CONUNDRUMS AT FINITE DENSITY*

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Extending the successes of lattice quantum chromodynamics (QCD) at zero as well as nonzero temperatures to nonzero density is extremely desirable in view of the quest for the QCD phase diagram both theoretically and experimentally. It turns out though to give rise to some conundrums whose resolution may assist progress in this exciting but difficult area, and should therefore be sought actively.

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1. Introduction

The theory of strong interactions, Quantum Chromo Dynamics (QCD), has intriguing properties such as confinement or chiral symmetry breaking which have been enigmas for over half a century. A major reason is, of course, the dominance of large coupling in such hadronic properties. Crucial clues in building physical pictures to understand them were provided by the studies of simple models such as the bag model or NJL model. The discovery of instanton solutions and the subsequent investigations of instanton-based models enhanced our understanding further by emphasizing the role of the zero and near-zero modes of the Dirac equation for interacting quarks. Investigating all these models in extreme environments such as high temperatures/densities led to a variety of phase diagrams of strongly interacting matter. It may not come as a surprise that even qualitative features of these model phase diagrams differed substantially, not to mention the quantitative details. For instance, the early sketches of the QCD phase diagram display separate deconfinement and chiral transitions for all temperatures and densities [1]. Nevertheless, they pointed to an interesting path to fathom chiral symmetry breaking and/or confinement.

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QCD formulated on a space-time lattice has yielded a more firm guidance in refining these pictures at finite temperatures to give us a reliable, in some cases even quantitative knowledge of the phase structure. However, extending this to finite densities or equivalently nonzero chemical potential, one encounters conundrums many of which are unrelated to the latticization and were hitherto still unknown to exist. These pose significant hurdles in excursions inside the diagram from the temperature axis. There is, of course, the famous fermion sign(phase) problem at nonzero baryon density or equivalently nonzero baryon chemical potential. The aim of this paper is to draw attention to the other, perhaps equally serious, problems.

2. The $\mu \neq 0$ problems: I. Divergences

Let us begin by recalling that the (baryonic) chemical potential is a Lagrange multiplier to enforce the constraint of (net baryon) number conservation in the grand canonical ensemble: $\partial_\mu J_\mu^B = 0$ is the current conservation equation and $N_B = \int \mathrm{d}^3 x J_0^B$ is the conserved charge. Following the same principle on lattice, one obtains [2] a point split version for the conserved number. Thus, introducing the chemical potential on the lattice amounts to multiplying the forward [backward] time-like links with $f(\mu a)$ [$g(\mu a)$], with $f(\mu a) = 1 + \mu a$ [$g(\mu a) = 1 - \mu a$] as seen in Fig. 1 for the naïve fermions. This form of f and g, which has been shown to remain the same for Wilson/Staggered/Improved local fermions as well, leads [2] to the following form of the energy density and quark number density for a gas of free quarks:

$$\begin{aligned} \epsilon &= c_0 a^{-4} + c_1 \mu^2 a^{-2} + c_3 \mu^4 + c_4 \mu^2 T^2 + c_5 T^4 \,, \\ n &= d_0 a^{-3} + d_1 \mu a^{-2} + d_3 \mu^3 + d_4 \mu T^2 + d_5 T^3 \,. \end{aligned} \tag{1}$$

Here, c_i and d_i are constants, a is the lattice spacing, and the subscript B of μ has been dropped for simplicity as well as to indicate that these expressions

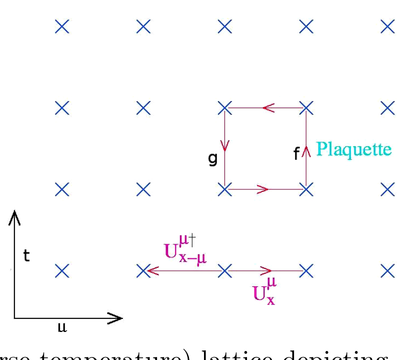

Fig. 1. Space-time (inverse temperature) lattice depicting a smallest loop (plaquette) with time links and a quark covariant derivative term.

hold for any conserved charge such as strangeness or electric charge. In the continuum limit of $a \to 0$, one obtains a leading quartic divergence and a subleading μ-dependent quadratic one. Subtracting off the vacuum contribution at $T = 0 = \mu$ eliminates the leading divergence in each case. However, the μ-dependent a^{-2} divergences persist in both the energy density and the quark number density. Note that these divergences are present for the free theory itself. As a solution to this problem, different forms of f and g have been proposed. The popular exponential choice [3], $f(\mu a) = \exp(\mu a)$ and $g(\mu a) = \exp(-\mu a)$ as well as another choice [2], $f(\mu a) = (1 + \mu a)/\sqrt{(1-\mu^2 a^2)}$ along with $g(\mu a) = (1-\mu a)/\sqrt{(1-\mu^2 a^2)}$, both lead to their corresponding $c_1 = 0 = d_1$, which then lead to finite results in the continuum limit. Indeed, the μ-dependent divergences are eliminated for all $f \cdot g = 1$ [4]. One anticipates this analytical proof of the lack of μ-dependent divergences for free quarks to hold true in any order-by-order perturbative inclusion of interactions with gluons. However, numerical simulations are needed, and were employed [5] to extend the proof for the non-perturbative interacting case as well, as shown in Fig. 2. Both the lack of any diverging behaviour as well as a unique continuum limit is evident in the data.

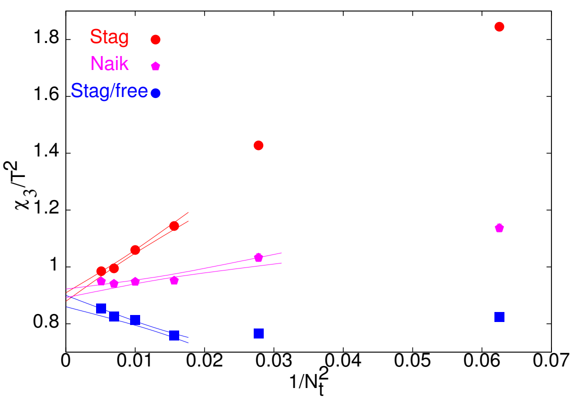

Fig. 2. Continuum limit for quark number susceptibilities with different actions. A linear behaviour of the data and convergence to a unique continuum limit indicates the absence of any divergence. Taken from Ref. [5].

A natural question arises as to why there are three (or more) lattice QCD actions when the continuum QCD has only one. The usual answer is universality. As long as all these actions reduce to the continuum QCD action in the limit of $a \to 0$, universality tells us that physics should be the same for all of them in that limit. Expanding the functions f, g in powers of μa, one finds that the three actions differ by terms of $\mathcal{O}(\mu^2 a^2)$ and higher which vanish in the $a \to 0$ limit and are thus *irrelevant* terms.

Paradox: These irrelevant terms vanish from action as $a \to 0$ but do eliminate divergences. This appears to be a violation of universality! On the other hand, since the divergence cancelling terms are absent in the continuum theory, as for the naïve case, one wonders whether the divergences are present in the continuum theory itself. As for any usual improved action, one hopes that universality will ensure physical results are unaffected but it seems prudent to check it in view of the above conundrum.

These modified/improved actions have a further problem. One can work out the current conservation equation for the Lagrangian with $\mu \neq 0$. It remains unchanged only for the linear μ-case. It acquires $\mu^2 a^2$ and higher order terms of even powers in all the other cases. Thus, integrating over spatial dimensions, one obtains a conserved charge on the lattice only for the linear μ-form. For all the divergence eliminating form of actions, one has **no** conserved charge on the lattice anymore! Consequently, $\mathcal{Z} \neq \exp(-\beta[\hat{H} - \mu\hat{N}])$ on the lattice for them and, therefore, one cannot define an *exact* canonical partition function on lattice from the $\mathcal{Z}$ defined this way. $\mathcal{Z} = \sum_n z^n \mathcal{Z}_n^C$ on the lattice only for the naïve linear μ-action. Once again, one has to hope that it is possible at least in the continuum limit of $a \to 0$ but clearly an explicit demonstration is necessary.

Most computational methods, if not all, consist of integrating out the quark fields, leading to the quark determinant. Due to its gauge-invariant nature, the determinant can be seen as a sum over all possible quark loops. Any μ-dependence for $\mathcal{Z}$ arises solely due to loops with time-like links, and hence is $\propto (f \cdot g)^l$, where l is the number of positive time-like links in the loop. This is illustrated for the simplest case of $l = 1$ in figure 1. Quark loops of *all* sizes and types contribute for the naïve case of f, $g = 1 \pm \mu a$, as is indeed the case also in the continuum. However, since $f \cdot g = 1$ for the other two actions, it is clear that only limited number of loops contribute. Indeed, only quark loops winding around the T-direction contribute to μ_B dependence for these cases. Again, if all the actions were to lead to the *same* physics, as they ought to, small quark loops which are topologically trivial must start also contributing, as $a \to 0$. It is far from clear how this may happen since for all non-vanishing a, the $f \cdot g = 1$ condition applies and these loops do *not* contribute to any μ-dependence. One possible way out maybe that the small loops sum up to a μ-independent constant, preferably zero. It is far from clear how this might come about in the interacting theory. This is yet another conundrum which universality suggests should resolve itself in the continuum limit, and needs to be verified by explicit computations.

3. Divergences exist in the continuum too

Let us recall that the conundrums discussed in the section above were related to the differences in the $f(\mu)$ and $g(\mu)$: $f \cdot g = 1 - \mu^2 a^2$ for the naïve linear case and $f \cdot g = 1$ for the other two. This, in turn, arose as the latter got rid of the μ-dependent divergences that arise for the former choice. Since in the continuum limit one finally has only the linear form, one may wonder whether the μ-dependent divergences exist in the continuum as well, and the lattice as a regulator is merely reproducing them systematically or whether the latticization itself introduces the divergences.

Indeed, it turns out that contrary to the common belief, the free theory divergences are **not** lattice artifacts. They exist in continuum too. Instead of the lattice regulator, one can employ a momentum cut-off Λ in the continuum theory to show [6] the presence of $\mu\Lambda^2$ terms in number density easily. We summarise below why one ought to expect them in the continuum itself.

The quark number density, or equivalently third of the baryon number density for a single flavour, is defined as

$$n = \frac{T}{V}\frac{\partial \ln \mathcal{Z}}{\partial \mu}|_{T=\text{fixed}} \tag{2}$$

with $\mathcal{Z}$ for free fermions given by

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \, \mathrm{e}^{\int_0^{1/T} \mathrm{d}\tau \int \mathrm{d}^3x \left[-\bar{\psi}(\gamma_\mu \partial_\mu + m - \mu\gamma_4)\psi\right]} . \tag{3}$$

Evaluating the quark number density, n, in the momentum space for the massless free quark gas, one has

$$n = \frac{2iT}{V}\sum_m \int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{(\omega_m - i\mu)}{p^2 + (\omega_m - i\mu)^2} \equiv \frac{2iT}{V}\int \frac{\mathrm{d}^3p}{(2\pi)^3}\sum_{\omega_m} F(\omega_m, \mu, \vec{p}) , \tag{4}$$

where $p^2 = p_1^2 + p_2^2 + p_3^2$ and $\omega_m = (2m+1)\pi T$. In the usual contour method, the sum over m or ω_m gets replaced as an integral in the complex ω-plane. Together with the subtracted vacuum ($\mu = 0$) contribution, one has in the complex ω-plane line integrals along the directed arms 3 and 1 in Fig. 3. Adding and subtracting the side arm line integrals, one obtains the canonical answer from the residue of the pole P in Fig. 3. One still has to evaluate the side arm contributions.

Let us introduce a cut-off Λ for all 4-momenta at $T = 0$ for a careful evaluation of the divergent arms 2 and 4 contributions in Fig. 3. The $\mu\Lambda^2$ terms can be seen to arise [6] from the arms 2 and 4

$$\int \frac{\mathrm{d}^3p}{(2\pi)^3}\left(\int_2 + \int_4\right)\frac{\mathrm{d}\omega}{\pi}\frac{\omega}{p^2+\omega^2} = -\frac{1}{2\pi}\int \frac{\mathrm{d}^3p}{2\pi^3}\ln\left[\frac{p^2+(\Lambda+i\mu)^2}{p^2+(\Lambda-i\mu)^2}\right] . \tag{5}$$

Utilising the fact that $\Lambda \gg \mu$, the integrand can be expanded in μ/Λ to discover that while the leading Λ^3 terms do indeed cancel there is a nonzero

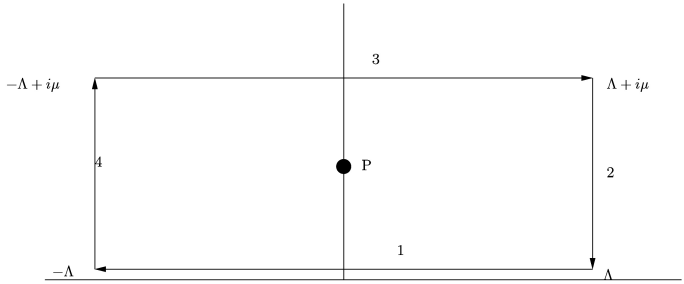

Fig. 3. The contour diagram for calculating the number density for free fermions at zero temperature. P denotes the pole.

coefficient for the subleading $\mu\Lambda^2$ term. It may be worth noting that the arms 2 and 4 make a finite contributions to the μ^3 term as well. One usually ignores the subleading contribution from the arms 2 and 4, amounting to a subtraction of the 'free theory divergence' in the continuum. This practice suggests a prescription of subtracting the free theory divergence by hand on the lattice as well. Such a prescription surely works in including the interactions in a perturbation theory. It has been tested in numerical simulations, and found to work excellently.

In order to test whether the divergence is truly absent in simulations, one needs to take the continuum limit $a \to 0$ or, equivalently, $N_T \to \infty$ at fixed $T^{-1} = aN_T$. For quenched QCD at $T/T_c = 1.25$ and 2 and for quark mass $m/T_c = 0.1$, lattices with $N_T = 4$, 6, 8, 10 and 12 were employed [6]. On 50–100 independent configurations, quark number susceptibility was computed. Since it is a derivative of the number density with μ, it should have a simple a^{-2} divergence. The $1/a^2$-term for free fermions on the corresponding $N^3 \times \infty$ lattice was subtracted from the computed values of the susceptibility in simulations. The results are displayed in Fig. 4 as a function of $1/N_T$. If

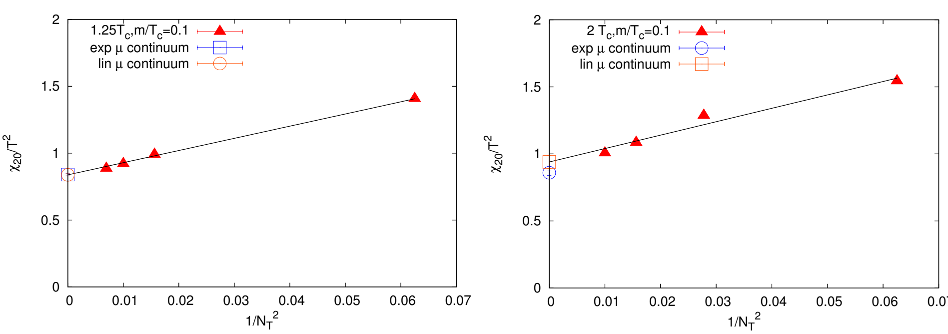

Fig. 4. The quark number susceptibility at $1.25\,T_c$ (left panel) and $2\,T_c$ (right panel) for $m/T_c = 0.1$. Taken from Ref. [6].

the interactions were to induce additional non-perturbative divergent contribution over and above the subtracted free theory ones, the susceptibility should behave as $\chi_{20}/T^2 = c_2(T)N_T^2 + c_1(T) + c_3(T)N_T^{-2} + \mathcal{O}(N_T^{-4})$. The divergent c_2-contribution would then lead to a rapid shoot-up near the χ_{20}/T^2-axis. c_1 is the expected continuum result with c_3 governing the approach to the limit.

A glance at both the panels of Fig. 4 shows an evident lack of any divergent rise in both or equivalently $c_2 \simeq 0$ for both temperatures, since both sets of data display only positive slope throughout. Furthermore, the extrapolated continuum result coincides with the earlier result obtained with the $\exp(\pm a\mu)$ action [7].

4. The $\mu \neq 0$ problem: II. Quark type

Placing quark fields on a lattice has the famous doubling problem. Mostly staggered quarks are used in lattice QCD simulations, as they possess some chiral symmetry. Consequently, the chiral condensate, $\langle\bar{\psi}\psi\rangle$, can be employed as an order parameter to investigate the QCD phase diagram as a function of T and μ_B. However, flavour and spin symmetry are broken for them. Moreover, flavour singlet $\mathrm{U}_A(1)$ symmetry is broken explicitly and thus the question of the $\mathrm{U}_A(1)$ anomaly is mute. On the other hand, the holy grail of phase diagram, namely, the QCD critical point needs two light flavours and the anomaly to persist [8] for the chiral transition on the $\mu_B = 0$ axis to be of second order, and hence it to be a cross over for physical light quarks. Domain Wall or Overlap quarks are, therefore, a better choice due to their "exact" chiral symmetry on the lattice. Although their nonlocality makes them computationally expensive, one can at least in principle employ them to study the QCD critical point. Defining chemical potential for them turns out, however, to be tricky. In particular, introducing chemical potential for either of them faces yet another conundrum related to the divergence problem discussed above.

The usual Wilson Dirac fermion matrix is at the heart of definition of both these nonlocal quarks. Adapting the exponential prescription for D^{Wilson}, Bloch and Wettig [9] introduced μ. This definition was shown to have no divergences in the free theory [10, 11]. Unfortunately, the BW prescription breaks the lattice chiral symmetry at any finite density [11], leaving us without any order parameter.

Luckily, a lattice action with continuum-like chiral symmetries for quarks at nonzero μ has been proposed already [12]. Since the massless continuum QCD action for nonzero μ can be written explicitly as a sum over right and left chiral modes of quarks, the key idea was to employ similar chiral projections for the Overlap quarks to construct the action at nonzero μ. It was shown to have exact chiral invariance on the lattice, and thus chiral condensate works as an order parameter for the entire T–μ_B plane [12]. Moreover, using the Domain Wall formalism, it was also shown why this is physically the right thing to do: it counts only the physical (wall) modes as the baryon number, while the BW action includes all the unphysical heavy modes as well.

It turns out, however, that this chirally-invariant Overlap action with nonzero μ is linear in μ, *i.e.*, comes with divergences. Furthermore, inventing the f, g in this case which will *(i)* eliminate the divergences and *(ii)* still preserve the exact chiral invariance on the lattice has so far not been possible. Recently, it has been shown that SLAC fermions, which too are nonlocal but possess exact chiral symmetry, also need a linear form in μ at finite density, and it too possesses these divergences [13]. Thus, the linear form seems the natural physical choice if chiral symmetries are to be exact on the lattice, although the resultant free theory has divergences. As in the previous section, these divergences can always be subtracted out especially if eliminating them using nonlinear forms for f, g leads to the conundrums already discussed.

5. The $\mu \neq 0$ problems: III. Topology

Instanton vacuum provides a nice physical picture of chiral symmetry breaking and the chiral phase transition [14]. Overlap Dirac operator spectra have been used to investigate topology and to understand the nature of the high temperature phase. In particular, the number of low quark eigenmodes get depleted [15] as T goes up and the number of exact zero modes, a measure of topological susceptibility, falls exponentially in the quark–gluon plasma phase. Naturally, one can envisage doing a similar study for the high density phase. However, it is not easy for QCD due to the sign problem.

QCD at nonzero isospin density as well as two colour QCD do not have a sign problem, as the quark determinant is real in each of these cases. A lot of work on both the cases has been done in studying the phase structure [16, 17]. In both these theories, it has been observed that an increase in number density and a drop in the chiral condensate occurs at the same $\mu_{\rm c}$. Interestingly though, the spectra of the corresponding low quark modes appear unaffected [18, 19] as a function of the corresponding μ even when one runs through $\mu_{\rm c}$ restoring the chiral symmetry. This observation in two different theories raises an interesting possibility that the chiral symmetry restoration is decoupled from a change in topology, and thus from perhaps the deconfinement transition, at finite density/chemical potential in general.

Figure 5 displays the eigenvalue distribution [18] on the log scale to highlight differences in the near-zero modes in the low and high density phases for the nonzero isospin case.

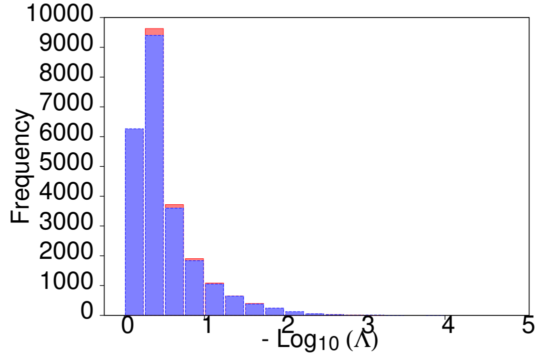

Fig. 5. A comparison of the near-zero quark mode distributions below and above the finite isospin chemical potential at which chiral symmetry restoration occurs. No visible difference is evident. Taken from Ref. [18], where further details can be found.

Similarly, very little or no change is visible in the number of exact zero modes or, equivalently, the topological susceptibility in both the cases [18, 19] across the corresponding chiral symmetry restoring transition.

6. Summary

Investigations at finite density using the reliable lattice QCD techniques face many hurdles, the most famous of which is the sign/phase problem of the quark determinant. We pointed out that the introduction of the chemical potential on the lattice itself is plagued with conundrums. Most of these, including the μ-dependent divergence, are not due to latticization. Indeed, lattice only reproduces faithfully what exists in the continuum field theory. Elimination of the divergence by modifications of action, as is commonly done, leads to apparent conflicts with universality which need to be resolved by carrying out continuum limit computations for many different ways of adding chemical potential.

The chiral and flavour invariance is crucial for the QCD critical point investigations. Eventually, one will have to employ the overlap quarks at finite density for reliable simulations. Doing so while retaining the chiral symmetry seems to lead to a linear μ-dependent action always. Subtraction of free theory divergences was demonstrated to suffice nonperturbatively and should be tested for the overlap action as well.

Numerical simulations suggest that the distribution of the topological charge, Q, changes very little in going from the low T and low density phase to the low T and high density phase as one goes across the isospin chemical potential $\mu_{\rm I}$ or $\mu^{N_{\rm c}=2}$ phase transitions, although the chiral condensate drops and number density picks up at each of these phase transitions. This is in contrast to the change of low-T to high-T phase, which exhibits an (exponential) fall-off. This may be a hint towards a possible separation of the chiral symmetry restoring transition and the deconfining phase at finite density. It will be challenging to check if this is indeed so for the finite density QCD.

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