation also has consequences for all other methods to tackle the sign problem. We argue for a choice closest to the continuum QCD as the best. In section 2, we recall the existing methods to place chemical potential on the lattice and demonstrate their failure with universality. The next section 3 is devoted to a discussion of their other attributes. We finally summarise our results.

2. Universality and Chemical Potential

The lattice QCD partition function in the path integral formalism is given by

$$Z = \int \mathcal{D}U_\mu \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S_G - S_F(ma, \mu_B)},$$

where $\psi(x)$, $\bar{\psi}(x)$ and $U_\mu(x)$ represent the quark, anti-quark at site $x$ and the gluon field on the link $(x, \hat{\mu})$ respectively. $S_G$ denotes a suitable choice for the gluonic action and $S_F$ is the quark action. We shall consider below the naive quark action but our considerations are easily generalized to other local actions such as the Wilson action, the staggered action or their improved versions. Similarly, we will consider only a single flavour with the baryonic chemical potential $\mu_B = 3\mu$ for simplicity, generalization to more flavours again being straightforward. Denoting by $ma$ the quark mass and by $\mu a$ its chemical potential, the fermionic action is given by $S_F = \bar{\psi} M(ma, \mu a) \psi$ with
M defined as below:

\[ S_F(ma, \mu a) = \sum_{x, \mu=1}^{3} \bar{\psi}(x) \gamma_\mu [U_\mu(x) \psi(x + \hat{\mu}) - U_\mu^\dagger(x - \hat{\mu}) \psi(x - \hat{\mu})] \] (2)

\[ + \sum_x \bar{\psi}(x) \gamma_4 \left[ f(\mu a) \cdot U_4(x) \psi(x + \hat{4}) - g(\mu a) \cdot U_4^\dagger(x - \hat{4}) \psi(x - \hat{4}) \right] \]

\[ + ma \psi(x) \psi(x) , \]

Three possible choices have so far been used in the literature \[21, 22, 23\] for the functions \(f\) and \(g\), denoted below by subscripts \(L\) (linear), \(E\) (exponential) and \(S\) (square root):

\[ f_L(\mu a) = 1 + \mu a , \quad g_L(\mu a) = 1 - \mu a \] (3)

\[ f_E(\mu a) = \exp(\mu a) , \quad g_E(\mu a) = \exp(-\mu a) \]

\[ f_S(\mu a) = (1 + \mu a)/\sqrt{1 - \mu^2 a^2} , \quad g_S(\mu a) = (1 - \mu a)/\sqrt{1 - \mu^2 a^2} . \]

Following the natural route of obtaining the conserved charge from the corresponding current conservation equation on the lattice leads to the naive linear choice \[23\] above. However, it has \(\mu\)-dependent quadratic divergences in the number density and the energy density even for the free quark gas. These can be eliminated by the other two options for \(f\) and \(g\). Indeed all functions satisfying \(f(\mu a) \cdot g(\mu a) = 1\) eliminate \[24\] those divergences. It is a straightforward exercise to check that all these actions lead to the same continuum action in the limit of vanishing lattice spacing \(a \to 0\) since their contribution to the action is formally of higher order in \(a\). In principle, this should ensure that the pressure is identical for all of them, provided the \(a \to 0\) limit is taken. The catch though is that mostly various derivatives of the pressure are evaluated and their computations are also necessarily performed for \(a \neq 0\). This turns out to have serious consequences as the \(k^{th}\) derivative of pressure can, and does, carry the memory of the terms up to \(O(\mu^k a^k)\) even as \(a \to 0\), as we show below.

Integrating the Grassmannian quark and antiquark fields, one has

\[ Z = \int \mathcal{D}U_\mu e^{-S_G} \operatorname{Det}M(ma, \mu a) . \] (4)

A derivative of \(\ln Z\) with \(\mu\) leads to the quark number density, or equiv-
alently (1/3) the baryon number density, defined by,

\[ n = \frac{T \partial \ln Z}{V \partial \mu} \bigg|_{T=\text{fixed}} \]

\[ = \frac{1}{N_t N_s^3 a^3} \langle \text{Tr} M^{-1} \cdot M' \rangle , \]

where \( M' \) is the derivative of the fermionic matrix \( M \) with respect to \( \mu a \), \( T = (N_t a)^{-1} \) is the temperature and \( V = N_s^3 a^3 \) is the volume. In the process of obtaining predictions for the signals of either the critical end point or the two-flavour chiral transition, one evaluates higher order derivatives of \( n \) to obtain various fluctuations such as the variance, skewness or kurtosis etc. In fact, coefficients of \( \mu^8 a^8 \) have been computed in attempts to locate the QCD critical point \[14\], and those of \( \mu^6 a^6 \) terms are expected to assist \[20\] in pinning down the hints of a critical point in the chiral limit of the two-flavour theory in the heavy ion collision data.

In general, a \( \mathcal{O}(\mu^k a^k) \) will clearly involve up to \( k \)-th derivative of the fermion matrix \( M \), and thus of \( f \) and \( g \). Using the condition \( f(\mu a) \cdot g(\mu a) = 1 \) along with the obvious \( f(0) = g(0) = 1 \) and \( f'(0) = -g'(0) = 1 \) (to ensure the \( \mu N \) form in the \( a \to 0 \) limit) conditions, one finds \( f''(0) + g''(0) = 2 \). Using the fact that particle-antiparticle symmetry implies \( f(\mu a) = g(-\mu a) \), one finds that the \( f^k(0) = (-1)^k g^k(0) \), and thus \( f''(0) = g''(0) = 1 \). Both \( f_E \) and \( f_S \) satisfy this. Unfortunately they differ in all the higher derivatives. There are no more conditions to fix the higher derivatives. Indeed, \( f'''(0) = 4 f''(0) - 3 \) is the only new relation one has. It is easy to verify from eq. (3) that \( f''_E(0) = 1 \) with \( f''_S(0) = 3 \) do satisfy this relation. Thus only the first derivative is identical for all the \( f \)’s in eq.(3). Already the second derivative \( f_E''(0) = 0 \) but the second derivative is identical for \( f_E \) and \( f_S \) and is unity. All further higher derivatives are different. Note these are all pure numbers, \( i. e. \), an approach to continuum limit will not change these derivatives themselves. This has consequences for the various higher order fluctuations of the conserved charge. They too will be different depending upon the choice of \( f \) from eq.(3) with no hope of their converging in the continuum limit. \textit{A priori} all \( f \) are on the same footing. This therefore appears to be then a serious violation of universality, as \( f''' \) and \( f'''' \) enter experimentally measurable quantities such as kurtosis or the \( \chi_6^B \).

One ought to have seen this coming after all since it is well-known \[23\] that \( f_L \) has quadratic \( \mu \)-dependent divergences but the other two do not. An easy
way to see this is to look at the expression for quark number susceptibility. It is given by

\[ \chi = \frac{1}{N_t N_s a^2} \left[ \langle (\text{Tr}M^{-1}M')^2 \rangle + \langle \text{Tr} (M^{-1}M'' - M^{-1}M'M^{-1}M') \rangle \right]. \tag{6} \]

Since \( f''_L = g''_L = 0 \) for the naive linear choice for all \( \mu a \), the first term in the second expectation value vanishes whereas \( f''(0) = g''(0) = 1 \) leads to a nonzero contribution from it for the other two actions. Indeed, it is precisely this term which ensures elimination of the divergence for them. It is important to note that the second derivative comes from \( \mathcal{O}(\mu^2 a^2) \) terms in \( f_E, f_S \) and \( g_E, g_S \) in eq.(3). These by themselves are irrelevant terms for the continuum limit of the pressure itself. However, they are not irrelevant at the susceptibility level. In particular, all of the terms enclosed in the square brackets in eq.(6) are parametrically independent of \( a \) and contribute formally equally. Each must vanish as \( a^2 \) in the continuum limit in order that \( \chi \) is nontrivial in that limit. Nevertheless, if one were to assume hypothetically that the \( \langle M^{-1}M'' \rangle \) term, which is the only term to have contribution from the \( \mu^2 a^2 \) term, itself somehow vanishes faster than the other terms in the \( a \to 0 \) limit, it is clear then that the result will be the same as the linear case for which \( \chi \) is divergent. We know, on the other hand, that the divergence in the \( a \to 0 \) limit is eliminated for the exponential and square root actions precisely due to the continued contribution of this term in the continuum limit, as demonstrated in [23] for the free quark gas and in [25] for the interacting case.

It should not come as a surprise that this phenomena recurs for higher order susceptibilities as well. One encounters even more prescription dependence at higher orders. Consider for example the fourth order susceptibility [13]:

\[ \chi^4 = \frac{1}{N_t N^3} \left[ \langle \mathcal{O}_{1111} + 6 \mathcal{O}_{112} + 4 \mathcal{O}_{13} + 3 \mathcal{O}_{22} + \mathcal{O}_4 \rangle - 3 \langle \mathcal{O}_{11} + \mathcal{O}_2 \rangle^2 \right]. \tag{7} \]

Here the notation \( \mathcal{O}_{ij...l} \) stands for the product, \( \mathcal{O}_i \mathcal{O}_j \cdots \mathcal{O}_l \). The relevant \( \mathcal{O}_i \)
for eq. (7) are \[13\]

\[ O_1 = \text{Tr} \ M^{-1} M', \]
\[ O_2 = -\text{Tr} \ M^{-1} M' M^{-1} M + \text{Tr} \ M^{-1} M'', \]
\[ O_3 = 2 \text{Tr} \ (M^{-1} M')^3 - 3 \text{Tr} \ M^{-1} M' M^{-1} M'' + \text{Tr} \ M^{-1} M''', \]
\[ O_4 = -6 \text{Tr} \ (M^{-1} M')^4 + 12 \text{Tr} \ (M^{-1} M')^2 M^{-1} M'' - 3 \text{Tr} \ (M^{-1} M'')^2 - 3 \text{Tr} \ M^{-1} M' M^{-1} M''' + \text{Tr} \ M^{-1} M'''. \]

Note that there is no explicit \( a \)-dependence on either side of the equation (7). \( \chi^4 \) is a pure number in the continuum limit. The traces run over all the lattice sites, get normalized by the lattice volume, and are thus pure numbers as well. Again \textit{a priori} none of the trace terms vanishes faster than any other in the continuum limit. Since \( O_3 \) and \( O_4 \) have terms with \( M''' \) and \( M'''' \), which in turn contain the \( f''' \), \( g''' \), \( f'''' \) and \( g'''' \), it is clear that for each choice out of the three in eq.(3), one will obtain a different value on the same set of dynamical gauge configurations. It is worth reminding that the differences due to the actions are pure numbers. For instance, \( f_E'''(0) = 1 \), \( f_S'''(0) = 3 \) while \( f_E''''(0) = 9 \), \( f_S''''(0) = 9 \). Thus \( \chi^4 \) onwards for all higher order susceptibilities one obtains results which depend on the choice of \( f \) and \( g \) and are thus not universal. Since \( \chi^n \propto a^{(n-4)} \), the overall behaviour of the corresponding RHS will naturally scale appropriately with \( a \), as seen for \( \chi \) in eq.(6). But all the individual terms of RHS can, and do, scale that way with none destined to vanish faster than the others as all are formally \( a \)-independent. Therefore, the three actions continue to give different results for all \( n \geq 5 \). It may happen that the corresponding \( \chi^n \), \( n \geq 5 \), vanishes in the continuum limit, as for the ideal quark gas, yielding then action independent results. In the interacting case though this is not the case in general.

This loss of universality is not limited only to the higher order fluctuations of the conserved charges computed using lattice QCD simulations. Recall that the pressure \( P \) is usually constructed as a series in \( \mu^B \) with these susceptibilities as the coefficients. Hence, the pressure, and consequently all thermodynamic quantities derived from it, are also similarly prescription dependent from the fourth order onwards. If one somehow computed the partition function itself directly, and obtained the continuum limit of the correspondingly evaluated pressure as its logarithm then it would not suffer from this loss of universality. On the other hand, any method which relies on computations of thermal expectation values of quark number susceptibilities will suffer from this problem.
In short, the quest to get rid of the $\mu$-dependent divergences lead to modification of the action in the Euclidean representation of the partition function, ostensibly by adding terms which are irrelevant in the continuum limit $\alpha \to 0$. The presence of the dimensional parameter $\mu$ in these terms, however, spoils this naive expectation of universality for quark number susceptibilities. Employing the $f_L$ and $g_L$ prescription has the advantage of being faithful to the continuum theory in reproducing the higher order fluctuations, but also has the disadvantage of a $\mu$-dependent divergence, again as in the continuum theory.

3. Conservation of Charge

Recall that invariance of an action under a global $U(1)$ symmetry leads to a current conservation equation, $\partial_\mu j^\mu(x) = 0$, and hence the conserved charge $N = \sum_\vec{x} j^4(\vec{x})$. It is worth noting that one can compute the current conservation equation after the addition of $\mu \bar{\psi}(x) \gamma_\mu \psi(x)$ term in the Lagrangian to find that the additional term does not alter the above current conservation equation, with the conserved charge remaining the same as it should.

For the lattice theory one can similarly demand invariance of eq.(2) under the global $U(1)$ symmetry: For $\psi' = \psi + \delta\psi$ and $\bar{\psi}' = \bar{\psi} + \delta\bar{\psi}$, $\delta S_F = 0$, where $\delta\psi = i\epsilon\psi$, and $\delta\bar{\psi} = -i\epsilon\bar{\psi}$ and $\epsilon$ is small. The resultant current conservation equation is easily worked out as $\sum_\mu [j^\mu(x - \hat{\mu}) - j^\mu(x)] = 0$ for the case $\mu a = 0$ when $f$ and $g$ are unity in general. Here $j^\mu(x) = [\bar{\psi}(x) \gamma_\mu U_\mu(x) \psi(x + \hat{\mu}) + \bar{\psi}(x + \hat{\mu}) \gamma_\mu U_\mu^\dagger(x) \psi(x)]$ is the point split version of the usual current one obtains in the continuum theory. The conserved charge is related to this point split $j^4$ in the same way and the addition of $\mu N$ term leads to the linear action with $f_L$ and $g_L$. For the case of $\mu \neq 0$, one can again follow the same procedure to work out the new current conservation equation.

A simple trick to write the generic $f$ and $g$ as $[(f + g)/2 \pm (f - g)/2]$ respectively makes it easy to follow the derivation. The $\delta S_F = 0$ equation can then be simplified similarly with two differences. $\delta S_F$ has an additional
term proportional to \([f(\mu a) - g(\mu a)]/2\), which is given by

\[
\delta S_F^{\text{add}}(ma, \mu a) = [f(\mu a) - g(\mu a)]/2 \sum_x \left[ \bar{\psi}(x) \gamma_4 U_4(x) \psi(x + \hat{4}) \right. \\
\left. + \bar{\psi}(x) \gamma_4 U^\dagger_4(x - \hat{4}) \psi(x - \hat{4}) \right. \\
\left. - \bar{\psi}(x - \hat{4}) \gamma_4 U_4(x - \hat{4}) \psi(x) - \bar{\psi}(x + \hat{4}) \gamma_4 U^\dagger_4(x) \psi(x) \right].
\]

Noting that \(x\) is a dummy sum variable, and substituting \(y = x \pm \hat{4}\) in the two terms on the third line of the eq. (9), it is easy to show that \(\delta S_F^{\text{add}}(ma, \mu a) = 0\). Secondly, the current conservation form of the full \(\delta S_F = 0\) has a difference with the \(\mu = 0\) case. The expression for \(j^4(x)\) is replaced by \(j^4_{\text{mod}}(x) = [f(\mu a) + g(\mu a)]/2 \left[ \bar{\psi}(x) \gamma_4 U_4(x) \psi(x + \hat{4}) + \bar{\psi}(x + \hat{4}) \gamma_4 U^\dagger_4(x) \psi(x) \right]\), resulting in the modified conserved charge being \(N_{\text{mod}} = \sum_x j^4_{\text{mod}}(x)\). Substituting the \(f\) and \(g\) from eq. (3), one can work out the consequences in each case. For the linear case, \(N_{\text{mod}} = N\) and thus remains unchanged. For the other two cases, namely the exponential and the square root forms, \(N_{\text{mod}}\) itself is \(\mu\)-dependent for nonzero \(a\), being \(\cosh(\mu a)N(\mu a = 0)\) and \(N(\mu a = 0)/\sqrt{1 - \mu^2 a^2}\) respectively. While in the continuum limit these functions can be expanded to obtain a quadratic \(a\)-approach to the standard conserved charge, the modifications persist for any finite \(a\) employed in the usual simulations. A conserved charge being dependent on the chemical potential itself may be dismissed as a lattice artifact but this does becomes a problem in defining the canonical partition function on the lattice.

Using fugacity \(z = \exp(\mu/T)\), one relates the grand canonical partition function to the canonical ones: \(Z^{\text{GC}} = \sum_n z^n Z^n_C\). Since \(z_{\text{lat}} = \exp(N_{\text{lat}} a\mu)\), such a relation is feasible only for the linear prescription of adding chemical potential. As one notices the conserved number ought to remain the same \(\mu\)-independent constant for such a relation. Since \(N_{\text{mod}}\) depends on \(\mu\) for the exponential case, a canonical ensemble with constant \(N_{\text{mod}}\) is not easily defined from the \(Z^{\text{GC}}\). Indeed, \(Z^{\text{GC}} \neq \sum_n z^n_{\text{lat}} Z^n_C\) in that case. This is of course also the case for all \(f\) and \(g\) which satisfy \(f \cdot g = 1\).

4. Summary

Current and future experimental programs on heavy ion collisions aim to measure fluctuations of conserved charges precisely. The STAR results
already exhibit intriguing structure in higher order proton number fluctuations such as kurtosis. Still higher order fluctuations ($\chi^B_6$) are anticipated to shed light on the nature of the chiral phase transition. Reliable theoretical predictions are needed for these for a trustworthy comparison. Lattice QCD at finite density is the best tool one currently has.

Defining a conserved charge, for instance the baryon number, from the corresponding conserved current defined on the lattice and adding it using the canonical Lagrange multiplier type linear chemical potential term in the fermion actions on the lattice is most natural. Its $\mu$-dependent divergences lead in the past to the proposals of other action, including the popular exponential action. We showed that these actions lead to different results for the same physical quantities, namely the higher order fluctuations starting from skewness, kurtosis and so on. These differences in the same physical quantity persist in the continuum limit of $a \to 0$, and therefore the actions designed to eliminate free theory $\mu$-dependent divergences violate universality. Only the action linear in $\mu$ has an unchanged current conservation equation and hence the same conserved charge for $\mu \neq 0$, as is also the case in the continuum theory. Other actions, including the popular exponential form, do not share these properties: the conserved charge on the lattice itself becomes a function of $\mu$. The usual definition of canonical partition function therefore does not hold for these forms. It would be an interesting challenge to devise a suitable compact form to define it on the lattice.

It may be worth noting that preservation of exact chiral invariance on the lattice seems feasible only for a linear form \cite{26} for the continuum-like overlap and the domain wall fermions. Since a $\mu$-dependent divergence exists already in the continuum for a gas of free fermions, and is subtracted there, it can similarly be subtracted out in simulations \cite{27}. Action with linear chemical potential term is thus unique in that it mimics the continuum behaviour faithfully for both local and nonlocal fermion actions. Modifying the local action to eliminate the divergence leads to a loss of universality for higher order susceptibilities.

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