Physics Letters B 749 (2015) 8–13

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Divergences in the quark number susceptibility: The origin and a cure

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ARTICLE INFO

Article history:
Received 10 April 2015
Received in revised form 4 July 2015
Accepted 16 July 2015
Available online 21 July 2015
Editor: J.-P. Blaizot

ABSTRACT

Quark number susceptibility on the lattice, obtained by merely adding a μN term with μ as the chemical potential and N as the conserved quark number, has a quadratic divergence in the cut-off a. We show that such a divergence already exists for free fermions with a cut-off regulator. While one can eliminate it in the free lattice theory by suitably modifying the action, as is popularly done, it can simply be subtracted off as well. Computations of higher order susceptibilities, needed for estimating the location of the QCD critical point, then need a lot fewer number of quark propagators at any order. We show that this method of divergence removal works in the interacting theory.

1. Introduction

The phase diagram of the strongly interacting matter described by Quantum Chromodynamics (QCD) has been a subject of intense research in the recent years. Usual weak coupling perturbative approach may work for sufficiently high temperatures. However, the gauge interactions are likely to be strong enough for temperatures close to Λ_{QCD}, the typical scale of QCD, necessitating strong coupling techniques. Lattice QCD is the most successful non-perturbative technique which has provided us with some interesting results pertaining to the phase diagram. It is now fairly well known from independent lattice studies that the transition from the hadron to the quark gluon plasma phase at zero baryon density is a crossover [1–3]. At non-zero density, or equivalently nonzero quark chemical potential μ, one has to face a sign problem: quark determinant is complex. This does not allow for an importance sampling based Monte Carlo study. Several ways have been advocated in the recent years to circumvent the sign problem in QCD [4–7]. From perturbative studies of model quantum field theories with the same symmetries as QCD [8] and chiral model investigations at $T << \mu$ [9], a critical end-point is expected in the QCD phase diagram. If present, the critical-end point would result in the divergence of the baryon number susceptibility. Thus its Taylor expansion [7] at finite baryon density as a series in μ_B/T can be used to compute the radius of convergence, and therefore, an estimate of the location of the critical end-point [10,11]. First such estimates of the radius of convergence of the Taylor series have predicted the critical end-point to be at $T_E/T_c = 0.94$ and $\mu_B/T_E = 1.8(1)$ [11]. Recently, a study on a finer lattice has suggested the continuum limit to be around $T_E/T_c = 0.94(1)$, $\mu_B/T_E = 1.68(5)$ [12]. In the heavy-ion experiments, the fluctuations of the net proton number could act as a proxy for the net baryon number. The STAR experiment at Brookhaven National Laboratory has reported the measurements for the fluctuations of the net proton number for a wide range of center of mass energy $\sqrt{s}$, of the colliding heavy ions between 7.7 and 200 GeV. At $\sqrt{s} = 19.6$ GeV the experimental data are observed [13] to deviate from the predictions of the proton fluctuations for models which do not have a critical end-point, and is similar to the lattice QCD-based predictions [14] for a critical point, signaling its possible presence. It would be thus important to have a thorough understanding of the systematics of the lattice QCD results and make them as much reliable as possible.

In addition to the usual suspects, such as continuum extrapolation or effects due to the finiteness of the lattice spacing, the scale-setting, and the statistical precision of the measurements, a key new important factor is that the radius of convergence estimate requires ratios of as many higher orders of quark number susceptibilities (QNSs) as possible. Currently the state of the art is the eighth order QNS [10,11]. It is very important to verify whether the existing results are stable if ratios of further higher order of QNS are taken into account. In order to calculate the QNS of order m, one has to take the mth-derivative of the free energy with respect to the quark chemical potential. Since the popular method

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http://dx.doi.org/10.1016/j.physletb.2015.07.036

of incorporating the chemical potential on the lattice is through $\exp(\pm\mu a)$ factors multiplying the forward and the backward temporal gauge links respectively of the fermion operator [15,16], there is an ever increasing proliferation of terms of varying sign as m increases. Their large number as well as the large cancellations amongst them at a specific order make it difficult to increase m beyond eight at present. Introducing the chemical potential by a μN-term, where N is the corresponding conserved charge, leads to both much fewer terms and lesser cancellations at the same m [17], thereby reducing the computational cost up to 60% at eighth order; more savings ought to accrue by going to even higher orders. Not only will this improve the precision of the location of the critical point but more precise Taylor coefficients and more terms in the Taylor expansion can potentially also lead to a better control of the QCD equation of state at finite baryon density which will be needed for the analysis of the heavy-ion data from the beam energy scan at RHIC as well as the future experiments at FAIR and NICA.

In this paper, we discuss whether such a linear in μ approach is viable or has unsurmountable problems by comparing with the usual exponential in μ method. In Section 2, we revisit the number density for non-interacting fermions in the continuum using a cut-off regulator. We point out that divergences appear already in the continuum free theory when the cut-off regulator is taken to infinity contrary to the common knowledge. We then discuss an approach to tackle this divergence in the free theory. By performing continuum extrapolation of the second and fourth order QNS for quenched QCD for the linear in μ method, we validate it in Section 3. This is the most important result of our paper. We discuss its possible consequences and the extensions to higher order QNS.

2. Thermodynamics of non-interacting fermions

QCD thermodynamics can be derived from its partition function, written in the path integral formalism [18] as,

$$\mathcal{Z} = \int \mathcal{D}A_\mu \mathcal{D}\bar{\psi}\mathcal{D}\psi \times e^{\int_0^{1/T} d\tau \int d^3x \left[-1/2\,\mathrm{Tr}(F^2_{\mu,\nu}) - \bar{\psi}(\gamma_\mu(\partial_\mu - igA_\mu) + m - \mu\gamma_4)\psi\right]}, \quad (1)$$

where ψ, $\bar{\psi}$ and A_μ represent the quark, anti-quark and the gluon fields respectively, whose the color indices are not written explicitly above. μ is the chemical potential for the net quark number with the corresponding conserved charge being $\int d^3x \bar{\psi}\gamma_4\psi$. Generalizations to various conserved flavor numbers is straightforward. For simplicity, we will consider only a single flavor with the baryonic chemical potential $\mu_B = 3\mu_q$. Appropriate derivatives of $\mathcal{Z}$ lead to various thermodynamical quantities, e.g., the quark number density, or equivalently (1/3) the baryon number density, is defined as,

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

Earlier attempts to discretize the above theory to investigate the finite baryon density physics on a space–time lattice revealed μ-dependent quadratic divergences in the number density and the energy density when the chemical potential is introduced in the quark Dirac operator by multiplying it with the corresponding conserved charge on the lattice. These divergences, which appear as a μ/a^2 term in the expression for the lattice number density with a as the lattice spacing, are present even if the gauge interactions are absent. Through explicit calculation of the number density for non-interacting fermions on the lattice, it was then shown [15,16,19] that suitable modification of the μN term in the action, eliminates these divergent terms on the lattice, and yields a finite $a \to 0$ continuum limit. Numerical studies of the QNS for the interacting theory subsequently confirmed that once the free theory divergences are thus eliminated, no further divergences arise [20,21]. A succinct way to describe all the various actions is to introduce functions $f(\mu a)[g(\mu a)]$ as the multiplying factors for the forward (backward) timelike gauge fields on the lattice. While for the naive discretization, $f = 1 + a\mu$ and $g = 1 - a\mu$ leads to a divergent baryonic susceptibility in the continuum limit, the choice $f = \exp(a\mu)$ and $g = \exp(-a\mu)$ does not.

Clearly since all derivatives of f and g are nonzero for the exponential case, whereas only the first derivative is nonzero for the linear case, higher order QNS are a lot simpler for the latter. Furthermore, for fermions with better chiral properties such as the Overlap fermions or the Domain Wall fermions, the exponential form leads to a loss [22] of the exact chiral symmetry on lattice for nonzero μ. Indeed the only chiral symmetry preserving form these fermions have for finite μ and a is the linear form [23]. This motivates us to revisit the issue of the nature and origin of these divergences when the chemical potential enters linearly instead of the exponential form. As we show below, the divergences are present for the continuum free fermions as well, and the lattice regulator simply faithfully reproduces them. While one can employ the freedom of lattice action to eliminate them, it is not necessary. Indeed, one can perhaps employ simpler subtraction methods to eliminate them, as we demonstrate in this paper.

2.1. Continuum free fermions

Results for the continuum free fermions are easily found in textbooks [18]. We review them below solely with the idea of pointing out explicitly the μ-dependent divergences present in them. For simplicity, we consider only massless fermions though this derivation can be easily extended for finite mass. The expression for the number density for free fermions is easily obtained from the definitions above as

$$n = 4iT \sum_{j=-\infty}^{\infty} \int \frac{d^3p}{(2\pi)^3} \frac{(\omega_j + i\mu)}{p^2 + (\omega_j + i\mu)^2} \equiv 4iT \sum_{j=-\infty}^{\infty} F(\omega_j, \mu)\,, \quad (3)$$

where $p^2 = p_1^2 + p_2^2 + p_3^2$ and $\omega_j = (2j+1)\pi T$. Here we choose the gamma matrices to be all Hermitian as is common in lattice studies. The continuum convention followed in the standard texts has only γ_4 as Hermitian and the other gamma matrices are anti-Hermitian. The expression in Eq. (3) can be evaluated by the usual trick of converting the sum over energy states to a contour integral. The Matsubara frequencies lie on the real ω-axis. Following [18] again, one can employ an infinitesimally small contour around the each pole on the real ω axis to represent the ω_j-sum, and obtain

$$2\pi T \sum_j F(\omega_j, \mu) = Lt_{\epsilon\to 0}\left[\int_{-\infty+i\epsilon}^{\infty+i\epsilon} \frac{F(\omega,\mu)d\omega}{e^{i\omega/T}+1} + \int_{\infty-i\epsilon}^{-\infty-i\epsilon} \frac{F(\omega,\mu)d\omega}{e^{i\omega/T}+1}\right]. \quad (4)$$

The line integrals in Eq. (4) can in turn be written in terms of contours in the upper and lower complex ω planes. Using the exact identity,