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A Fresh Look at the Chemical Potential on the Lattice

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Lattice techniques are the most reliable ones to investigate the QCD phase diagram in the temperature-baryon density (chemical potential) plane. These techniques are, however, well-known to be saddled with a variety of problems at nonzero density. I address here the old question of placing the baryonic (quark) chemical potential on the lattice and point out its important consequences for the current and future experimental searches of the QCD critical point.

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1. Introduction

Quantum chromodynamics (QCD) is now widely accepted as the theory of strong interactions. However, simple phenomenological models were in vogue much before its heralding. In view of the strong non-perturbative nature of the hadronic world these models continue to be employed for qualitative, and at times even quantitative, understanding of the underlying physics. The behaviour of strongly interacting matter under extreme temperatures and/or densities is one such area. Based on chiral symmetries of QCD and the corresponding Nambu-Jona Lasinio type of models the expected phase diagram for 2 light and one moderately heavy quark has emerged [1], as displayed in Figure 1. One of its fundamental aspect is the critical point in T-μ_B plane, where μ_B is the baryon chemical potential which governs the net baryon density.

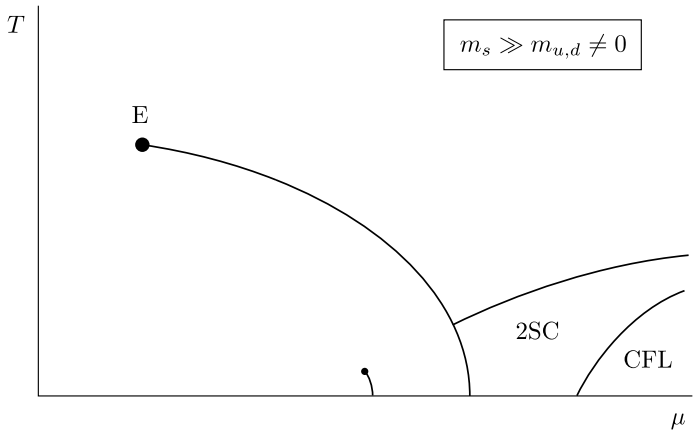

Figure 1: A typical QCD phase diagram in the T-μ_B plane, showing the QCD critical point for $m_u = m_d >> m_s$. Taken from Ref. [1].

A lot of theoretical and experimental attention has been focused on locating the QCD critical point, and in devising its characteristic signatures. In particular, it was suggested that higher moments of fluctuations are enhanced near a critical point and a non-monotonic behaviour in them as a function of colliding energy could be a signal for criticality [2]. Inspired by lattice QCD results, employing baryonic higher order fluctuations was advocated [3]. Exciting experimental results [4] from the STAR collaboration on net proton fluctuations seemed intriguingly like the theoretical expectations [3]. Sixth order baryonic fluctuations have been advocated as a possible tool to establish the expected $O(4)$-criticality for the two-flavour QCD at nonzero temperatures with $\mu_B = 0$ [5]. Finally, various methods to determine the location of the critical point using lattice techniques, specifically the Taylor series method, need higher order baryonic fluctuations. It thus appears worthwhile to examine the higher order quark number susceptibilities (QNS) carefully which we set out to do here.

2. The $\mu \neq 0$ problems

It is well-known that the fermionic determinant becomes complex for nonzero quark chemical potential. This leads to the well-known sign/phase problem due to the lack of positivity of the

measure of the corresponding path integral. Several approaches have been proposed, many of which rely eventually on using the higher derivatives of determinant related to the QNS. To that extent our arguments below would apply to many of them, though for definiteness we will focus on the Taylor series expansion method where successive higher order terms are needed to improve it systematically.

Mostly staggered fermions are used in the investigations of QCD phase diagram. These do not have a well defined flavour number or the $U_A(1)$ symmetry on the lattice. While these may be attained in the continuum limit on large lattices, it is debatable as to how well the present days lattice simulations perform from this perspective. Model considerations suggest that two light quark flavour QCD with an anamoly contribution which decreases slowly with temperature at zero chemical potential leads to a QCD critical point in the temperature-baryon density phase diagram. Higher number of light flavours or a sharp drop in the anamoly contribution may lead only to a first order transition line in the phase diagram. Domain wall quarks or the overlap quarks have the same symmetries as the continuum quarks but do not have a unique local quark current, making it difficult to define the chemical potential for them. There have been proposals in the literature with their associated problems. We argue that the problem of definition of chemical potential generically affects all types of fermions, and that demanding universality of the QNS leads us to a definition valid for all types.

For simplicity, we shall consider the simplest case of naıve fermions as the arguments below can be easily extended to all others with similar consequences. Recall that the naıvely discretized fermionic action is

$$S^F = \sum_{x,x'} \bar{\psi}(x) \left[\sum_{\mu=1}^{4} D^\mu(x,x') + ma\delta_{x,x'} \right] \psi(x'),$$

where

$$D^\mu(x,x') = \frac{1}{2}\gamma^\mu \left[U^\mu_x \delta_{x,x'-\hat{\mu}} - U^{\mu\dagger}_{x'} \delta_{x,x'+\hat{\mu}} \right].$$

It clearly has a $U(1)$ phase rotation symmetry. Under $\psi' = \exp(i\alpha)\psi$ and $\bar{\psi}' = \bar{\psi}\exp(-i\alpha)$, with $0 \le \alpha < 2\pi$ and constant, it remains invariant. As usual, one can easily follow the canonical method to write the corresponding current conservation equation, $\sum_\mu \Delta_\mu J^{lat}_\mu = 0$, and obtain from it the conserved charge in the naturally point-split form. Switching on the gauge fields, $U^\mu(x)$, the conserved quark/baryon charge in QCD is $N = \sum_x \bar{\psi}(x)\gamma^4[U^4_x\psi(x+\hat{4}) + U^{4\dagger}_{x-\hat{4}}\psi(x-\hat{4})]/2$. Adding the baryonic chemical potential to the action therefore amounts to weights $f(a\mu) = 1 + a\mu$ and $g(a\mu) = 1 - a\mu$ to forward and backward time links respectively in the full lattice QCD action. Even for the free case, $\forall U^\mu(x) = I$, this action leads to μ-dependent a^{-2} divergences in the $a \to 0$ limit in energy density ϵ, and quark number density n. In particular, one has

$$\begin{aligned} \epsilon &= \mathbf{c_0 a^{-4}} + \mathbf{c_1}\mu^2\mathbf{a^{-2}} + c_3\mu^4 + c_4\mu^2T^2 + c_5T^4 \\ n &= \mathbf{d_0 a^{-3}} + \mathbf{d_1}\mu\mathbf{a^{-2}} + d_3\mu^3 + d_4\mu T^2 + d_5T^3. \end{aligned} \tag{1}$$

Subtracting off the vacuum contribution at $T = 0 = \mu$, eliminates the leading divergence in each case but the μ-dependent divergence persists. This has been, of course, known since long, and proposals to eliminate these divergences also exist. Hasenfratz and Karsch [6] as well as Kogut et al.

[7] proposed to modify the weights f and g to $\exp(\pm a\mu)$ to obtain finite results while simultaneously Bilić-Gavai [8] showed $(1 \pm a\mu)/\sqrt{(1 - a^2\mu^2)}$ also lead to finite results. Indeed, in general *any* set of functions f, g, satisfying $f(a\mu) \cdot g(a\mu) = 1$ with $f(0) = f'(0) = 1$ suffices to eliminate the μ-dependent divergence [9].

It is worth emphasizing that the analytical proof of elimination of divergences was provided *only* for free quarks [6, 8, 9], and thus also for perturbation theory. Numerical computations had to be performed to show that it worked for the non-perturbative interacting case as well [10].

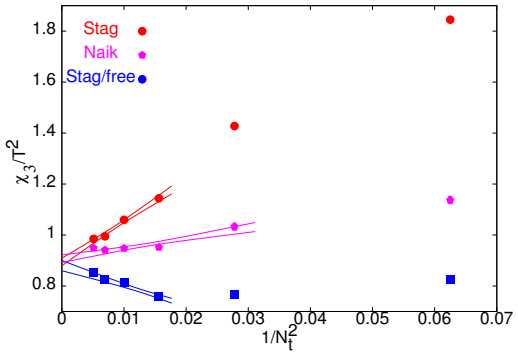

Figure 2: Continuum limit for quark number susceptibilities with different actions. A linear behaviour of the data and convergence to a unique continuum limit indicates the absence of any divergence. Taken from Ref. [10].

Figure 2 displays the results of [10] for the continuum limit of quark number susceptibilities with different actions computed for $\mu = 0$ at a constant temperature of $2T_c$. Since $\chi \sim \partial n/\partial\mu$, it too has a quadratic divergence which naturally is μ-independent. Furthermore, at fixed temperature $T^{-1} = N_t \cdot a$, the continuum limit of $a \to 0$ is equivalent to $N_t \to \infty$. The data in Figure 2 exhibit a linear behaviour and converge to a unique limit to the expected result at that temperature. Since a rising curve to infinity as $1/N_t \to 0$ would be the signal of a divergence, the absence of divergence is demonstrated in a non-perturbative manner as well for all $f(a\mu) \cdot g(a\mu) = 1$ choices of the weight factors as the χ is the same for all of them.

One may naturally wonder why this type of divergence was not encountered in the continuum theories. Specifically, one may attribute it to the latticization. A question then arises as to why, and how, does lattice introduce this divergence. An argument was provided [6] in the early work, stating that the divergence arises on the lattice due to the lack of a "formal" gauge symmetry. In the continuum theory, the μ term in the action appears as if it is a 4^{th} component of a constant gauge field. The simple naıve choice for the weights does not respect such formal global gauge invariance on the lattice while all the forms above where divergences are eliminated do have this formal gauge symmetry.

$$f(a\mu) \cdot g(a\mu) = 1 \Leftrightarrow F(a\mu) = \exp(\ln f(a\mu)), G(a\mu) = \exp(-\ln f(a\mu)). \tag{2}$$

It is important to note that even this formal analogy with the global gauge transformation strictly speaking needs an imaginary chemical potential and is thus invalid for the physically interesting case of the real chemical potential. Not surprisingly, it turns out to be **wrong** as well: Latticization

does not introduce divergence. It merely assists in spotting what exists in the continuum already [11]. Techniques such as contour integrals in the continuum have an inbuilt way to eliminate these divergences, either by subtraction or by a suitable regulator-based prescription. It has been demonstrated [11] that a similar subtraction scheme can be used on the lattice to remove the divergent contributions, leading to finite results in the $a \to 0$ limit also for the action with the linear chemical potential.

3. Universal Or Unique?

As discussed above, there are three different lattice action for finite density QCD, including the naıve one, for all of which divergences can be eliminated from the continuum limit result. A priori, the multiplicity of lattice actions corresponding to the same continuum QCD action is a familiar phenomenon. Indeed, the entire program of improvement of action, which aims to obtain better results even for not so small a, relies on the concept of *universality* which assures the same universal results for all physical quantities in the $a \to 0$ limit. As we will argue below, there are subtleties in the case of finite density actions which raise the question posed in the heading of this section.

Recall that the three lattice actions for $\mu \neq 0$ are characterised by the three different weight factors $f(\mu a)[g(\mu a)]$ for all the forward [backward] time-like links. Denoting them by L, E and S for their linear, exponential and square root forms, the corresponding weights are given by

$$\begin{aligned} f_L(\mu a) &= 1 + \mu a\,, & g_L(\mu a) &= 1 - \mu a \\ f_E(\mu a) &= \exp(\mu a)\,, & g_E(\mu a) &= \exp(-\mu a) \\ f_S(\mu a) &= (1 + \mu a)/\sqrt{1 - \mu^2 a^2}\,, & g_S(\mu a) &= (1 - \mu a)/\sqrt{1 - \mu^2 a^2}\,. \end{aligned} \tag{3}$$

Considering the classical continuum limit of the actions incorporating these weight factors, it is easy to verify that all of them have the same form at $O(\mu a)$. Indeed, these actions all differ in terms starting $O(\mu^2 a^2)$. Universality of physical results is assured if all these terms are irrelevant. Alternatively, if these actions produce different results, one ought to worry whether these terms are indeed irrelevant, and can thus be legitimately be added to the action at all. Assuming that they are irrelevant leads to the following paradox. It has been shown that the L-action has divergences mentioned earlier, which have to be subtracted by hand while the other two do not have them in an apparent violation of universality. Furthermore, since the divergences do exist in the continuum theory, as demonstrated in Ref. [11], one wonders how/whether they will reappear for the actions with f_E or f_S as $a \to 0$. As a next step to assess how universal the physical results from these actions are let us examine [12] the quark number susceptibility at $\mu = 0$ in some details in order to understand this difference. It is given by

$$\chi = \frac{1}{N_t N_s^3 a^2}\left[\left\langle\left(\mathrm{Tr}M^{-1}M'\right)^2\right\rangle + \left\langle \mathrm{Tr}\left(M^{-1}M'' - M^{-1}M'M^{-1}M'\right)\right\rangle\right], \tag{4}$$

Here M is the quark matrix (inverse propagator) and $M'(M'')$ is its first(second) derivative with respect to μ. We shall consider $\chi(\mu = 0)$, and therefore M, M' & M'' above are evaluated at $\mu = 0$. None of the terms depends on a explicitly [$S_F(a\mu) = \bar{\psi}M(a\mu)\psi$]. All the terms inside the

bracket are dimensionless, with the a^2 factor in the denominator supplying the dimension of χ. In the continuum limit of $a \to 0$, *all* the terms must vanish at least as a^2 for a nontrivial continuum limit of χ. Of course, if any term vanishes as a^n, $n \geq 3$, it will be irrelevant in the continuum limit while $n \leq 1$ would lead to a divergence. While comparing the three χ's, it should be noted that M' is the same for all f's while $M'' = 0$ for f_L and nonzero for others. Thus the presence of quadratic divergence for the linear form can be attributed to the vanishing of its M'' term, implying that the other two terms together have a^0 as the leading behaviour. The exponential and square root form have the same nonzero M'' at $\mu = 0$, coming from the $\mu^2 a^2$ terms in them. Its presence precisely cancels the a^0 piece of the other two terms leading to a divergence-free result for χ, as has been demonstrated for both the free theory(analytically) [6, 8, 9] and the quenched QCD (numerically) [10]. Therefore the M'' term must also have a^0, and it is ruled out that it vanishes faster than a^2 for any action. Hence, the difference in the results remains even in the continuum limit, in spite of M'' arising from an apparent **irrelevant** term in the action, namely $O(\mu^2 a^2)$ term.

It is clear that this problem of *non-universal* results worsens as one computes higher order fluctuations. Each successive order will have terms with the corresponding higher derivative of M, which in turn means higher derivatives of f (since $g = 1/f$ is assumed to cancel the divergences). While $f_E''(0) = f_S''(0)$, it is easy to show that $f_E'''(0) = f_E''''(0) = 1$ but $f_S'''(0) = 3$. Moreover, $f_S''''(0) = 9$ [12]. Indeed, $f_E^n(0) \neq f_S^n(0)$ for all $n > 2$. Let us recall that the third and fourth order baryon number susceptibilities, which are themselves related to various quark number susceptibilities up to the corresponding order, are crucially used in locating [13] the QCD critical point, both theoretically and experimentally. In fact, one hopes to improve upon the current results by incorporating as many higher orders as possible. Furthermore, the sixth order baryonic fluctuations have been advocated as signature for the $O(4)$ criticality [5] which too will need up to sixth order of the quark number susceptibilities.

As we argued above, the theoretical results for all these fluctuations *depend* on which f one uses irrespective of the choice to eliminate the divergence by the $f \cdot g = 1$ condition or by subtraction. One has the embarrassing situation of having as many predictions for physically measurable quantities as the number of f ! Thus the desire to eliminate the divergences by the $f \cdot g = 1$ condition does not appear to be in accord with universality.

Trying to understand the reasons beneath this violation of universality, we note that μ, being dimensionful, one has to ensure that it has a fixed value in physical units as $a \to 0$. Recall that in order to achieve the continuum limit at a fixed temperature $T = 1/N_t a$ in physical units one needs to take $a \to 0$ *along with* $N_t \to \infty$. Thus not only a but $Ta = 1/N_t$ are two separate scales which need to be tuned appropriately. Similarly, one will have to treat a and μa as separate scales which will have to be approach zero by themselves such that μ is held the same in physical units. At the purely classical level, where one examines the approach of the lattice action to that in the continuum, the additional $O(\mu^2 a^2)$ term can be easily seen to vanish **iff** $a \to 0$ limit is the same as $\mu a \to 0$. At the quantum expectation level, on the other hand, we expect μ/T to be held fixed as $a \to 0$, making $\mu a \to 0$ a separate limit. The n^{th} derivatives of P will be, by definition, sensitive to the corresponding $\mu^n a^n$ terms in P for $n \geq 2$, exposing their relevant nature in the corresponding susceptibilities, and consequently to pressure. It needs to be emphasized that while the entire effort to modify the f_L and g_L from their natural linear prescription, which can be derived from an underlying conserved current on the lattice, was motivated by the question of divergences in eq,(2),

the non-universality pointed out above has nothing to do with the diverging terms. It is primarily related to the question of adding term to all orders in μa with the assumption/hope that universality will make their contribution irrelevant. The elimination of divergence is, in fact, a proof that it is not so, *i.e.*, μa being a separate scale which needs to be tuned in the continuum limit these terms are relevant. We advocate that it is more advisable to use the **unique** f_L and g_L in lattice computations than to sacrifice universality.

Changing from the linear form to either the exponential or the square root form leads to a further problems. The actions with either f_E or with f_S has no conserved charge anymore [12]. Following the canonical method to derive current conservation for actions with or without chemical potential terms in the continuum, or on the lattice, it is easy to prove this. Both in the continuum and for the f_L,g_L lattice action, the *same* current conservation equation results[12] for $\mu \neq 0$ as for $\mu = 0$, and thus the conserved charge is unaffected by $\mu \neq 0$ terms, as it must. On the other hand, for f_E and f_S-actions with $\mu \neq 0$ one gets a conserved charge that itself depends on μ ! As a direct consequence, $Z \neq \sum_n z^n Z_n^C$ on the lattice for these two actions. This is possible only if the $a \to 0$ and $\mu a \to 0$ limits are identical for *all* μ. This implies that one cannot define an *exact* canonical partition function on lattice from the Z defined this way for the actions employing the exponential or the square root forms. Only for the linear μ-case one has an exactly conserved charge on the lattice, and thus an *exact* canonical partition function $Z = \sum_n z^n Z_n^C$ on the lattice.

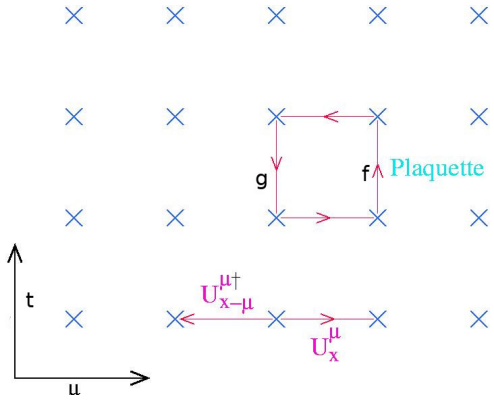

Figure 3: Illustration of the weight factors in the t-μ plane (μ =1,2,3).

The $f \cdot g = 1$ condition introduces differences in the μ-dependence of the partition function Z which again seem to survive the $a \to 0$ continuum limit. Given the fact only timelike links acquire a nontrivial weight factor at $\mu \neq 0$, it is obvious that any μ-dependence for Z arises solely due to loops with time-like links, and hence is $\propto (f \cdot g)^l$, where l is the number of forward or backward links in a Wilson loop. Figure 3 illustrates this for $l = 1$, the timelike plaquette. Since $f_L \cdot g_L = 1 - \mu^2 a^2$, quark loops of **all** sizes and types contribute to the μa dependence for the Z. This is similar to the expectation in the continuum as well where time-like Wilson loops of **all** sizes would contribute. However, only quark loops winding around the T direction contribute to μ dependence for the other two cases since $f \cdot g = 1$. The μ-dependence thus arises from only a topologically distinct class of Wilson lines, raising the same universality violation issue again. Of course, only explicit calculations may show what is the fate of the topologically trivial Wilson loops of all sizes and whether they somehow add up to a μ-independent expression. At least, this

apparent paradox suggests that it is crucial to check if universality is obeyed for all three actions perhaps by considering other theories which do not have the sign problem for nonzero μ.

4. Summary

Prescriptions to modify weights for nonzero chemical potential in the lattice actions which satisfy $f \cdot g = 1$, where $f(\mu a)[g(\mu a)]$ is the weight factor for a forward [backward] timelike gauge link, such as the popular exponential form, violate universality for quark number susceptibilities. As their order increases, further non-universal results arise depending on the exponential[6, 7] or the square root form [8]. Employing them leads to f-dependent results even in the continuum limit for fluctuations measurable in, and of great interest to, heavy ion collision experiments.

μ-dependent divergences, for elimination of which the condition was invented, are not unique to lattice regularization. Indeed, lattice only reproduces faithfully what exists in the continuum field theory. Following the example of continuum field theory, one can subtract the free theory divergences by hand, and this process has been shown to suffice even nonperturbatively [11]. The linear form preserves the quark/baryonic current conservation on the lattice, and retains the same conserved quark/baryon number for all μ. On the other hand, the conserved charge depends on μa for the other two. As a result the canonical partition function can meaningfully be defined on the lattice exactly only for the linear form.

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