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Fluctuations of the quark number and of the chiral condensate

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The distributions of the quark number and chiral condensate over the gauge fields are computed for QCD in Euclidean space at nonzero quark chemical potential. As both operators are non-Hermitian the distributions are in the complex plane. Moreover, because of the sign problem, the distributions are not real and positive. The computations are carried out within leading order chiral perturbation theory and give a direct insight into the delicate cancellations that take place in contributions to the total baryon number and the chiral condensate.

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I. INTRODUCTION

The phase diagram of strongly interacting matter is determined by the behavior of the chiral condensate $\langle\sigma\rangle$ and the quark number $\langle n\rangle$. These quantities signal the breakdown of chiral symmetry and the formation of baryonic matter. Not only are the expectation values of σ and n of interest, but also their fluctuations are central to our understanding of strongly interacting matter since they may be visible in fluctuations of the observables measured in heavy ion collisions [1–4].

In Euclidean space, both σ and n are complex when evaluated at nonzero chemical potential for a typical gauge field background. The reason why n and σ take complex values is that the fermion determinant at nonzero chemical potential is complex: if we write $\det(D+\mu\gamma_0+m)=r\exp(i\theta)$, we have

$$n \equiv \frac{d}{d\mu}\,\mathrm{logdet}(D+\mu\gamma_0+m) = \frac{d}{d\mu}\log r + i\frac{d}{d\mu}\theta,$$
$$\sigma \equiv \frac{d}{dm}\,\mathrm{logdet}(D+\mu\gamma_0+m) = \frac{d}{dm}\log r + i\frac{d}{dm}\theta. \tag{1}$$

The fluctuations therefore take place in the complex σ- and n-plane. Since the fermion determinant is also complex valued for nonzero chemical potential, fluctuations in all directions of the complex σ- and n-plane contribute to the expectation values $\langle\sigma\rangle$ and $\langle n\rangle$, which, of course, are real. A description of fluctuations of σ and n is contained in their distributions P_σ and P_n. Here, we derive these distributions analytically to leading nontrivial order in chiral perturbation theory. From (1), we see that the imaginary part of the quark number operator is directly related to the phase of the fermion determinant. We therefore expect that the cancellations due to fluctuations of the phase are tightly linked to the distribution of the quark number in the imaginary direction. The results presented below confirm this expectation.

Chiral perturbation theory [5] is the low energy limit of QCD which describes the strongly interacting theory in terms of weakly interacting Goldstone modes corresponding to the spontaneous breakdown of chiral symmetry. Since the pions have zero quark charge, the expectation value of the quark number in chiral perturbation theory is automatically zero. The square of the quark number

$$\langle n_q^2\rangle = \frac{1}{Z}\frac{d^2}{d\mu^2}Z = \langle n^2\rangle + \left\langle\left(\frac{dn}{d\mu}\right)\right\rangle \tag{2}$$

is of course also zero since in chiral perturbation theory the partition function Z is independent of μ. The distribution of the values which the quark number operator takes as the gauge fields fluctuate is, however, nontrivial even when evaluated within chiral perturbation theory. To see that this is necessarily the case, let us consider the second moment of n i.e. $\langle n^2\rangle = \int dxdy(x+iy)^2P_n(x+iy)$. If the second moment is nonzero the distribution P_n is nontrivial, i.e. not a two dimensional δ-function at the origin of the complex n-plane.

Let us emphasize that $\langle n^2\rangle$ is not the average of the square of the quark number, see (2), rather the second moment must be thought of as

$$\langle n^2\rangle = \frac{1}{Z}\frac{d}{d\mu_u}\frac{d}{d\mu_d}Z \tag{3}$$

evaluated at degenerate chemical potentials and quark masses for the up and down quark. Even though there is an equal number of quarks and antiquarks associated with each pion, the vacuum expectation value of $\langle n^2\rangle$, is nonzero if there are correlations between the quarks and the antiquarks of different flavor. Confinement of quarks and antiquarks into pions strongly suggests that such a correlation exists in chiral perturbation theory, and in fact $\langle n^2\rangle$ takes a nonzero value even at $\mu=0$, see for example [6]. At zero chemical potential $\langle n^2\rangle$ coincides with the off-diagonal quark number susceptibility which has been computed analytically by high temperature perturbation theory [7] as well as by numerical lattice simulations [8].

Since this is a likely source of confusion let us again stress that P_n gives the distribution of n, defined in (1), over the ensemble of gauge fields: If one makes a frequency plot of the values obtained for n in a lattice QCD ensemble of gauge fields the shape which emerges is described by P_n. The first moment measured on this distribution gives the average quark number. The second moment measured on this distribution, however, only gives the first of the two terms which combine to give the square of the quark number, cf. (2). If we phrase this in terms of the eigenvalues z_k of $\gamma_0(D+m)$ we have

$$n_q = n = \sum_k \frac{1}{z_k+\mu}, \qquad n_q^2 = \sum_{k\neq l} \frac{1}{z_k+\mu}\frac{1}{z_l+\mu}, \\ n^2 = \sum_{k,l} \frac{1}{z_k+\mu}\frac{1}{z_l+\mu} = \Big[\sum_k \frac{1}{z_k+\mu}\Big]^2. \tag{4}$$

So $\langle n_q^2\rangle$ is not the average of a square and consequently not the second moment of a distribution over the gauge fields. The reason is that n_q^2 contains correlations due to the Pauli principle.

On a more technical level, the reason for the μ dependence of $P_n(x+iy)$ can bee seen from the generating function of the distributions. These involve quarks with different chemical potentials, i.e. the isospin chemical potential, $\mu_1-\mu_2$, is nonzero and couples nontrivially in the generating functions. This point will be explained explicitly below. The success of chiral perturbation theory in predicting the behavior of QCD at nonzero chemical potential has been demonstrated clearly by recent comparisons to lattice QCD results both in the p-regime [9–12] and the ϵ-regime [13–17].

The phase of the fermion determinant may lead to exponentially large cancellations in the computation of expectation values. If we would try to measure this expectation value numerically with lattice QCD simulations, we would be confronted with numerical errors which are exponentially hard to handle. This is *the QCD sign problem* and severely limits first principle studies of the QCD phase diagram (see [18] for recent reviews of the QCD sign problem).

The results for the distributions that are derived below give a direct insight in the cancellations caused by the sign problem. For example, the vanishing value of the baryon number (within chiral perturbation theory) is obtained only after a delicate cancellation between the contribution from Re$[n]$ and from Im$[n]$. The range of the fluctuations in the complex quark number plane which must be taken into account, in order to obtain the total baryon number, grows like the four volume. In contrast, the width of the distribution for the ensemble where the phase of the fermion determinant is ignored (the phase-quenched ensemble) only scales like the square root of the volume. The numerical challenge faced by lattice QCD is to go from the phase-quenched (simulation) ensemble to the full (target) ensemble. One therefore needs to sample the far tails of the distributions. The analytic insight we have obtained here can in this way help to understand the limitations of present lattice gauge simulations at nonzero chemical potential and give hints for future developments. Besides the reweighting method [19–21] discussed here, the results obtained are also relevant for the complex Langevin method [22–26] as well as for the density of states method [27–30].

Throughout the paper we will work with two flavors. We refer to the this theory as the $N_f = 1+1$ theory. The phase-quenched theory is referred to as $1+1^*$ since the absolute square of the fermion determinant corresponds to a quark and a conjugate quark.

This paper is organized as follows. First, we consider the region where 2μ is less than the pion mass and the mean fields do not depend on the chemical potential. We derive the distribution of the quark number operator as well as that of the chiral condensate. Results are given both for QCD with dynamical quarks and for the partially quenched case. Implications for lattice QCD are discussed in Sec. VI. Before concluding, we discuss the distribution of the quark number operator and chiral condensate for larger values of the chemical potential. The distribution of the quark number for imaginary chemical potential is evaluated in the Appendix.

II. GENERAL DEFINITIONS AND KNOWN RESULTS FROM *CPT*

Before starting the actual computation of the distributions, in this section we introduce notations and explain why chiral perturbation theory can give information about QCD at nonzero quark chemical potential.

The quark number operator is the logarithmic derivative of the fermion determinant with respect to the quark chemical potential $\mu = \mu_1 + \mu_2$

$$n(\mu) \equiv \mathrm{Tr}\frac{\gamma_0}{D+\mu\gamma_0+m}, \tag{5}$$

while for σ we differentiate with respect to the quark mass (we consider degenerate flavors)

$$\sigma(\mu) \equiv \mathrm{Tr}\frac{1}{D+\mu\gamma_0+m}. \tag{6}$$

At low temperatures, the QCD partition function and its low energy limit in the form of a chiral Lagrangian are independent of μ until the chemical potential is sufficient to balance the energy required to create a baryon. Since the expectation value of the quark number and the chiral condensate are derivatives of the partition function with respect to μ, they are independent of μ when evaluated in chiral perturbation theory. On the contrary, expectation values that cannot be written as derivatives of the partition function with respect to μ may still depend on the chemical potential. This happens when the generating function

for the operator under consideration includes quarks with different values of the chemical potential.

To illustrate this let us compute the expectation value of n^2, the cross correlation introduced above. In order to obtain n^2 we start from the generating function

$$Z_{1+1}(\mu, \mu_1) = \langle \det(D + \mu\gamma_0 + m) \det(D + \mu_1\gamma_0 + m) \rangle \tag{7}$$

and differentiate with respect to the two different chemical potentials

$$\langle n^2 \rangle_{1+1} = \frac{1}{Z_{1+1}(\mu, \mu)} \lim_{\mu_1 \to \mu} \frac{d}{d\mu} \frac{d}{d\mu_1} Z(\mu, \mu_1). \tag{8}$$

Since the chemical potentials in the generating function are different, there is a nonzero component of the isospin chemical potential $\mu - \mu_1$. It is this component that induces a nontrivial chemical potential dependence in chiral perturbation theory and hence a nonzero result after differentiation with respect to μ and μ_1. Since the free energy is an even function of the isospin chemical potential (for degenerate quark masses) it takes two derivatives to obtain a nonzero value for $\mu_1 \to \mu$.

To one-loop order in chiral perturbation theory, we have

$$\frac{Z_{1+1}(\mu, \mu_1)}{Z_{1+1}(\mu, \mu)} = e^{G_0(\mu, \mu_1) - G_0(\mu = 0)}, \tag{9}$$

where the one-loop free energy is (the divergent part of G_0 is independent of μ and does not contribute)

$$G_0(\mu, -\tilde{\mu}) = \frac{V m_\pi^2 T^2}{\pi^2} \sum_{n=1}^{\infty} \frac{K_2(\frac{m_\pi n}{T})}{n^2} \cosh\left(\frac{(\mu + \tilde{\mu})n}{T}\right). \tag{10}$$

Thus

$$\langle n^2 \rangle_{1+1} = \lim_{\mu_1 \to \mu} \frac{d}{d\mu} \frac{d}{d\mu_1} G_0(\mu, \mu_1). \tag{11}$$

This quantity is usually referred to as the off diagonal quark number susceptibility and is denoted by χ^B_{ud}.

Below we will use the notation $\Delta G_0(\mu_1, \mu_2) = G_0(\mu_1, \mu_2) - G_0(0, 0)$ and

$$\begin{aligned} \nu_I &\equiv \frac{d}{d\mu_1} \Delta G_0(\mu_1, -\mu)|_{\mu_1 = \mu}, \\ \chi^B_{ud} &\equiv \frac{d^2}{d\mu_1 d\mu_2} \Delta G_0(\mu_1, \mu_2)|_{\mu_1 = \mu_2 = \mu}, \\ \chi^I_{ud} &\equiv \frac{d^2}{d\mu_1 d\mu_2} \Delta G_0(-\mu_1, \mu_2)|_{\mu_1 = \mu_2 = \mu}, \end{aligned} \tag{12}$$

for the μ derivatives of the free energy and

TABLE I. The first and second moment of n and σ to one-loop order in chiral perturbation theory for $\mu < m_\pi/2$. The absolute value of the mean field result for the chiral condensate is denoted by Σ. In the partially quenched (PQ) ensemble, the operators of the full theory are evaluated for a gauge field background where the phase of the fermion determinant is ignored.

	$\mathcal{E} = 1 + 1$	$\mathcal{E} = \mathrm{PQ}$
$\langle n \rangle_\mathcal{E}$	0	ν_I
$\langle n^2 \rangle_\mathcal{E}$	χ^B_{ud}	$\nu_I^2 + \chi^B_{ud}$
$\lvert\langle \sigma \rangle_\mathcal{E}\rvert$	$\Sigma + 2\delta\Sigma^B$	$\Sigma + \delta\Sigma^I + \delta\Sigma^B$
$\langle \sigma^2 \rangle_\mathcal{E}$	$\chi^B_S + (\Sigma + 2\delta\Sigma^B)^2$	$\chi^B_S + (\Sigma + \delta\Sigma^B + \delta\Sigma^I)^2$

$$\begin{aligned} \delta\Sigma^B &= \frac{d}{d\tilde{m}} \Delta G_0(\mu, \mu, m, \tilde{m})|_{\tilde{m} = m}, \\ \delta\Sigma^I &= \frac{d}{d\tilde{m}} \Delta G_0(\mu, -\mu, m, \tilde{m})|_{\tilde{m} = m}, \\ \chi^B_S &= \frac{d^2}{d\tilde{m} dm} \Delta G_0(\mu, \mu, m, \tilde{m})|_{\tilde{m} = m}, \\ \chi^I_S &= \frac{d^2}{d\tilde{m} dm} \Delta G_0(\mu, -\mu, m, \tilde{m})|_{\tilde{m} = m}, \end{aligned} \tag{13}$$

for the one-loop contributions to the chiral condensate and chiral susceptibility. Also for the chiral susceptibility it is understood that we will only consider the off diagonal component. Note that all of these quantities are extensive. For quantities labeled by B, we have that $\mu_q = \mu$ and $\mu_I = 0$, and for the quantities labeled with I $\mu_q = 0$ and $\mu_I = \mu$. The quark mass dependence of G_0 is through m_π via the Gell-Mann–Oakes–Renner relation

$$m_\pi^2 = \frac{\Sigma(m + \tilde{m})}{F^2}. \tag{14}$$

Let us also stress that all quantities with superscript B are independent of the chemical potential (in one-loop chiral perturbation theory).

In Table I we give results for one-loop chiral perturbation theory valid for $\mu < m_\pi/2$. The label PQ refers to the result obtained in a partially quenched ensemble. By definition this ensemble is generated with the absolute value of the fermion determinant but we keep the μ dependence of n and σ as in the ordinary theory. We will use each of these results to check the distributions of the quark number operator and the chiral condensate.

III. THE DISTRIBUTION OF THE QUARK NUMBER OPERATOR

In this section, we compute the distribution of the quark number in the 1 + 1 theory. Since

$$\begin{aligned} n(\mu)^* &= \left(\mathrm{Tr} \frac{\gamma_0}{D + \mu\gamma_0 + m}\right)^* \\ &= -\mathrm{Tr} \frac{\gamma_0}{D - \mu\gamma_0 + m} = -n(-\mu) \end{aligned} \tag{15}$$

the quark number operator is in general complex (it is purely imaginary at $\mu = 0$). The fluctuations of the quark number thus occur in the complex plane. We first derive the distribution of the real part, $(n(\mu) - n(-\mu))/2$, and of the imaginary part, $(n(\mu) + n(-\mu))/2$, of the quark number. Then, finally, we compute the full distribution in the complex quark number plane. As we shall see, the distribution in the complex plane factorizes into the distribution of the real part and the distribution of the imaginary part.

A. The distribution of the real part of the quark number

Here, we derive the distribution of the real part of the quark number defined by

$$P^{1+1}_{\mathrm{Re}[n]}(x) \equiv \left\langle \delta\left(x - \frac{1}{2}(n(\mu) - n(-\mu))\right)\right\rangle_{1+1}, \tag{16}$$

within one-loop chiral perturbation theory for $\mu < m_\pi/2$.

First, we represent the δ-function as an integral

$$P^{1+1}_{\mathrm{Re}[n]}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{-ixk}\langle e^{+i(k/2)(n(\mu)-n(-\mu))}\rangle_{1+1}. \tag{17}$$

Then, we expand the exponential of the trace

$$\langle e^{i(k/2)(n(\mu)-n(-\mu))}\rangle_{1+1} = \sum_{j=0}^{\infty}\frac{(ik/2)^j}{j!}\langle (n(\mu) - n(-\mu))^j\rangle_{1+1}. \tag{18}$$

This shows that a probability distribution is determined by its moments which we will compute next.

In order to compute the trace to the jth power we need to introduce $2j$ replica quarks (see [31] for an introduction to the replica trick in chiral perturbation theory)

$$\langle (n(\mu) - n(-\mu))^j\rangle_{1+1} = \lim_{\mu_i\to\mu}\lim_{n_i\to 0}\frac{1}{n_1\cdots n_j}d_{\mu_1}\cdots d_{\mu_j} \times\left\langle\prod_{i=1}^{j}\det(D+\mu_i\gamma_0+m)^{n_i}\det(D-\mu_i\gamma_0+m)^{n_i}\right\rangle_{1+1}. \tag{19}$$

In one-loop chiral perturbation theory, the replicated generating function for the real part is given by (this is where the assumption $\mu < m_\pi/2$ enters: for $\mu > m_\pi/2$ the generating function is in a Bose condensed phase, see Se. VII)

$$\left\langle\prod_{i=1}^{j}\det(D+\mu_i\gamma_0+m)^{n_i}(D-\mu_i\gamma_0+m)^{n_i}\right\rangle_{1+1} = \exp\left(\sum_{l\le m=1}^{j} 2n_l n_m(G_0(\mu_l,\mu_m) + G_0(-\mu_l,\mu_m)) + \sum_{l=1}^{j} 2n_l(G_0(\mu_l,\mu) + G_0(-\mu_l,\mu))\right). \tag{20}$$

We now take $d_{\mu_1}\cdots d_{\mu_j}$ of the generating function, evaluate it at $\mu_i = \mu$, and take the replica limits $n_i \to 0$. Note that the term linear in the n_k's includes $G_0(-\mu_l,\mu)$, and the derivative with respect to μ_l does *not* vanish at $\mu_l = \mu$. Therefore terms with even as well as odd values of j contribute when we evaluate the derivative $d_{\mu_1}\cdots d_{\mu_j}$ at $\mu_l = \mu$. All terms with the same number of pairs from the first sum in (20) give the same contribution to the jth moment. The combinatorial factor for choosing b pairs out of j is

$$\binom{j}{2b}\frac{(2b)!}{b!2^b}. \tag{21}$$

For the moments, we thus find [recall the notation (12)]

$$\begin{aligned}\langle (n(\mu) - n(-\mu))^j\rangle_{1+1} &= \sum_{b=0}^{\mathrm{Int}(j/2)}\binom{j}{2b}(2b-1)!![2(\chi^B_{ud}+\chi^I_{ud})]^b(2\nu_I)^{j-2b}\\ &= \sum_{b=0}^{\mathrm{Int}(j/2)}\binom{j}{2b}(2\nu_I)^{j-2b}\frac{1}{\sqrt{\pi(\chi^B_{ud}+\chi^I_{ud})}}\int_{-\infty}^{\infty}du(2u)^{2b}e^{-u^2/(\chi^B_{ud}+\chi^I_{ud})}\\ &= \frac{1}{\sqrt{\pi(\chi^B_{ud}+\chi^I_{ud})}}\int_{-\infty}^{\infty}dx(2x)^j e^{-(x-\nu_I)^2/(\chi^B_{ud}+\chi^I_{ud})},\end{aligned} \tag{22}$$

where $\mathrm{Int}(j/2)$ is the integer part of $j/2$. These are the moments of a Gaussian distribution centered at ν_I. The distribution of the real part of the quark number is thus given by

$$P^{1+1}_{\mathrm{Re}[n]}(x) = \frac{1}{\sqrt{\pi(\chi^B_{ud}+\chi^I_{ud})}}e^{-(x-\nu_I)^2/(\chi^B_{ud}+\chi^I_{ud})}. \tag{23}$$

We see that $P^{1+1}_{\mathrm{Re}[n]}(x)$ is properly normalized. The expectation value of the real part of the quark number equals the isospin

number in the phase-quenched theory evaluated at μ

$$\langle \mathrm{Re}[n]\rangle_{1+1} = \int_{-\infty}^{\infty} dx x P^{1+1}_{\mathrm{Re}[n]}(x) = \nu_I, \tag{24}$$

and the average of the square of the real part of the quark number is given by

$$\begin{aligned}\langle (\mathrm{Re}[n])^2\rangle_{1+1} &= \int_{-\infty}^{\infty} dx x^2 P^{1+1}_{\mathrm{Re}[n]}(x) \\ &= \nu_I^2 + \frac{1}{2}(\chi^B_{ud} + \chi^I_{ud}).\end{aligned} \tag{25}$$

Note that fluctuations of the quark number in the real direction vanish at $\mu = 0$. The reason is that the width of the distribution of the real part of n goes to 0 for $\mu \to 0$.

B. The distribution of the imaginary part of the quark number

In this subsection, we derive the distribution of the imaginary part of the quark number defined by

$$P^{1+1}_{\mathrm{Im}[n]}(y) \equiv \left\langle \delta\left(y + i\frac{1}{2}(n(\mu) + n(-\mu))\right)\right\rangle_{1+1}, \tag{26}$$

within one-loop chiral perturbation theory for $\mu < m_\pi/2$.

As in the previous subsection, the distribution is determined by its moments which can be shown by representing the δ-function as an integral

$$P^{1+1}_{\mathrm{Im}[n]}(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{-iyk}\langle e^{(k/2)(n(\mu)+n(-\mu))}\rangle_{1+1} \tag{27}$$

and expanding the exponential

$$\langle e^{(k/2)(n(\mu)+n(-\mu))}\rangle_{1+1} = \sum_{j=0}^{\infty}\frac{1}{j!}\left\langle\left(\frac{k}{2}(n(\mu)+n(-\mu))\right)^j\right\rangle_{1+1}. \tag{28}$$

The jth power of $\mathrm{Im}[n]$ can be computed by introducing j fermionic replica quarks and j bosonic replica quarks

$$\begin{aligned}\langle (n(\mu)+n(-\mu))^j\rangle_{1+1} = \lim_{\mu_i\to\mu}\lim_{n_i\to 0}\frac{1}{n_1\cdots n_j}d_{\mu_1}\cdots d_{\mu_j} \\ \times\left\langle\prod_{i=1}^{j}\frac{\det(D+\mu_i\gamma_0+m)^{n_i}}{\det(D-\mu_i\gamma_0+m)^{n_i}}\right\rangle_{1+1}.\end{aligned} \tag{29}$$

Note that the ratio of the two determinants makes up the phase factor, $\det(D(\mu))/\det(D(-\mu)) = \exp(2i\theta(\mu))$. From Eq. (1), we see that the phase indeed generates the imaginary part of n after differentiation with respect to the chemical potential.

The replicated generating function within one-loop chiral perturbation theory is given by

$$\begin{aligned}&\left\langle\prod_{i=1}^{j}\frac{\det(D+\mu_i\gamma_0+m)^{n_i}}{\det(D-\mu_i\gamma_0+m)^{n_i}}\right\rangle_{1+1} \\ &= \exp\Bigg(\sum_{l\le m=1}^{j} 2n_l n_m(G_0(\mu_l,\mu_m) - G_0(-\mu_l,\mu_m)) \\ &\quad + \sum_{l=1}^{j} 2n_l(G_0(\mu_l,\mu) - G_0(-\mu_l,\mu))\Bigg),\end{aligned} \tag{30}$$

where we used that $\mu < m_\pi/2$ so that pion condensates are absent in the generating function.

We now take $d_{\mu_1}\cdots d_{\mu_j}$ of the generating function, evaluate it at $\mu_i = \mu$, and take the replica limit $n_i \to 0$. The only difference with the previous section is the minus sign in front of $G_0(-\mu_l,\mu_m)$ and $G_0(-\mu_l,\mu)$. We thus find the moments

$$\begin{aligned}\langle (n(\mu)+n(-\mu))^j\rangle_{1+1} &= \sum_{b=0}^{\mathrm{Int}(j/2)}\binom{j}{2b}(2b-1)!![2(\chi^B_{ud}-\chi^I_{ud})]^b(-2\nu_I)^{j-2b} \\ &= \sum_{b=0}^{\mathrm{Int}(j/2)}\binom{j}{2b}(-2\nu_I)^{j-2b}\frac{(-1)^b}{\sqrt{\pi(\chi^I_{ud}-\chi^B_{ud})}}\int_{-\infty}^{\infty} du(2u)^{2b}e^{-u^2/(\chi^I_{ud}-\chi^B_{ud})} \\ &= \frac{1}{\sqrt{\pi(\chi^I_{ud}-\chi^B_{ud})}}\int_{-\infty}^{\infty} dy(2iy)^j e^{(iy+\nu_I)^2/(\chi^I_{ud}-\chi^B_{ud})}.\end{aligned} \tag{31}$$

These are the moments of a Gaussian distribution centered at $i\nu_I$. Notice that $\chi^I_{ud} - \chi^B_{ud} > 0$, which follows from the explicit expression for the one-loop result [see Eq. (11)]. Since

$$\mathrm{Im}\, n(\mu) = \frac{1}{2i}(n(\mu) + n(-\mu)), \tag{32}$$

the distribution of the imaginary part of the quark number is given by

$$P^{1+1}_{\mathrm{Im}[n]}(y) = \frac{1}{\sqrt{\pi(\chi^I_{ud}-\chi^B_{ud})}}e^{(iy+\nu_I)^2/(\chi^I_{ud}-\chi^B_{ud})}. \tag{33}$$

Note that the distribution takes complex values, as could be expected because of the phase of the fermion determinant. Moreover, we have that $P^{1+1}_{\mathrm{Im}[n]}(y)$ is properly normalized,

that the expectation value of the imaginary part of the quark number equals i times the isospin number in the phase-quenched theory

$$\langle \mathrm{Im}[n] \rangle_{1+1} = \int_{-\infty}^{\infty} dy y P^{1+1}_{\mathrm{Im}[n]}(y) = i\nu_I, \tag{34}$$

and finally, that the average of the square of the imaginary part of the quark number is given by

$$\begin{aligned}\langle (\mathrm{Im}[n])^2 \rangle_{1+1} &= \int_{-\infty}^{\infty} dy y^2 P^{1+1}_{\mathrm{Im}[n]}(y) \\ &= -\nu_I^2 + \frac{1}{2}(\chi^I_{ud} - \chi^B_{ud}).\end{aligned} \tag{35}$$

In contrast to the real part, the width of the fluctuations of the imaginary part of n, $(\chi^I_{ud} - \chi^B_{ud})^{1/2}$, remains nonzero for $\mu \to 0$.

C. The distribution of the quark number

We finally turn to the distribution of the full quark number defined by

$$\begin{aligned}P^{1+1}_n(x,y) \equiv \Big\langle \delta\Big(x - \frac{1}{2}(n(\mu) - n(-\mu))\Big) \\ \times \delta\Big(y + i\frac{1}{2}(n(\mu) + n(-\mu))\Big)\Big\rangle_{1+1},\end{aligned} \tag{36}$$

within one-loop chiral perturbation theory for $\mu < m_\pi/2$. In this section, we show that this distribution factorizes into the distribution of the real and imaginary part of the quark number.

Factorization occurs if the moments factorize. This can be easily seen by writing the probability distribution as an integral over the characteristic function, i.e.

$$\begin{aligned}P^{1+1}_n(x,y) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dk_x dk_y e^{-ixk_x} \\ \times e^{-iyk_y}\langle e^{i(k_x/2)(n(\mu)-n(-\mu))} \\ \times e^{(k_y/2)(n(\mu)+n(-\mu))}\rangle_{1+1}.\end{aligned} \tag{37}$$

If the moments of the real and imaginary parts of the quark number factorize, the expectation values of the exponents in between the brackets will factorize.

The relevant moments follow from a replicated generating function as follows:

$$\begin{aligned}&\langle (n(\mu) + n(-\mu))^j (n(\mu) - n(-\mu))^k \rangle_{1+1} \\ &= \lim_{n_i \to 0} \frac{1}{n_1 \cdots n_{j+k}} d_{\mu_1} \cdots d_{\mu_{j+k}} \\ &\times \Big\langle \prod_{l=1}^{j} \det(D + \mu_l\gamma_0 + m)^{n_l} \det(D - \mu_l\gamma_0 + m)^{n_l} \\ &\times \prod_{l=j+1}^{j+k} \frac{\det(D + \mu_l\gamma_0 + m)^{n_l}}{\det(D - \mu_l\gamma_0 + m)^{n_l}} \Big\rangle_{1+1} \Big|_{\mu_i = \mu}.\end{aligned} \tag{38}$$

When we compute this replicated generating function in one-loop chiral perturbation theory a big simplification takes place: The contributions from Goldstone particles with one quark from the first two determinants and the other from one of the two determinants in the ratio exactly cancel. The reason is that the one-loop contribution of such mixed fermionic Goldstone particles occurs with the same combinatorial factor as the mixed bosonic Goldstone particles but with the opposite sign. This was first observed in [6] where it was formulated as the absence of correlations between the phase factor and the magnitude of the fermion determinant to one-loop order in chiral perturbation theory. Hence the moments of the real and imaginary part of the quark number factorize.

The probability distribution therefore factorizes as

$$\begin{aligned}P^{1+1}_n(x,y) &= P^{1+1}_{\mathrm{Re}[n]}(x) P^{1+1}_{\mathrm{Im}[n]}(y) \\ &= \frac{1}{\pi\sqrt{(\chi^I_{ud})^2 - (\chi^B_{ud})^2}} e^{-(x-\nu_I)^2/(\chi^I_{ud}+\chi^B_{ud})} \\ &\times e^{(iy+\nu_I)^2/(\chi^I_{ud}-\chi^B_{ud})}.\end{aligned} \tag{39}$$

To check this first main result let us first note that since the distributions of the real and imaginary parts of the quark number are normalized, also the product is normalized. Moreover, the expectation value of the quark number is zero

$$\begin{aligned}\langle n \rangle_{1+1} &= \int dxdy(x+iy) P^{1+1}_n(x,y) \\ &= \int dx x P^{1+1}_{\mathrm{Re}[n]}(x) + i\int dy y P^{1+1}_{\mathrm{Im}[n]}(y) \\ &= \nu_I + ii\nu_I = 0.\end{aligned} \tag{40}$$

We see that the total quark number (which necessarily is zero in chiral perturbation theory) is obtained only after a detailed cancellation between the contribution from the real part and the imaginary part. Such a detailed cancellation also occurs when we compute the average of n^2

$$\begin{aligned}\langle n^2 \rangle_{1+1} &= \int dxdy(x+iy)^2 P^{1+1}_n(x,y) \\ &= \int dx x^2 P^{1+1}_{\mathrm{Re}[n]}(x) - \int dy y^2 P^{1+1}_{\mathrm{Im}[n]}(y) \\ &\quad + 2i\int dx x P^{1+1}_{\mathrm{Re}[n]}(x) \int dy y P^{1+1}_{\mathrm{Im}[n]}(y) \\ &= \nu_I^2 + \frac{1}{2}(\chi^I_{ud} + \chi^B_{ud}) - \Big(-\nu_I^2 + \frac{1}{2}(\chi^I_{ud} - \chi^B_{ud})\Big) \\ &\quad + 2i\nu_I i\nu_I = \chi^B_{ud}.\end{aligned} \tag{41}$$

Note that, even though the distribution of the baryon number depends on the isospin density and off diagonal susceptibility, these quantities drop out when evaluating the moments of the quark number operator.

Finally, we note that since $\chi^I_{ud} + \chi^B_{ud} \to 0$ for $\mu \to 0$, the quark number distribution becomes localized on the

imaginary axis for $\mu = 0$. This is in perfect agreement with the fact that the quark number operator is anti-Hermitian for $\mu = 0$ cf. Equation (15).

IV. THE PQ DISTRIBUTION OF THE QUARK NUMBER OPERATOR

In this section, we give the result for the partially quenched distribution of the quark number. To derive this, all we need to notice is how the terms that mix the replica quarks and physical quarks contribute to the generating function.

Real part: For the real part we consider Eq. (20) where the expectation value is now taken in the $1 + 1^*$ theory. Since $G_0(\mu_l, \mu)$ is invariant under a change of the sign of both chemical potentials, we get exactly the same mixing between the replica sector and the physical sector as before. Hence the final answer for the distribution of the real part of n is again the same

$$P^{\mathrm{PQ}}_{\mathrm{Re}[n]}(x) = P^{1+1}_{\mathrm{Re}[n]}(x). \tag{42}$$

Imaginary part: The generating function for the imaginary part (30) changes when we consider the partially quenched case. This time the two physical flavors make up an absolute square of the fermion determinant while the replica flavors make up the phase factor. As we have seen before, there are no correlations between these two factors within one-loop chiral perturbation theory. The generating function for the imaginary part of the quark number in the partially quenched case is thus given by Eq. (30) but without the single sum which mixes the replica and the physical sector. Hence there are no linear terms after differentiation and the final result is obtained from Eq. (33) by setting $\nu_I = 0$

$$P^{\mathrm{PQ}}_{\mathrm{Im}[n]}(y) = \frac{1}{\sqrt{\pi(\chi^I_{ud} - \chi^B_{ud})}} e^{-y^2/(\chi^I_{ud} - \chi^B_{ud})}. \tag{43}$$

As it should be (since we take vacuum expectation values in the $1 + 1^*$ theory), both distributions are real and positive. The full distribution is again the product of these two since the factorization only involves replicated flavors. Thus we find

$$\begin{aligned} P^{\mathrm{PQ}}_n(x, y) &= P^{\mathrm{PQ}}_{\mathrm{Re}[n]}(x) P^{\mathrm{PQ}}_{\mathrm{Im}[n]}(y) \\ &= \frac{1}{\pi\sqrt{(\chi^I_{ud})^2 - (\chi^B_{ud})^2}} e^{-(x-\nu_I)^2/(\chi^I_{ud} + \chi^B_{ud})} \\ &\quad \times e^{-y^2/(\chi^I_{ud} - \chi^B_{ud})}. \end{aligned} \tag{44}$$

As a cross-check, we see that

$$\langle n^{\mathrm{PQ}} \rangle_{1+1^*} = \nu_I \tag{45}$$

and

$$\langle (n^{\mathrm{PQ}})^2 \rangle_{1+1^*} = \chi^B_{ud} + \nu_I^2 \tag{46}$$

are in agreement with Table I.

In Sec. VI, we make use of these results when discussing the problems faced by numerical lattice QCD at $\mu \neq 0$.

V. THE DISTRIBUTION OF THE CHIRAL CONDENSATE

In this section, we derive the distribution of σ and study how the chiral condensate $\langle \sigma \rangle$ builds up. As was the case for the quark number, the operator σ is not Hermitian

$$\begin{aligned} \sigma(\mu)^* &= \left(\mathrm{Tr} \frac{1}{D + \mu\gamma_0 + m} \right)^* \\ &= \mathrm{Tr} \frac{1}{D - \mu\gamma_0 + m} = \sigma(-\mu). \end{aligned} \tag{47}$$

Therefore we derive the distribution in the complex σ plane. We start by computing the distribution of the real and of the imaginary part separately. The distribution of the full chiral condensate then follows as the product of the two. This is precisely the same which happened for the baryon density. In fact, the derivation for σ is almost identical to the one for the quark number.

To see that the derivation is analogous to that for the baryon number, let us start with the distribution of $\mathrm{Re}[\sigma]$ and derive the generating function. We evaluate the distribution

$$P^{1+1}_{\mathrm{Re}[\sigma]}(x) \equiv \left\langle \delta\left(x - \frac{1}{2}(\sigma(\mu) + \sigma(-\mu)) \right) \right\rangle_{1+1} \tag{48}$$

for $\mu < m_\pi/2$ to one-loop order in chiral perturbation theory.

The δ-function can be represented as an integral

$$P^{1+1}_{\mathrm{Re}[\sigma]}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ixk} \langle e^{+i(k/2)(\sigma(\mu) + \sigma(-\mu))} \rangle_{1+1} \tag{49}$$

and the exponential is expanded

$$\langle e^{i(k/2)(\sigma(\mu) + \sigma(-\mu))} \rangle_{1+1} = \sum_{j=0}^{\infty} \frac{1}{j!} \left\langle \left(i\frac{k}{2}(\sigma(\mu) + \sigma(-\mu)) \right)^j \right\rangle_{1+1}, \tag{50}$$

so that the distribution follows from the moments.

The moments can again be expressed in terms of a replicated generating function. This time, the replica index labels the masses $m_1, \ldots, m_j$,

$$\langle(\sigma(\mu)+\sigma(-\mu))^j\rangle_{1+1} = \lim_{m_i\to m}\lim_{n_i\to 0}\frac{1}{n_1\cdots n_j}d_{m_1}\cdots d_{m_j} \times\left\langle\prod_{i=1}^{j}\det(D+\mu\gamma_0+m_i)^{n_i}(D-\mu\gamma_0+m_i)^{n_i}\right\rangle_{1+1}. \tag{51}$$

We now need to keep track of the mass dependence of the replicated generating function

$$\left\langle\prod_{i=1}^{j}\det(D+\mu\gamma_0+m_i)^{n_i}(D-\mu\gamma_0+m_i)^{n_i}\right\rangle_{1+1} = \exp\Bigg(\sum_{l\le m=1}^{j}2n_ln_m(G_0(\mu,\mu,m_l,m_m) + G_0(-\mu,\mu,m_l,m_m)) + \sum_{l=1}^{j}2n_l[m_l\Sigma + (G_0(\mu,\mu,m,m_l)+G_0(-\mu,\mu,m,m_l))]\Bigg). \tag{52}$$

Compared to the generating function for Re$[n]$ in Eq. (20) there are two differences: (1) The replica index now labels the quark masses instead of the chemical potentials. (2) The term linear in the replica number contains the mean field value Σ of the chiral condensate. However, the entire structure of the generating function remains, and the combinatorics associated with the differentiation is identical to that for the quark number. Only now, the physical quantities appearing in the expressions are the chiral condensates and the chiral susceptibilities. We get

$$P^{1+1}_{\mathrm{Re}[\sigma]}(x) = \frac{1}{\sqrt{\pi(\chi^I_S+\chi^B_S)}}e^{-(x-\Sigma-\delta\Sigma^B-\delta\Sigma^I)^2/(\chi^I_S+\chi^B_S)}, \tag{53}$$

where we used the definitions in (13).

Likewise, the distribution for the imaginary part of σ

$$P^{1+1}_{\mathrm{Im}[\sigma]}(y) \equiv \left\langle\delta\left(y+i\frac{1}{2}(\sigma(\mu)-\sigma(-\mu))\right)\right\rangle_{1+1}, \tag{54}$$

follows form that for the imaginary part of the quark number simply by reidentifying the physical quantities which appear in the final expression

$$P^{1+1}_{\mathrm{Im}[\sigma]}(y) = \frac{1}{\sqrt{\pi(\chi^I_S-\chi^B_S)}}e^{(iy-\delta\Sigma^B+\delta\Sigma^I)^2/(\chi^I_S-\chi^B_S)}. \tag{55}$$

Notice the absence of the mean field value of the chiral condensate. In the generating function, the mean field contribution from the fermionic replicas cancels against the one from the replicated bosonic quarks. In agreement with the Hermiticity property (47), we see that the width of $P^{1+1}_{\mathrm{Im}[\sigma]}$ vanishes for $\mu\to 0$ while the width of the distribution of the real part remains nonzero. From the explicit expression for G_0 it can be easily shown that $\chi^I_S-\chi^B_S>0$.

Since the structure of the generating function is unchanged the full distribution

$$P^{1+1}_{\sigma}(x,y) \equiv \left\langle\delta\left(x-\frac{1}{2}(\sigma(\mu)+\sigma(-\mu))\right)\times\delta\left(y+i\frac{1}{2}(\sigma(\mu)-\sigma(-\mu))\right)\right\rangle_{1+1} \tag{56}$$

again factorizes

$$P^{1+1}_{\sigma}(x,y) = P^{1+1}_{\mathrm{Re}[\sigma]}(x)P^{1+1}_{\mathrm{Im}[\sigma]}(y). \tag{57}$$

Thus we have

$$P^{1+1}_{\sigma}(x,y) = \frac{1}{\pi\sqrt{(\chi^I_S)^2-(\chi^B_S)^2}}e^{-(x-\Sigma-\delta\Sigma^B-\delta\Sigma^I)^2/(\chi^I_S+\chi^B_S)} \times e^{(iy-\delta\Sigma^B+\delta\Sigma^I)^2/(\chi^I_S-\chi^B_S)}. \tag{58}$$

As a check of this second main result, we compute the chiral condensate

$$\langle\sigma\rangle_{1+1} = \int_{-\infty}^{\infty}dxdy(x+iy)P^{1+1}_{\sigma}(x,y) = \Sigma+2\delta\Sigma^B \tag{59}$$

and the square of the condensate

$$\langle\sigma^2\rangle_{1+1} = \int_{-\infty}^{\infty}dxdy(x+iy)^2P^{1+1}_{\sigma}(x,y) = \chi^B_S+(\Sigma+2\delta\Sigma^B)^2. \tag{60}$$

We see that the dependence on Σ^I and χ^I_S has canceled and the results obtained in Table I are reproduced. The cancellations take place in exactly the same manner as for the baryon density. We conclude that in both cases the μ dependence of the fluctuations are induced through a coupling to the isospin charge of the pions. These strong fluctuations in the real part and in the imaginary part combine and leave the physical observable independent of the chemical potential.

Finally, we give also the partially quenched distribution of the chiral condensate

$$P^{\mathrm{PQ}}_{\sigma}(x,y) = \frac{1}{\pi\sqrt{(\chi^I_S)^2-(\chi^B_S)^2}}e^{-(x-\Sigma-\delta\Sigma^B-\delta\Sigma^I)^2/(\chi^I_S+\chi^B_S)} \times e^{-y^2/(\chi^I_S-\chi^B_S)}. \tag{61}$$

The partially quenched expectation values from Table I

$$\langle\sigma\rangle_{\mathrm{PQ}} = \Sigma+\delta\Sigma^B+\delta\Sigma^I \tag{62}$$

and

$$\langle\sigma^2\rangle_{\mathrm{PQ}} = \chi^B_S+(\Sigma+\delta\Sigma^B+\delta\Sigma^I)^2 \tag{63}$$

follow from Gaussian integrations over the distribution function.

We will use both the partially quenched results and the full results to explain how to deal with some of the numerical problems encountered in lattice QCD at nonzero chemical potential.

VI. NUMERICAL LATTICE QCD AT NONZERO μ

Above, we have derived the full and partially quenched distributions of the quark number operator for $\mu < m_\pi/2$. Here, we discuss how these results can be of use when measuring the quark number operator by numerical lattice QCD.

The main problem encountered in numerical lattice QCD at nonzero chemical potential is that operators may acquire their expectation values by virtue of extremely delicate cancellations caused by the complex valued fermion determinant in the path integral. To illustrate the problem, let us look at the distribution of the quark number operator, Eq. (39). Notice that the distribution itself takes complex values, i.e. it is not a probability measure. This feature is also shared by the unquenched eigenvalue density of the Dirac operator [32,33] and the distribution of the phase of the fermion determinant [6]. These complex oscillations are all important in order to separate the physics of nonzero baryon chemical potential [34] from that at isospin chemical potential. Common to the three examples mentioned above is that the amplitude of the complex oscillations is exponentially large in the volume. Moreover, in all three cases, one must integrate over on the order of V periods of the oscillations in order to obtain a reliable value of the baryon density or chiral condensate. Let us illustrate this explicitly using the results derived above.

The unquenched distribution of the quark number $P_n^{1+1}(x, y)$ takes complex values, and, as we have seen in Eq. (40), both the real part and the imaginary part contribute to the baryon density. The magnitudes are equal to ν_I, but the signs are opposite so that the total quark number vanishes. Since the complex oscillations are associated with the imaginary part y of the quark number $n = x + iy$, let us ask: How large should $y_{\max}$ be in order that

$$\int_{-y_{\max}}^{y_{\max}} dy i y P_{\mathrm{Im}[n]}^{1+1}(y) \sim -\nu_I. \tag{64}$$

The answer is

$$y_{\max}^2 - \nu_I^2 \gg \chi_{ud}^I - \chi_{ud}^B. \tag{65}$$

Since $\nu_I \sim V$ and $\chi_{ud}^I - \chi_{ud}^B \sim V$, we find that $y_{\max}$ has to be only slightly larger than ν_I. As the period of the oscillations is of order unity, we conclude that we have to include on the order of V oscillations in the integral. This can be a hard task to control numerically unless we know the analytical form of the distributions. The results presented here give this form to leading order. There will be corrections to this form in order to induce a nonzero baryon number, but one should still expect large cancellations between contributions from the real part and the imaginary part.

Not only can results from chiral perturbation theory help to understand the detailed cancellations occurring in the integral, they can also give hints on which part of the integrand one needs to sample numerically in lattice

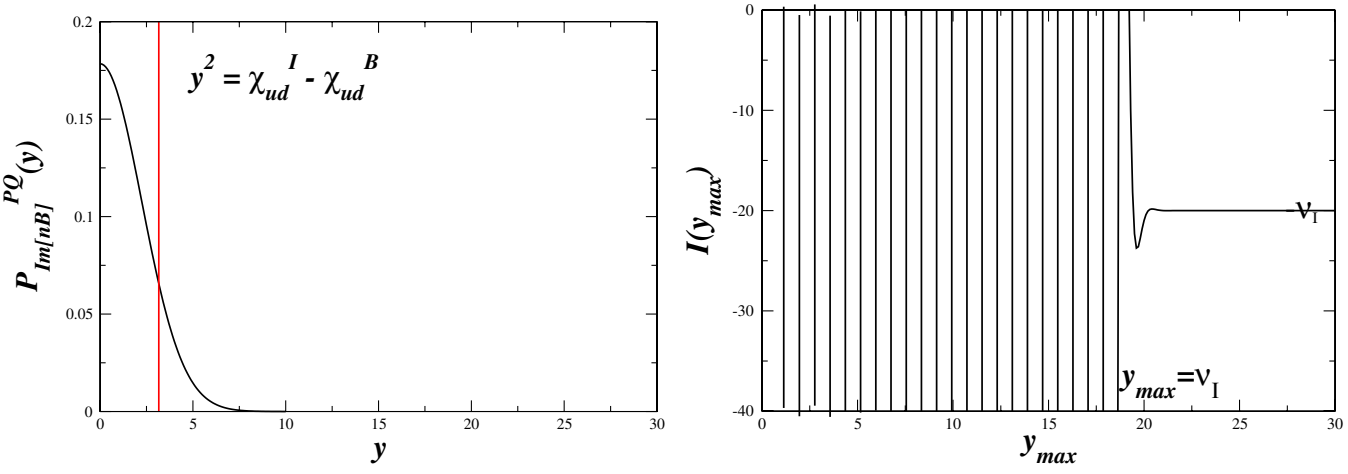

FIG. 1 (color online). Left panel: The distribution of the imaginary part of the quark number in the partially quenched simulation ensemble. Right panel: The contribution to the quark number in the 1 + 1 target theory from the imaginary part of n as a function of $y_{\max}$, see Eq. (64). Only when $y_{\max}$ is larger than ν_I do we find that the contribution from the imaginary part cancels the one from the real part and leaves $\langle n \rangle_{1+1} = 0$. If $\nu_I \sim V$ is much larger than the width of the PQ distribution $\sqrt{\chi_{ud}^I - \chi_{ud}^B} \sim \sqrt{V}$, then there is a serious overlap problem. For the plot, we have chosen $\nu_I = 20$ and $\chi_{ud}^I - \chi_{ud}^B = 10$, and we already see that, unless one also samples the far end of the tail, the configurations generated in the PQ simulation ensemble do not have the values of $\mathrm{Im}[n]$ required for the cancellation of the baryon number.

QCD: Imagine that we have generated an ensemble of configurations for the phase-quenched weight. Then for the configurations in our simulation ensemble, the quark number n is distributed according to $P_n^{\rm PQ}(x, y)$ as given in Eq. (44). Within the width of this distribution only on the order of $\sqrt{V}$ oscillations takes place. The reweighting from the simulation ensemble to the full theory (target ensemble) therefore has to lift the far tail of the phase-quenched distribution. (For illustration, see Fig. 1.)

Even though the sign problem makes it hard to approach the thermodynamic limit $V \to \infty$, it is worth it to keep in mind that in a given numerical simulation we work with a finite volume where the sign problem may be tractable depending on the value of T and μ. We will address this issue in [35].

In the complex Langevin [22–26] approach to the QCD sign problem, the real and the imaginary part of the quark number are themselves complex. In particular, this means that the imaginary part y is not constrained to the real axis. Rather as we now show, y will fluctuate parallel to the real y axis but shifted into the complex y plane by $i\nu_I$. To show this, we start from the complex action, obtained from the one-loop result for the distribution of the quark number

$$S = -\log[P^{1+1}_{{\rm Im}[n]}(y)] = -(iy + \nu_I)^2/(\chi^I_{ud} - \chi^B_{ud}), \quad (66)$$

where we made use of the result in Eq. (33). The flow equations for $y = a + ib$ are given by (the step size is denoted by ϵ)

$$\begin{aligned} a_{n+1} &= a_n - \epsilon\,{\rm Re}\left[\frac{dS}{dy}\right]_{y=a_n+ib_n} + \sqrt{\epsilon}\eta_n \\ &= a_n - \epsilon\frac{2a_n}{\chi^I_{ud} - \chi^B_{ud}} + \sqrt{\epsilon}\eta_n \end{aligned} \quad (67)$$

and

$$b_{n+1} = b_n - \epsilon\,{\rm Im}\left[\frac{dS}{dy}\right]_{y=a_n+ib_n} = b_n - \epsilon\frac{2(b_n - \nu_I)}{\chi^I_{ud} - \chi^B_{ud}}. \quad (68)$$

Note that a and b decouple: a fluctuates about zero while b quickly moves to ν_I and stays there, since there is no noise η to kick it around. The complex Langevin algorithm therefore will essentially replace

$$\int_{-\infty}^{\infty} dy y P^{1+1}_{{\rm Im}[n]}(y) \quad (69)$$

by

$$\int_{-a_{\rm max}}^{a_{\rm max}} da(a + i\nu_I)e^{-a^2/(\chi^I_{ud} - \chi^B_{ud})}, \quad (70)$$

where $a_{\rm max}$ is the width of the region sampled by the algorithm. Since the flow equation for a is just that of the ordinary real Gaussian $\exp(-a^2/(\chi^I_{ud} - \chi^B_{ud}))$ and completely decoupled from the imaginary part, the complex Langevin algorithm should not have any problems in sampling this. In other words, $a_{\rm max}$ is a good deal larger than $\sqrt{\chi^I_{ud} - \chi^B_{ud}}$ and the integral is close to $i\nu_I$ as desired. Again there will be corrections to the one-loop results derived here and complex Langevin must be able to take these into account correctly in order to obtain the correct average quark number. However, as long as the average quark number is much smaller than ν_I, the fluctuations in the complex y plane should be expected to take place in the neighborhood of $i\nu_I$. A similar example of a possible usefulness of complex Langevin was presented in [36,37].

For purely imaginary values of the chemical potential the sign problem is absent, and the quark number operator is imaginary. In A, we work out the distribution of the quark number for imaginary values of the chemical potential. The result is a Gaussian centered at zero. It is certainly true that simulations at imaginary μ [38–40] are easier—the reason is the positivity of the measure. This suggests that simulations at imaginary μ are as easy as simulations at $\mu = 0$. Analytical and numerical studies show that the analytic continuation is well under control at least for $\mu/T < 1$ [38–40], and it would be interesting to interpret this result in the light of the distributions discussed here. Analytic continuation to real μ has also been studied in models without the sign problem [41].

VII. DISTRIBUTIONS FOR $\mu > m_\pi/2$

The chiral expansion of the generating functions relevant for the baryon distribution take a different form when $\mu > m_\pi/2$. In this domain, the chemical potential induces a Bose condensate with a nonzero isospin number even at the mean field level. The derivation presented above is therefore not valid for $\mu > m_\pi/2$. In this section, we discuss the distributions of the quark number and the chiral condensate for $\mu > m_\pi/2$.

A. The fluctuations of the chiral condensate ($\mu > m_\pi/2$)

For $\mu > m_\pi/2$, the quark mass is inside the spectrum of $D + \mu\gamma_0$ [33,42–44]. Since an eigenvalue of $D + \mu\gamma_0$ can come very close to the quark mass, the fluctuations of the chiral condensate are much larger when $\mu > m_\pi/2$. In order to quantify the fluctuations of the chiral condensate let us consider the moments of the real and the imaginary part of σ. To start we consider the quenched case.

The odd moments of ${\rm Im}[\sigma]$: Because the quenched weight does not depend on the sign of μ the odd moments vanish

$$\langle(\sigma - \sigma^*)^{2p+1}\rangle = 0. \quad (71)$$

It follows that the quenched distribution of the imaginary part of the chiral condensate must be an even function; that is: $P^{(N_f=0)}_{{\rm Im}[\sigma]}(y)$ is symmetric in y.

The even moments of ${\rm Im}[\sigma]$: The even moments are nonzero. In fact, as we now show, they are divergent. To

see this, let us first consider the second moment of the imaginary part

$$\langle(\sigma-\sigma^*)^2\rangle = 2\langle\sigma^2\rangle - 2\langle\sigma\sigma^*\rangle. \tag{72}$$

If we express σ in terms of the eigenvalues z_k of $D+\mu\gamma_0$

$$\sigma = \sum_k \frac{1}{z_k+m} \tag{73}$$

we see that $\langle\sigma\sigma^*\rangle$ includes an absolute squared pole, which gives rise to a logarithmic singularity. So we have

$$\langle(\sigma-\sigma^*)^2\rangle = -2\langle\sigma\sigma^*\rangle + \mathcal{O}(\epsilon^0). \tag{74}$$

Obviously, the logarithmic singularity is only present when the quark mass is inside the support eigenvalue density. In fact, it can be shown explicitly within chiral random matrix theory that the divergent part of the second moment is proportional to the eigenvalue density evaluated at the quark mass

$$\begin{aligned}\langle(\sigma-\sigma^*)^2\rangle &= -2\left\langle\sum_k \frac{1}{|z_k+m|^2}\right\rangle \\ &= -2\int_{C_\epsilon} d^2z\rho(z,z^*)\frac{1}{|z+m|^2} \\ &= 4\pi\log(\epsilon)\rho_{N_f=0}(z=m,z^*=m) \\ &= \log(\epsilon)\theta(|\mu|-m_\pi/2)\frac{V\Sigma^2}{\mu^2F^2}.\end{aligned} \tag{75}$$

Here, C_ϵ is the complex plane excised by a sphere of radius ϵ centered at $-m$. The quenched eigenvalue density is the leading order result from chiral perturbation theory [43]. We conclude that the quenched second moment of $\mathrm{Im}[\sigma]$ is logarithmically divergent if the quark mass is inside the support of the eigenvalue density, i.e. if $\mu > m_\pi/2$.

The higher even moments of σ have more severe divergences. The most divergent term is the one with the same powers of σ and σ^*, so that

$$\langle(\sigma-\sigma^*)^{2p}\rangle \simeq (-1)^p\frac{(2p)!}{p!p!}\langle(\sigma\sigma^*)^p\rangle. \tag{76}$$

In order to understand this better, let us work out the details explicitly for $p=2$. Again, we keep only the leading divergence

$$\begin{aligned}\langle(\sigma-\sigma^*)^4\rangle &= 6\langle(\sigma\sigma^*)^2\rangle \\ &= 6\left\langle\sum_{g,h,j,k}\frac{1}{z_g+m}\frac{1}{z_h+m}\frac{1}{z_j^*+m}\frac{1}{z_k^*+m}\right\rangle.\end{aligned} \tag{77}$$

The most singular terms are the diagonal terms with $g=h=j=k$ which lead to a $1/\epsilon^2$ singularity which dominates the integral over the spectral density.

Because the most divergent term is also given by the diagonal part of the sum for $p>2$, it is always proportional to the eigenvalue density. We thus obtain the general relation (for $p=2,3,4,\ldots$)

$$\begin{aligned}\langle(\sigma-\sigma^*)^{2p}\rangle \sim (-1)^p\frac{(2p)!}{p!p!}\frac{1}{2(p-1)\epsilon^{2(p-1)}} \\ \times\theta(|\mu|-m_\pi/2)\frac{V\Sigma^2}{4\pi\mu^2F^2}.\end{aligned} \tag{78}$$

We conclude that $P^{(N_f=0)}_{\mathrm{Im}[\sigma]}(y)$ must be symmetric in y in order that the odd moments vanish, and it must have a $1/|y|^3$ tail to reproduce the observed singularities. When the quark mass is outside the spectrum of the Dirac operator the same argument applies, but now the spectral density at $z=m$ is exponentially suppressed, and the singular terms vanish in the thermodynamic limit. While the singularities tell us about the tail of the distribution, the leading divergent behavior of the moments does not contain sufficient information to obtain $P^{(N_f=0)}_{\mathrm{Im}[\sigma]}(y)$ for smaller y. We have verified the $1/|y|^3$ tail of $P^{(N_f=0)}_{\mathrm{Im}[\sigma]}(y)$ by a numerical simulation of quenched chiral random matrix theory.

So far we have considered the quenched case. As a first step toward the fully unquenched theory, let us consider the phase-quenched theory. In this case, the absolute square of the fermion determinant in the measure, $\prod_j|z_j^2+m^2|^2$, shifts the singularities. We now have

$$\langle(\sigma-\sigma^*)^2\rangle_{1+1^*} \sim \epsilon^0, \tag{79}$$

$$\langle(\sigma-\sigma^*)^4\rangle_{1+1^*} \sim \log(\epsilon), \tag{80}$$

and

$$\langle(\sigma-\sigma^*)^{2p}\rangle_{1+1^*} \sim \frac{1}{\epsilon^{2(p-2)}} \tag{81}$$

for $p>2$. This implies that the far tail of the distribution of $\mathrm{Im}[\sigma]$ drops of like $1/|y|^5$. The distribution is again even since the odd moments still vanish because the absolute square of the fermion determinant does not depend on the sign of the chemical potential.

Finally, let us briefly look at the unquenched case. Let us for simplicity take $N_f=1$. With a single determinant in the measure, the odd moments no longer vanishes. Moreover, the odd moments can now also diverge. For example,

$$\langle(\sigma-\sigma^*)^3\rangle_{N_f=1} = -\langle\sigma^2\sigma^*\rangle_{N_f=1} \sim \log(\epsilon). \tag{82}$$

Again, the $\log(\epsilon)$ singularity is only present when the quark mass is inside the support of the spectral density, i.e. for $\mu > m_\pi/2$. In general, we have

$$\langle(\sigma-\sigma^*)^{2p+1}\rangle_{N_f=1} \sim \frac{1}{\epsilon^{2(p-1)}} \tag{83}$$

for $p>1$. The diverging odd moments show that the unquenched distribution of $\mathrm{Im}[\sigma]$ is not an even function of y. We expect that the unquenched distribution of $\mathrm{Im}[\sigma]$ takes complex values.

Unfortunately, due to the divergences, we have not been able to derive the full distribution of the imaginary part of the chiral condensate for $\mu > m_\pi/2$.

For the real part of σ, the main difference is that the odd moments are nonzero. The leading divergent part of the even moments is the same (up to a sign) as for the imaginary part.

B. Fluctuations of the quark number ($\mu > m_\pi/2$)

The general arguments which gave us information about the distribution of the chiral condensate also apply to the quark number for $\mu > m_\pi/2$. For $\mu > m_\pi/2$, we have that μ is inside the support of the spectrum of $\gamma_0(D + m)$ [45], and this again leads to enhanced fluctuations. A rerun of the general arguments presented above show that also the quenched distribution of the real and of the imaginary part of the baryon number has an inverse cubic tail. Rather than repeating the arguments, let us instead discuss the cancellations which ensure that the total baryon number remains zero in the unquenched case (as must be true in chiral perturbation theory).

Let us first consider the real and imaginary part of the quark number density for the quenched or phase-quenched case. The imaginary part of the quark number is given by

$$2i\,\mathrm{Im}[n] = \mathrm{Tr}\frac{\gamma_0}{\gamma_0(D+m)+\mu} + \mathrm{Tr}\frac{\gamma_0}{\gamma_0(D+m)-\mu}. \tag{84}$$

Because the spectrum of $\gamma_0(D + m)$ is reflection symmetric about the imaginary axis, and the average spectrum for the quenched and phase-quenched theory is reflection symmetric both about the real and the imaginary axis, we find that also for $\mu > m_\pi/2$

$$\langle \mathrm{Im}[n]\rangle_{N_f=0} = \langle \mathrm{Im}[n]\rangle_{1+1^*} = 0. \tag{85}$$

The real part of the quark number is given by

$$2\,\mathrm{Re}[n] = \mathrm{Tr}\frac{\gamma_0}{\gamma_0(D+m)+\mu} - \mathrm{Tr}\frac{\gamma_0}{\gamma_0(D+m)-\mu}. \tag{86}$$

This is the isospin density with a nonvanishing expectation value in the quenched and phase-quenched theory for $\mu > m_\pi/2$ because of pion condensation. At mean field level in chiral perturbation theory, the isospin density is [46]

$$\nu_I = \langle \mathrm{Re}[n]\rangle_{1+1^*} = 2\mu F^2\left[1 - \left(\frac{m_\pi^2}{4\mu^2}\right)^2\right]. \tag{87}$$

We now consider the unquenched case with $N_f = 2$. In the supersymmetric formalism, the generating function for $\mathrm{Re}[n]$ is given by

$$Z(\mu_1,\mu_2) = \left\langle \frac{\det(\gamma_0(D+m)+\mu_2)\det(\gamma_0(D+m)-\mu_2)\det^2(\gamma_0(D+m)+\mu_1)}{\det(\gamma_0(D+m)+\mu_1)\det(\gamma_0(D+m)-\mu_1)} \right\rangle \tag{88}$$

with

$$2\langle \mathrm{Re}[n]\rangle_{1+1} = \frac{d}{d\mu_2}\log Z(\mu_1,\mu_2)|_{\mu_1=\mu_2=\mu}. \tag{89}$$

The generating function undergoes a phase transition to a pion condensed phase at $\mu = m_\pi/2$. It can be interpreted as the average phase factor at μ_1 for the phase-quenched theory at μ_2. Such averages were studied in [47]. At the mean field level, the generating function factorizes as

$$Z(\mu_1,\mu_2) = \frac{\langle \det(\gamma_0(D+m)+\mu_2)\det(\gamma_0(D+m)-\mu_2)\det^2(\gamma_0(D+m)+\mu_1)\rangle}{\langle \det(\gamma_0(D+m)+\mu_1)\det(\gamma_0(D+m)-\mu_1)\rangle}. \tag{90}$$

The imaginary part of the quark number for two flavors can also be obtained from the generating function

$$2i\langle \mathrm{Im}[n]\rangle_{1+1} = \frac{d}{d\mu_1}\Big|_{\mu_1=\mu_2=\mu} \log Z(\mu_1,\mu_2) \tag{91}$$

with

$$Z(\mu_1,\mu_2) = \left\langle \frac{\det(\gamma_0(D+m)+\mu_1)\det(\gamma_0(D+m)+\mu_2)\det(\gamma_0(D+m)-\mu_2)}{\det(\gamma_0(D+m)-\mu_1)} \right\rangle. \tag{92}$$

The partition function (92) is a phase-quenched average phase factor which was studied in [39]. At the mean field level, this partition function factorizes as

$$Z(\mu_1, \mu_2) = \frac{\langle \det^2(\gamma_0(D+m)+\mu_1)\det(\gamma_0(D+m)+\mu_2)\det(\gamma_0(D+m)-\mu_2)\rangle}{\langle \det(\gamma_0(D+m)-\mu_1)\det(\gamma_0(D+m)+\mu_1)\rangle}. \quad (93)$$

We observe that the real and imaginary part of the quark number are obtained from the same generating function. The mean field analysis of partition function (90) was outlined in [48]. It is determined by the action

$$S = \frac{1}{4}F^2\,\mathrm{Tr}[U,B][U^{-1},B] - \mathrm{Tr}M\Sigma(U+U^{-1}) \quad (94)$$

with the baryon matrix and the mass matrix given by

$$B = \mathrm{diag}(\mu_1, \mu_1, \mu_2, -\mu_2), \qquad M = \mathrm{diag}(m, m, m, m). \quad (95)$$

The ansatz for the mean field can be written as [48]

$$U = R_{kl}^{-1}(\beta_{kl})R_{4k}(\alpha_k)R_{kl}(\beta_{kl}) \quad (96)$$

with $k = 1, 2, 3$ and $l \neq k$. Here, $R_{pq}(\alpha)$ is a rotation in the pq plane by angle α. There is one important difference with [48], though. Because the quark masses are equal and the chemical potential are put equal after differentiation, the integration over β_k cannot be done by a saddle point approximation but has to be performed exactly.

In total there are 6 different saddle points. For $\mu_1 = \mu_2$, the action of each of the saddle point is the same and the dependence on β_k cancels. Therefore the integral over β_k has to be performed exactly for $\mu_1 \neq \mu_2$, whereas the α_k are determined by the saddle point equation.

For the real part of the quark number we obtain:

$$2\langle \mathrm{Re}[n]\rangle_{1+1} = -(12+4)c\mu F^2[\cos^2\bar{\alpha} - 1], \quad (97)$$

where the first term (i.e. 12) originates from the rotation matrices that mix $-\mu_2, \mu_2, \mu_1$ and the second term (i.e. 4) from the rotation matrices that mix $-\mu_2, \mu_1, \mu_1$. The real constant c is a normalization factor. The solution of the saddle point equation is given by [46]

$$\cos\bar{\alpha} = \frac{m_\pi^2}{4\mu^2}. \quad (98)$$

With this, we have

$$\langle \mathrm{Re}[n]\rangle_{1+1} = 8c\mu F^2\left[1 - \left(\frac{m_\pi^2}{4\mu^2}\right)^2\right], \quad (99)$$

which is proportional to the isospin density in the Bose condensed phase of the phase-quenched theory at mean field level,cf. (87).

For the imaginary part of the quark number, we obtain contributions both from the numerator and the denominator of the generating function. The contribution that originates from the numerator is given by

$$(4+4)\mu F^2[\cos^2\bar{\alpha} - 1], \quad (100)$$

where again the first and second term correspond to rotation matrices that mix $-\mu_2, \mu_2, \mu_1$ and that mix $-\mu_2, \mu_1, \mu_1$ in this order. The contribution from the denominator is given by

$$-24c\mu F^2[\cos^2\bar{\alpha} - 1]. \quad (101)$$

Since the real and imaginary parts are obtained from the same generating function, the constant c in the expressions is the same. For the imaginary part of the quark number, we thus obtain

$$2i\langle \mathrm{Im}[n]\rangle_{1+1} = 16c\mu F^2[\cos^2\bar{\alpha} - 1]. \quad (102)$$

As must be true in chiral perturbation theory, the sum of the real and imaginary part of the quark number vanishes. Here, we have shown this by explicitly computing both contributions. As for $\mu < m_\pi/2$, we have found that the two terms are proportional to the isospin density in the phase-quenched theory. For $\mu > m_\pi/2$, however, the isospin density is far greater due to Bose condensation of pions.

VIII. CONCLUSIONS

The distribution of the quark number operator and the chiral condensate for Euclidean QCD at nonzero chemical potential has been derived to leading order in chiral perturbation theory. As the two operators take on complex values, the distributions are over the complex plane. Moreover, because of the phase factor of the fermion determinant, the distributions are not real and positive. We have shown how the complex oscillations of the unquenched distributions lead to large cancellations when evaluating the baryon density and chiral condensate. These cancellations give a direct insight into the problems faced by numerical lattice QCD at nonzero chemical potential. Of course, the net contribution from pions to the average baryon density is zero within chiral perturbation theory. Nevertheless, pions contribute manifestly to the distribution of the quark number and the chiral condensate and hence to the noise produced in numerical lattice gauge simulations at nonzero chemical potential.

Most of the results were derived for $\mu < m_\pi/2$ to one-loop order in chiral perturbation theory. Then the distributions of the chiral condensate and the quark number take a Gaussian form as one might expect from the central limit theorem. The unquenched distribution of the imaginary part of these observables takes on complex values. For example, for the imaginary part of the quark number, this distribution is a Gaussian that is shifted in the imaginary direction by an amount proportional to the volume (the isospin number in the phase-quenched theory when evaluated at the same value of the chemical potential). This is, of course, not possible in an ordinary reweighting scheme and the final results for the baryon density instead relies on

detailed cancellations after taking into account the far tail of the distribution. However, within the complex Langevin method the real and imaginary parts of the baryon density are complexified and the imaginary part could fluctuate around i times a quantity of order the volume.

For $\mu > m_\pi/2$, the distributions of the real and the imaginary part of the quark number and chiral condensate develop a power law tail. This extreme enhancement of the fluctuations is a direct consequence of the quark mass being inside the spectral support of the Dirac operator $D + \mu\gamma_0$ and the chemical potential being inside the support of $\gamma_0(D + m)$.

The analytical results provided here may help in interpreting state of the art lattice simulations at nonzero chemical potential. They can be used as a benchmark for attempts to link the fluctuations of the baryon number to the presence of the tricritical point. Since we have understood fluctuations produced, the pions this may help in optimizing and developing numerical approaches to reduce this source of noise.

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APPENDIX A: IMAGINARY CHEMICAL POTENTIAL

In this appendix, we give the result for the distribution of the quark number operator when evaluated at purely imaginary values of the chemical potential. The fermion determinant is real for imaginary chemical potential, and numerical simulations are possible for an even number of flavors [38–40]. In this case, the quark number operator is anti-Hermitian even when $i\mu$ is nonzero

$$n(i\mu)^* = \left(\mathrm{Tr}\frac{\gamma_0}{D + i\mu\gamma_0 + m}\right)^* = -\mathrm{Tr}\frac{\gamma_0}{D + i\mu\gamma_0 + m} = -n(i\mu). \quad \text{(A1)}$$

The distribution is therefore one-dimensional

$$P^{1+1,i\mu}_{n(i\mu)}(y) \equiv \langle\delta(y + in(i\mu))\rangle_{1+1,i\mu}. \quad \text{(A2)}$$

The derivation of the distribution for $\mu < m_\pi/2$ to one-loop order in chiral perturbation theory is simpler than for real μ since now there are no terms $n(-i\mu)$ which can couple to the isospin charge of the pions. We find

$$P^{1+1,i\mu}_{n(i\mu)}(y) = \frac{1}{\sqrt{\pi|\chi^B_{ud}|}} e^{-y^2/|\chi^B_{ud}|}. \quad \text{(A3)}$$

As must be true within chiral perturbation theory, we find that

$$\langle n(i\mu)\rangle_{1+1,i\mu} = 0. \quad \text{(A4)}$$

Note also that the width of the distribution is independent of μ. As χ^B_{ud} is extensive, the distribution of the quark density becomes a δ-function at the origin in the thermodynamic limit.

We also get

$$\langle n(i\mu)^2\rangle_{1+1,i\mu} = |\chi^B_{ud}|. \quad \text{(A5)}$$

One can, of course, also consider the distributions of $n(i\mu) \pm n(-i\mu)$ which will be the analytic continuations of the distributions of the analytic part of the real and imaginary parts of n.

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