Imaginary chemical potentials and the phase of the fermionic determinant

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A numerical technique is proposed for an efficient numerical determination of the average phase factor of the fermionic determinant continued to imaginary values of the chemical potential. The method is tested in QCD with eight flavors of dynamical staggered fermions. A direct check of the validity of analytic continuation is made on small lattices and a study of the scaling with the lattice volume is performed.

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I. INTRODUCTION

Lattice QCD simulations in presence of a finite density of baryonic matter are hindered by the well known sign problem. Consider for instance the QCD partition function

\[ Z(\mu, \mu) = \int D\!U e^{-\mathcal{S}[U]} (\det M[U, \mu])^2 \]

\[ = \int D\!U e^{-\mathcal{S}[U]} \det M[U, \mu]^2 e^{i\theta} \]

(1)

describing two flavors of quarks (or eight flavors in the case of staggered flavors) which are given an equal chemical potential \( \mu \): the determinant of the fermionic matrix \( M \) is in general complex \( (\theta \neq 0) \) for \( \mu \neq 0 \) and Monte Carlo simulations are not feasible. Various possibilities have been explored to circumvent the problem, like reweighting techniques \([1, 2, 3]\), the use of an imaginary chemical potential either for analytic continuation \([4, 5, 6, 7, 8, 9, 10]\) or for reconstructing the canonical partition function \([11, 12, 13]\). Taylor expansion techniques \([14, 15]\) and non-relativistic expansions \([16, 17, 18]\).

The same is not true in the case of a finite isospin density, i.e. when quarks are given opposite chemical potentials. Indeed, due to the property \( \det M[U, -\mu] = \det M[U, \mu]^\ast \), the partition function

\[ Z(\mu, -\mu) = \int D\!U e^{-\mathcal{S}[U]} |\det M[U, \mu]|^2 \]

(2)

has a positive measure. That is also known as phase quenched QCD. The average value of the phase factor of the fermionic determinant, \( \langle e^{i\theta} \rangle_{\mu, -\mu} \), where the index indicates the partition function the expectation value refers to, gives a direct measurement of the severity of the sign problem. \( \langle e^{i\theta} \rangle \sim 0 \) will signal the stage at which the complex nature of the determinant will imply a significant difference between finite baryonic density and finite isospin density, as well a poor reliability of reweighting techniques (see Ref. \([19]\) and references therein).

It clearly follows from Eqs. (1) and (2) that the average phase factor is the expectation value of the ratio of two determinants; it can also be expressed as the ratio of two partition functions:

\[ \langle e^{i\theta} \rangle_{\mu, -\mu} = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle_{(\mu, -\mu)} = \frac{Z(\mu, \mu)}{Z(\mu, -\mu)}. \]

(3)

Its direct numerical computation reveals a difficult numerical task as the lattice volume \( V \) increases, since it involves the numerical evaluation of fermionic determinants.

It has been proposed recently \([20, 21]\) to study the analytic continuation of the average phase factor to imaginary values of the chemical potential

\[ \langle e^{i\theta} \rangle_{i\mu, -i\mu} = \left\langle \frac{\det M(i\mu)}{\det M(-i\mu)} \right\rangle_{(i\mu, -i\mu)} = \frac{Z(i\mu, i\mu)}{Z(i\mu, -i\mu)} \]

\[ = \frac{\int D\!U e^{-\mathcal{S}[U]} \det M[U, i\mu] \det M[U, -i\mu]}{\int D\!U e^{-\mathcal{S}[U]} \det M[U, i\mu] \det M[U, -i\mu]} \]

(4)

where \( Z(i\mu, i\mu) \) and \( Z(i\mu, -i\mu) \) are the analytic continuation of the partition functions at finite baryonic and isospin chemical potentials respectively, which are both suitable for numerical simulations since \( \det M[U, i\mu] \) is always real. Numerical difficulties however are present also in this case: the observable to be averaged is still expressed in terms of fermionic determinants. Moreover in principle sampling problems deriving from a bad overlap between the two statistical distributions described by \( Z(i\mu, i\mu) \) and \( Z(i\mu, -i\mu) \) may arise. In Ref. \([21]\) the fermionic determinant has been estimated on the basis of the lowest lying eigenvalues of the fermionic matrix.

In the present paper we propose a new technique which, making use of numerical strategies developed in different contexts, permits an exact evaluation of the average phase factor with a reasonable scaling of the required CPU time as the lattice volume is increased. In doing this we will fully exploit the possibility of performing numerical simulations of the partition function \( Z(i\mu_1, i\mu_2) \) for generic values of \( \mu_1 \) and \( \mu_2 \).

In Section \([22]\) we illustrate two different possible methods, which are then numerically tested and compared in Section \([23]\) for the theory with 8 staggered flavors.
II. THE METHOD

The evaluation of the average phase factor, expressed like in Eq. (3) or Eq. (4) as the ratio of two different partition functions, resembles similar problems which are encountered in quite different contexts, like the evaluation of disorder parameters in statistical models and in lattice gauge theories. Explicit examples are given by monopole disorder parameters or by the ’t Hooft loop, which enters in various studies about color confinement. The major problem in those cases is the small overlap between the statistical distributions corresponding to two different partition functions, resulting in a poor sampling efficiency. Powerful techniques have been developed in different partition functions, resembling similar problems which are possible to determine further derivatives of \( \rho \) in order to improve the integration accuracy.

As a different method we consider rewriting \( \langle e^{i2\theta} \rangle_{\mu\nu} \) as the product of \( N \) intermediate ratios:

\[
\langle e^{i2\theta} \rangle_{\mu\nu} = \frac{Z(i\mu, i\nu)Z(\mu, -i\mu)}{Z(i\mu, -i\mu)Z(\mu, -i\mu)} \cdots \frac{Z_N}{Z_0} = \prod_{k=1}^{N} r_k(9)
\]

where \( Z_N = Z(i\mu, i\mu) \), \( Z_0 = Z(i\mu, -i\mu) \) while

\[
Z_k \equiv \int DU e^{-S_G[U]} \det M[U, i\mu] \det M[U, i(-\mu + k\delta\nu)](10)
\]

with \( \delta\nu = 2\mu/N \). The idea is to compute each single ratio \( r_k \) by a different Monte Carlo simulation. Apart from the increased overlap among each couple of partition functions, an improvement comes also from the simpler form in which the observable appearing in each ratio \( r_k \) can be rewritten, for large enough \( N \). Indeed we have:

\[
r_k = \langle \det M(i(\nu + k\delta\nu)) / \det M(i\nu) \rangle_{(i\mu, i\nu)}(11)
\]

where \( \nu = -\mu + (k-1)\delta\nu \) and

\[
A[U, \nu, \delta\nu] \equiv M[U, i\nu]^{-1} M[U, i(\nu + \delta\nu)].
\]

If \( \delta\nu \) is small, the matrix \( A[U, \nu, \delta\nu] \) is very close to the identity matrix \( \text{Id} \) for each configuration \( U \). We can therefore expand the logarithm in Eq. (13) thus rewriting the following approximate expression for \( r_k \):

\[
r_k \simeq \left\langle \exp \left( \text{Tr}(A - \text{Id}) - \frac{1}{2} \text{Tr}(A - \text{Id})^2 + \ldots \right) \right\rangle(13)
\]

Each trace in the exponential can be evaluated by a noisy estimator as follows:

\[
\text{Tr}(A[U] - \text{Id})^n \simeq \frac{1}{K} \sum_{j=1}^{K} \eta_{(j)}^{(1)} \eta_{(j)}^{(2)} \ldots \eta_{(j)}^{(n)}(14)
\]

where \( \eta_{(j)}^{(1)} \) is a random vector satisfying \( \langle \eta_{(j)}^{(1)} \eta_{(j)}^{(2)} \rangle_\eta = \delta_{i_1 i_2} \). The computation of each noise estimate in Eq. (14) can be made faster if, when applying the matrix \( A[U] = M[U, i\nu]^{-1} M[U, i(\nu + \delta\nu)] \) to the vector \( \eta_{(j)}^{(1)} \) (or to \( A[U] - \text{Id} \) at higher orders), \( \eta_{(j)}^{(2)} \) itself is taken as a starting tentative solution for the inverter giving \( M[U, i\nu]^{-1} \langle M[U, i(\nu + \delta\nu)]\eta_{(j)}^{(1)} \rangle: \) the guess is better and better as \( \delta\nu \to 0 \).

The second method is not conceptually different from the first one: finite free energy differences are computed...
in this case instead of derivatives. However the numerical procedure is different and it is not clear a priori which approach is more convenient. In the second case no numerical integration must be performed, however one has the drawback that the exponential of a noisy unbiased estimator is biased, hence a large number $K$ of vectors must be used and the final result must be checked to be independent of $K$. Moreover the systematic error involved in the truncation of the logarithm expansion, Eq. (13), must be properly estimated and kept under control.

III. NUMERICAL RESULTS

We have tested our methods for the theory with 8 staggered flavors of mass $am = 0.1$. We will present results obtained on $L_s^3 \times L_t$ lattices with $L_t = 4$ and $L_s = 4, 8, 16$. At zero chemical potential this theory presents a strong first order deconfinement/chiral transition, the critical coupling being $\beta_c \sim 4.7$ for $L_t = 4$. We have performed simulations both in the deconfined region ($\beta = 4.8$) and in the low temperature confined region ($\beta = 4.6$). On the smallest lattice ($L_s = 4$) we will compare our results directly with those obtained at real isospin chemical potential by a direct evaluation of the determinant phase. Numerical simulations have been performed mostly on the APEmille facility in Pisa. The INFN apeNEXT facility in Rome has been used for the results on the largest lattice. The standard exact HMC algorithm [28] has been used with trajectories of length 1.

A collection of the results obtained for imaginary chemical potentials is reported in Table I.

FIG. 1: $\rho(\nu)$ for various values of $\mu$ at $\beta = 4.8$ and $L_s = 4$.

FIG. 2: $\rho(\nu)$ for various values of $\mu$ at $\beta = 4.6$ and $L_s = 4$.

FIG. 3: $\rho(\nu)$ for various values of $\mu$ at $\beta = 4.8$ and $L_s = 16$.

FIG. 4: $r_k^+$ (blank triangles) and the inverse of $r_k^-$ (blank circles) defined in Eq. (15), together with their geometric mean, i.e. $\sqrt{r_k}$ (filled circles). Data are showed for $L_s = 4$, $\mu = 0.05$, $\nu = -0.045$ and $\delta \nu = 0.005$.
A. Systematic errors and comparison of the methods

In Figs. 1 [2] and 3 we report various determinations of \( \rho(\nu) \) (minus the imaginary part of the baryon number, Eq. (7)) obtained on discrete sets of points.

It is apparent that \( \rho(\nu) \) is a very smooth function of \( \nu \) in all explored cases and independently of the lattice size and of the explored phase (confined or deconfined)\(^1\). In most cases it can even be approximated by a linear function; therefore numerical integration turns out to be an easy task. We have adopted a simple linear interpolation between consecutive points to obtain the results given in Table I; the reported errors derive from standard error propagation of the statistical errors of the single data points. We have verified, by changing the order of the interpolating polynomial, that the systematic error related to the interpolation-integration procedure is negligible with respect to the statistical one.

Concerning the second method described in Section II, we have adopted a standard trick \(^2\) in order to reduce systematic effects. Each partial ratio \( r_k \) in Eq. (9) has been rewritten as

\[
 r_k = \frac{\left\langle \text{det} M(i(\nu + \delta \nu)) \right\rangle_{i\mu,i\nu}}{\left\langle \text{det} M(i\nu) \right\rangle_{i\mu,i\nu}} = \frac{r_k^+}{r_k^-} = \frac{\left\langle \text{det} M(i(\nu + \delta \nu))/\text{det} M(i(\nu + \frac{\pi}{2})) \right\rangle_{i\mu,i\nu,i\nu + \frac{\pi}{2}}}{\left\langle \text{det} M(i(\nu))/\text{det} M(i(\nu + \frac{\pi}{2})) \right\rangle_{i\mu,i\nu,i\nu + \frac{\pi}{2}}}. \tag{15}
\]

\( r_k \) can again be evaluated in a single simulation and a jackknife analysis has to be applied to obtain a correct error estimate. Two major benefits derive in this case. First, the reduced value \( \delta \nu/2 \) greatly improves the convergence of the logarithm expansion in Eq. (13). Second, the bias introduced by the finite number of noisy estimators, see Eqs. (13) and (14), gets largely cancelled in the ratio. That is apparent from Fig. 4, where we plot \( r_k^+ \) and the inverse of \( r_k^+ \) defined in Eq. (13), and their geometric mean (i.e. \( \sqrt{r_k} \)), as a function of the number \( K \) of noise vectors, in one particular sample case. It is clear that, while the single factors have a relatively slow convergence, their product is stable from \( K = 5 \) on. We have however always used \( K = 30 \) in our determinations.

Regarding the logarithm expansion, Eq. (13), we have always adopted a third order approximation: in all cases the discrepancy with the result obtained at the second order is at least one order of magnitude smaller than the statistical uncertainty. The fact that the systematic error related to this expansion is well under control can be also appreciated from Table I second and third row, showing that the determination of \( \langle e^{2\theta} \rangle_{i\mu} \) is stable against the variation of the number of intermediate ratios.

Let us now come to the comparison between the two methods. While they always give perfectly compatible results, thus confirming the absence of appreciable systematics, it is clear from Table I that, with a comparable numerical effort (in the last column we give the total number of Monte-Carlo trajectories used for each determination), the method described by Eq. (8) (integration of the derivative) furnishes more accurate determinations. We have therefore chosen this method in order to perform more extensive studies of \( \langle e^{2\theta} \rangle_{i\mu} \).

B. Test of analytic continuation

The average phase factor computed at finite isospin chemical potential, at variance with that computed in the quenched theory, is expected \(^2\) to be an analytic function of \( \mu^2 \) around \( \mu^2 = \mu^2 \). We can test directly analytic continuation by comparing our results with direct determinations of \( \langle e^{2\theta} \rangle \) performed at real chemical potentials: this is done only for the smallest lattice \( (L_s = 4) \), where the second determination is easily affordable.

\begin{table}[h]
\begin{tabular}{|c|c|c|c|}
\hline
\( L_s \) & \( \beta \) & \text{Im(}\mu\text{)} & \text{method} & \text{HMC trajs} \\
\hline
4 & 4.8 & 0.025 & DER(10) & 100522(42) & 700k \\
4 & 4.8 & 0.025 & RAT(5) & 100300(18) & 150k \\
4 & 4.8 & 0.025 & DER(10) & 10028(11) & 300k \\
4 & 4.8 & 0.025 & direct & 10033(11) & 40k \\
4 & 4.8 & 0.05 & DER(20) & 10108(11) & 800k \\
4 & 4.8 & 0.05 & RAT(10) & 10122(16) & 500k \\
4 & 4.8 & 0.075 & DER(15) & 10266(17) & 350k \\
4 & 4.8 & 0.10 & DER(20) & 10454(16) & 700k \\
4 & 4.8 & 0.20 & DER(16) & 1283(8) & 700k \\
4 & 4.8 & 0.025 & DER(10) & 10184(19) & 150k \\
4 & 4.8 & 0.025 & DER(10) & 101900(50) & 60k \\
16 & 4.8 & 0.025 & DER(10) & 10732(85) & 40k \\
16 & 4.8 & 0.025 & DER(15) & 1053(33) & 40k \\
16 & 4.8 & 0.05 & DER(10) & 1368(30) & 40k \\
4 & 4.6 & 0.025 & DER(5) & 10061(10) & 200k \\
4 & 4.6 & 0.05 & DER(10) & 102704(15) & 350k \\
\hline
\end{tabular}
\caption{Collection of determinations of the average phase factor continued to imaginary values of \( \mu \) for various parameter sets and computation methods. In the fourth column the method used to obtain the determination is described: DER(N) stands for the integration of the first derivative \( \rho \) determined on a discrete set of (N+1) points, Eq. (8); RAT(N) stands for the evaluation of N intermediate ratios \( r_k \), Eq. (9). Finally on the smallest lattices also a direct determination of the expectation value in Eq. (4) is reported for comparison.}
\end{table}

\(^1\) Clearly one expects a non-smooth behaviour if \( Z(\mu, \nu) \) and \( Z_0 \equiv Z(\mu, -\nu) \) belong to two different phases, so that some transition is met when \( \nu \) goes from \( -\nu \) to \( \nu \), however in these cases analytic continuation itself is not applicable.

\(^2\) It is even in \( \mu \) for symmetry reasons.
We plot in Fig. [5] results obtained at $\beta = 4.6$ and $\beta = 4.8$. The whole set of results obtained at real chemical potentials ($\mu^2 > 0$) and imaginary chemical potentials ($\mu^2 < 0$) can be described by a simple quadratic behaviour

$$\langle e^{\i\theta} \rangle = 1 + A\mu^2$$

in a range $|\mu^2| \leq 0.01$, with $A = -4.41(9)$ and $\chi^2$/d.o.f. $\simeq 1.5$ for $\beta = 4.8$ and $A = -10.2(3)$ and $\chi^2$/d.o.f. $\simeq 1.8$ for $\beta = 4.6$. If the range of values is extended a quartic term is necessary

$$\langle e^{\i\theta} \rangle = 1 + A\mu^2 + B\mu^4$$

as shown in the figure. We obtain, at $\beta = 4.8$, $A = -4.48(8)$, $B = 15.7 \pm 2.5$ and $\chi^2$/d.o.f. $\simeq 1.3$.

Analyticity around $\mu^2 = 0$ is therefore well verified. We stress that at $\beta = 4.8$ our largest value of the imaginary chemical potential is still below the first Roberge-Weiss phase transition at $\text{Im}(\mu) = \pi/(3L_\gamma)$, hence within the expected range of validity of analytic continuation for $\mu^2 < 0$ at high temperatures.

We have performed numerical simulations at different values of $L_s$ in order to test both the behaviour of $\langle e^{\i\theta} \rangle$ and the efficiency of our method as the lattice volume is increased.

In Fig. [6] we report determinations performed at fixed values of $i\mu$ and variable $L_s$ at $\beta = 4.8$. A behaviour

$$\langle e^{\i\theta} \rangle = 1 + CL_s^2$$

well describes the data with $\gamma \sim 2.5$ for both values of $i\mu$.

Concerning the numerical efficiency, we notice that to obtain comparable uncertainties (of the order of 10 %) for $\langle e^{\i\theta} \rangle - 1$, on the largest lattice ($16^3 \times 4$) we needed a CPU time which is less than one order of magnitude bigger than what needed on the smallest lattice ($4^3$). Considering that the two lattice volumes differ by a factor 64, we deduce that, at least for the quark mass considered in the present study, our method requires a numerical effort which scales in an affordable way with the lattice size.

### IV. CONCLUSIONS

We have presented two different techniques, described respectively by Eq. [5] and Eq. [6], for an efficient numerical determination of the average phase factor of the fermionic determinant continued to imaginary values of the chemical potential. We have applied both methods to QCD with 8 dynamical staggered flavors, verifying the absence of uncontrolled systematic effects and performing a comparison of the efficiencies, with the conclusion that the method based on the integration of the imaginary part of the baryon density, Eq. [5], is numerically more convenient. A fair good scaling of the efficiency is observed as the lattice volume is increased. We have also directly tested, on small lattices, the analyticity of the average phase factor around $\mu^2 = 0$. The method proposed and tested in the present paper will be used in the future to perform more extensive studies, with more physical quark masses and number of flavors, of the average phase factor continued to imaginary chemical potentials.
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