PROCEEDINGS OF SCIENCE

How the Quark Number fluctuates in QCD at small chemical potential

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We discuss the distribution of the quark number over the gauge fields for QCD at nonzero quark chemical potential. As the quark number operator is non-hermitian, the distribution is over the complex plane. Moreover, because of the fermion determinant, the distribution is not real and positive. The computation is carried out within leading order chiral perturbation theory and gives direct insight into the delicate cancellations that take place in contributions to the total baryon number.

The XXVIII International Symposium on Lattice Field Theory, Lattice2010
June 14-19, 2010
Villasimius, Italy

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1. Introduction

First principle predictions for the QCD phase diagram would be of great value as a benchmark for the international experimental heavy ion program. In principle, we know precisely how to proceed: start from the grand canonical partition function,

$$Z_{1+1} = \int dA\, \det{}^2(D+\mu\gamma_0+m)\, e^{-S_{\rm YM}}, \tag{1.1}$$

and study the baryon number as a function of the chemical potential, μ, and temperature for quark masses m (for notational simplicity we consider the two flavor theory in these proceedings). As the phase transitions occur in the non perturbative domain it is natural to turn to lattice QCD. While we know exactly how to include the chemical potential on the lattice [1, 2], in practice, our studies are limited by the fact that the fermion determinant at nonzero values of the chemical potential becomes complex

$$\det{}^2(D+\mu\gamma_0+m) = |\det(D+\mu\gamma_0+m)|^2 e^{2i\theta}. \tag{1.2}$$

This *sign problem* invalidates the standard Monte Carlo method which is at the hart of lattice QCD. The sign problem is not only hard because the average of the phase factor is exponentially small [3], it is also challenging because much of our intuition for statistical systems leads to wrong conclusions at non zero μ. Most prominently, a probabilistic argument leads one to conclude that the chiral condensate is continuous as a function of the quark mass at $m = 0$ for any non zero value of μ [4]. Rather, as the solution [5] of this Silver Blaze problem shows, it is imperative that we consider distribution functions that take complex values. Only through extreme complex oscillations of the eigenvalue density of the Dirac operator is it possible to understand how the discontinuity of the chiral condensate remains non zero in the presence of the chemical potential. Here we will show [6] that the extreme complex oscillations take place also in the chiral condensate and the baryon number and that they are essential to get the correct physical results.

For simplicity we will here focus on the baryon number, which in a single gauge field configuration is given by

$$n \equiv \frac{d}{d\mu}\log\det(D+\mu\gamma_0+m). \tag{1.3}$$

Our goal is to determine the distribution $\langle\delta(n-n')\rangle$ of the baryon number over the gauge fields. We will show that this distribution takes complex values and that the extreme oscillations are essential to obtain the correct average baryon number

$$\langle n\rangle = \int dn'\, n'\, \langle\delta(n-n')\rangle. \tag{1.4}$$

This direct insight into the sign problem also allow us to address how complex Langevin works in this case.

In order to understand better the distribution $\langle\delta(n-n')\rangle$ of the baryon number operator over the gauge fields, let us first understand its first two moments. For the first moment there is no source of confusion: The average quark number is the first moment

$$\frac{1}{2}\frac{1}{Z_{1+1}}\,\frac{d}{d\mu}\,Z_{1+1} = \langle n\rangle. \tag{1.5}$$

However, the second derivative with respect to μ

$$\frac{1}{4}\frac{1}{Z_{1+1}}\ \frac{d^2}{d\mu^2}\ Z_{1+1} = \langle n^2\rangle + \frac{1}{2}\langle\left(\frac{dn}{d\mu}\right)\rangle, \tag{1.6}$$

is *not* the second moment of the distribution $\langle\delta(n-n')\rangle$. Rather, the average of the square of n can be written as

$$\langle n^2\rangle = \frac{1}{Z}\ \frac{d}{d\mu_u}\frac{d}{d\mu_d}\ Z_{1+1}\Big|_{\mu_u=\mu_d=\mu}, \tag{1.7}$$

where we distinguished the chemical potentials for the two flavors and differentiated with respect to each one before setting them equal.

When we express the traces in terms of the eigenvalues, z_k, of $\gamma_0(D+m)$

$$\begin{aligned}
\frac{1}{2}\frac{1}{Z_{1+1}}\ \frac{d}{d\mu}\ Z_{1+1} &= \left\langle\sum_k \frac{1}{z_k+\mu}\right\rangle \\
\frac{1}{4}\frac{1}{Z_{1+1}}\ \frac{d^2}{d\mu^2}\ Z_{1+1} &= \left\langle\sum_{k,l}\frac{1}{z_k+\mu}\frac{1}{z_l+\mu} - \frac{1}{2}\sum_k\frac{1}{(z_k+\mu)^2}\right\rangle \\
\langle n^2\rangle &= \left\langle\sum_{k,l}\frac{1}{z_k+\mu}\frac{1}{z_l+\mu}\right\rangle = \left\langle\Big[\sum_k\frac{1}{z_k+\mu}\Big]^2\right\rangle,
\end{aligned} \tag{1.8}$$

it becomes obvious that (1.6) is *not* the average of a square and in particular it is *not* the second moment of the distribution of n over the gauge fields. The distribution $\langle\delta(n-n')\rangle$ is nevertheless of great interest since it gives direct insights in the sign problem.

As a final point before we turn to the results, note that the quark number takes complex values

$$n(\mu)^* = \left(\mathrm{Tr}\frac{\gamma_0}{D+\mu\gamma_0+m}\right)^* = -n(-\mu). \tag{1.9}$$

Hence, the distribution $\langle\delta(n-n')\rangle$ is in the complex n plane

$$P_n(x,y) \equiv \langle\delta\left(x-\mathrm{Re}[n]\right)\delta\left(y-\mathrm{Im}[n]\right)\rangle, \tag{1.10}$$

and the average baryon number is given by the integral of $(x+iy)$ weighted by the distribution $P_n(x,y)dxdy$.

2. The distribution of n from Chiral Perturbation Theory

Despite the fact that pions have zero baryon charge the distribution of the baryon number over the gauge fields is non trivial when computed within Chiral Perturbation Theory. Certainly in Chiral Perturbation Theory we have that

$$\frac{1}{2}\frac{1}{Z_{1+1}}\ \frac{d}{d\mu}\ Z_{1+1} = \langle n\rangle = 0 \quad \text{and} \quad \frac{1}{Z_{1+1}}\ \frac{d^2}{d\mu^2}\ Z_{1+1} = 0, \tag{2.1}$$

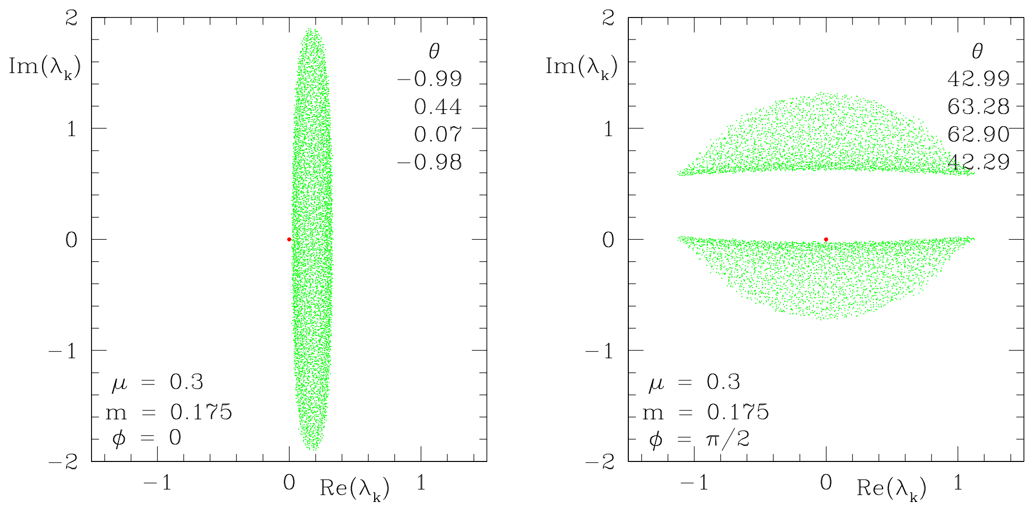

Figure 1: Scatter plot of the spectrum of a Random Matrix Dirac operator for $\mu = m_\pi/2$; **left:** the eigenvalues of $D+\mu\gamma_0+m$ **right:** the eigenvalues of $i(\gamma_0(D+m)+\mu)$. In both cases the support of the spectrum has reached the origin indicated by the red point. Beyond this point, ie. for $\mu > m_\pi/2$ the distribution of the chiral condensate and the baryon has power law tails. (A similar phenomenon is expected to happen for lattice QCD with Wilson fermions in the Aoki phase [8].)

but the average of the square of n is non zero

$$\langle n^2 \rangle = \frac{d^2}{d\mu_1 d\mu_2} G_0(\mu_1,\mu_2)\Big|_{\mu_1=\mu_2=\mu} \neq 0, \tag{2.2}$$

since the 1-loop free energy is

$$G_0(\mu_1,\mu_2) = V\frac{m_\pi^2 T^2}{\pi^2}\sum_{n=1}^{\infty}\frac{K_2(\frac{m_\pi n}{T})}{n^2}\cosh(\frac{\mu_1-\mu_2}{T}n). \tag{2.3}$$

So $\langle\delta(n-n')\rangle$ must necessarily be non trivial in Chiral Perturbation Theory.

In order to compute the full distribution $P_n(x,y)$ it is necessary to evaluate all moments

$$\langle \mathrm{Re}[n]^k \mathrm{Im}[n]^j \rangle \tag{2.4}$$

in Chiral Perturbation Theory. The details are given in [6] and involve an interesting combinatorial use of the replica trick [7]. For the computation it is essential to specify whether the chemical potential is larger or smaller than $m_\pi/2$, since in the replicated generating functions additional condensates appear at this scale. Also from the perspective of the eigenvalues of the Dirac operator it is clear that the case $\mu < m_\pi/2$ must be very different from the one with $\mu > m_\pi/2$, see figure 1.

We first discuss the distribution of n for $\mu < m_\pi/2$. To one-loop order in Chiral Perturbation Theory the distribution factorizes [6]

$$P_n(x,y) = P_{\mathrm{Re}[n]}(x)P_{\mathrm{Im}[n]}(y), \tag{2.5}$$

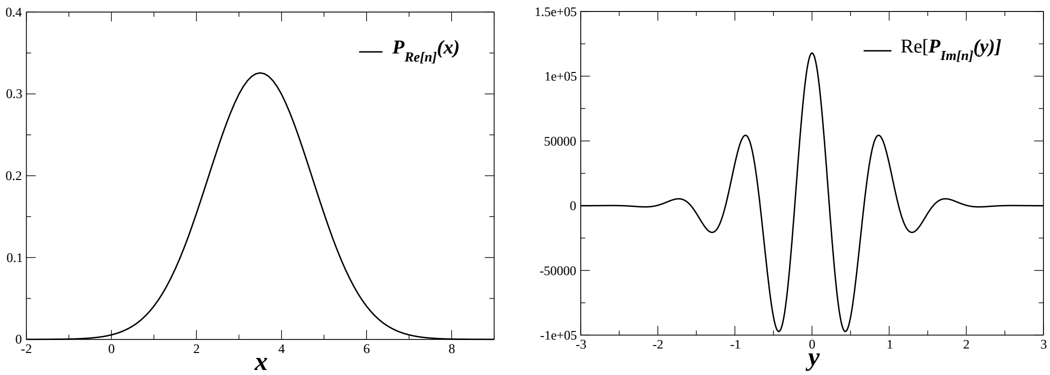

Figure 2: The distribution of the baryon number over the gauge fields in the grand canonical ensemble. For $\mu < m_\pi/2$ the distribution factorizes into the distribution of the real part (left figure) and the imaginary part (right figure). The distribution of the imaginary part takes complex values, shown is the real part. Note the difference in the scales on the vertical axis. The amplitude of the distribution of the imaginary part of n grows exponentially with the volume.

where the two factors take simple Gaussian forms

$$P_{\mathrm{Re}[n]}(x) \;=\; \frac{1}{\sqrt{\pi(\chi^B_{ud}+\chi^I_{ud})}}e^{-(x-\nu_I)^2/(\chi^B_{ud}+\chi^I_{ud})} \tag{2.6}$$

$$P_{\mathrm{Im}[n]}(y) \;=\; \frac{1}{\sqrt{\pi(\chi^I_{ud}-\chi^B_{ud})}}e^{-(y-i\nu_I)^2/(\chi^I_{ud}-\chi^B_{ud})}. \tag{2.7}$$

Note in particular that $P_{\mathrm{Im}[n]}(y)$ takes complex values. It is quite natural that the sign problem manifest it self in the distribution of the imaginary part of n since

$$n \;\equiv\; \frac{d}{d\mu}\log\det(D+\mu\gamma_0+m) = \frac{d}{d\mu}\log|\det(D+\mu\gamma_0+m)|+i\frac{d}{d\mu}\theta. \tag{2.8}$$

In the above expression for the distribution of n we have made use of the notation

$$\begin{aligned}
\nu_I \;&\equiv\; \frac{d}{d\mu_1}\Delta G_0(\mu_1,-\mu)\Big|_{\mu_1=\mu} \qquad (2.9)\\
\chi^B_{ud} \;&\equiv\; \frac{d^2}{d\mu_1 d\mu_2}\Delta G_0(\mu_1,\mu_2)\Big|_{\mu_1=\mu_2=\mu}\\
\chi^I_{ud} \;&\equiv\; \frac{d^2}{d\mu_1 d\mu_2}\Delta G_0(-\mu_1,\mu_2)\Big|_{\mu_1=\mu_2=\mu},
\end{aligned}$$

where the free energy difference is (note that $\chi^I_{ud}+\chi^B_{ud}>0$ and $\chi^I_{ud}-\chi^B_{ud}>0$)

$$\Delta G_0(\mu_1,\mu_2) = V\frac{m_\pi^2T^2}{\pi^2}\sum_{n=1}^{\infty}\frac{K_2(\frac{m_\pi n}{T})}{n^2}\left[\cosh(\frac{\mu_1-\mu_2}{T}n)-1\right]. \tag{2.10}$$

Since all of the above quantities are extensive the amplitude of $P_{\mathrm{Im}[n]}(y)$ grows exponentially with the volume, the width grows like $\sqrt{V}$, while the period of the oscillations are of order V^0. For a plot of the distribution see figure 2. The extreme oscillations of $P_{\mathrm{Im}[n]}(y)$ are essential in order to obtain zero expectation value of the quark number in Chiral Perturbation Theory

$$\begin{aligned} \langle n \rangle &= \int dxdy\ (x+iy)P_n(x,y) \\ &= \int dx\ xP_{\mathrm{Re}[n]}(x) + i\int dy\ yP_{\mathrm{Im}[n]}(y) \\ &= \nu_I + ii\nu_I = 0 \end{aligned} \tag{2.11}$$

The detailed cancellation between the contribution from the real part and the imaginary part is only possible if the phase of the fermion the determinant is accounted for properly. Similar cancellations also take part for the higher moments of the baryon number as well as for the moments of the chiral condensate, see [6] for details.

3. Complex Langevin

One use of the results for the distribution of the baryon number is to illustrate how the complex Langevin method can deal with sign problems in simple models. Clearly the distribution of the imaginary part of the baryon number over the gauge fields is the challenging part. Therefore, let us ask if complex Langevin is able to do the simple one dimensional integral

$$\int dy\, y\, P_{\mathrm{Im}[n]}(y), \tag{3.1}$$

that is, to measure the contribution to the average baryon number from the imaginary part of n.

To this end we define the complex Langevin action for $y = \mathrm{Im}[n]$ as

$$S = -\log[P_{\mathrm{Im}[n]}(y)] = -(iy+\nu_I)^2/(\chi^I_{ud} - \chi^B_{ud}). \tag{3.2}$$

The next step is to complexify $\mathrm{Im}[n]$ as $y = a + ib$ and write down the flow equations for a and b

$$\begin{aligned} a_{n+1} &= a_n - \varepsilon\frac{2a_n}{\chi^I_{ud} - \chi^B_{ud}} + \sqrt{\varepsilon}\eta_n \\ b_{n+1} &= b_n - \varepsilon\frac{2(b_n - \nu_I)}{\chi^I_{ud} - \chi^B_{ud}}. \end{aligned} \tag{3.3}$$

Note that the flow equations decouple. The equation for a is that of a Gaussian for which complex Langevin works perfectly. That of b simply shifts y by ν_I in the imaginary direction. Since there is no noise in the imaginary direction, the complex Langevin method effectively shifts the contour of the y-integral by a term of order V in the imaginary direction. After the shift, a simple integral over a Gaussian without oscillations is left and the complex Langevin method has no problem in evaluating this. Clearly the shift of the contour is the only reasonable thing to do in this case, the strength of the complex Langevin method is that it can make this shift automatically. A similar example was worked out in [9] and [10].

For $\mu > m_\pi/2$ the chemical potential enters the spectral support of $\gamma_0(D+m)$ and the distribution of the baryon number develops power law tails [6]. Nevertheless, complex Langevin is also able to deal with the sign problem for one dimensional QCD [11] in this region.

4. Summary

The interplay between lattice QCD and analytical studies of QCD is essential to understand QCD at nonzero chemical potential. Due to the sign problem, the standard methods of lattice QCD only have a limited range of applicability. In order to study dense strongly interacting matter from first principles new numerical methods must be invented and put to use. To understand how such methods can be designed it is essential to understand how the sign problem affects physical observables such as the baryon number and the chiral condensate.

Here we have derived the distribution of the baryon number over the gauge fields from Chiral Perturbation Theory. We have shown that the distribution takes complex values and is strongly oscillating. These oscillations were shown to be central to the detailed cancellations which take place when forming the average baryon number. The distributions also give detailed information on the overlap problem as will be discussed in [12]. Here we have used the distribution of the baryon number to show how the complex Langevin method can deal with sign problems. An important point to take away from this is that the complex Langevin method works equally well independent of the volume and hence independently of the strength of the sign problem. Similarly, in the well known cases [13] where the complex Langevin method fails it does so independently of the volume.

It is also possible to compute the distribution of the baryon number *over the phase of the fermion determinant* within Chiral Perturbation theory [14]. Also in this case the complex and oscillating nature of the distribution is essential in order to obtain the correct physics at nonzero chemical potential. That calculation also directly demonstrates that all phases of the fermion determinant are important.

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