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Imaginary chemical potentials and the phase of the fermionic determinant

Simone Conradi and Massimo D'Elia

Dipartimento di Fisica dell'Università di Genova and INFN, Sezione di Genova, Via Dodecaneso 33, I-16146 Genova, Italy

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

$$Z(\mu, \mu) \equiv \int \mathcal{D}U e^{-S_G[U]}(\det M[U, \mu])^2 = \int \mathcal{D}U e^{-S_G[U]}|\det M[U, \mu]|^2 e^{i2\theta}, \qquad (1)$$

describing two flavors of quarks (or eight flavors in the case of staggered fermions) which are given an equal chemical potential μ: 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 [1–3], the use of an imaginary chemical potential either for analytic continuation [4–10] or for reconstructing the canonical partition function [11–13], Taylor expansion techniques [14,15], and nonrelativistic expansions [16–18].

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

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

has a positive measure. That is also known as phase quenched QCD. The average value of the phase factor of the fermionic determinant, $\langle e^{i2\theta}\rangle_{(\mu,-\mu)}$, where the index indicates the partition function the expectation value refers to, gives a direct measurement of the severeness of the sign problem. $\langle e^{i2\theta}\rangle \sim 0$ signals the stage at which the complex nature of the determinant implies a significant difference between finite baryonic density and finite isospin density, as well as 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 and it can also be expressed as the ratio of two partition functions:

$$\langle e^{i2\theta}\rangle_\mu \equiv \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle_{(\mu,-\mu)} = \frac{Z(\mu, \mu)}{Z(\mu, -\mu)}. \qquad (3)$$

Its direct numerical computation becomes difficult 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

$$\langle e^{i2\theta}\rangle_{i\mu} \equiv \left\langle \frac{\det M(i\mu)}{\det M(-i\mu)} \right\rangle_{(i\mu,-i\mu)} = \frac{Z(i\mu, i\mu)}{Z(i\mu, -i\mu)} = \frac{\int \mathcal{D}U e^{-S_G[U]} \det M[U, i\mu] \det M[U, i\mu]}{\int \mathcal{D}U e^{-S_G[U]} \det M[U, i\mu] \det M[U, -i\mu]}, \qquad (4)$$

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 μ_1 and μ_2.

In Sec. II we illustrate two different possible methods, which are then numerically tested and compared in Sec. III 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, both related to the investigation of 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 both cases, consisting in either determining derivatives of the disorder parameters, from which the ratio of partition functions can then be reconstructed after integration [22–24], or in making use of various reweighting techniques, like that of rewriting the original ratio in terms of intermediate ratios which are more easily evaluable [25–27].

In the present case the major difficulty derives from a direct computation of the observables, which is expressed in terms of fermionic determinants, but sampling problems may, in principle, worsen the situation also in this case, especially in the large volume limit. In the following we will describe the application of both kinds of techniques described above to the present case, and try to understand by numerical simulations which of them is best suited for this context.

We describe at first how to reconstruct $\langle e^{i2\theta}\rangle$ in terms of derivatives. Consider the modified ratio

$$R_\mu(\nu) = \frac{Z(i\mu, i\nu)}{Z(i\mu, -i\mu)}, \tag{5}$$

where

$$Z(i\mu, i\nu) \equiv \int \mathcal{D}U e^{-S_G[U]} \det M[U, i\mu] \det M[U, i\nu]. \tag{6}$$

It is clear that $R_\mu(-\mu) = 1$, while $R_\mu(\mu)$ is the original ratio. It can be easily verified that

$$\begin{aligned}\rho(\nu) &\equiv \frac{d}{d\nu} \ln R_\mu(\nu) = \frac{d}{d\nu} \ln Z(i\mu, i\nu) \\ &= \left\langle i \,\mathrm{Tr}\left(M^{-1}(i\nu)\frac{d}{d(i\nu)}M(i\nu)\right)\right\rangle_{(i\mu,i\nu)}.\end{aligned} \tag{7}$$

The last quantity is nothing but i times the average number of quarks coupled to the chemical potential $i\nu$: the latter is purely imaginary for symmetry reasons, hence $\rho(\nu)$ is real, and can be computed using a noisy unbiased estimator. The average phase factor can then be obtained by integration

$$\langle e^{i2\theta}\rangle_{i\mu} = \exp\left(\int_{-\mu}^{\mu} \rho(\nu) d\nu\right) \tag{8}$$

and no quark determinant must be explicitly computed.

In practice, the derivative $\rho(\nu)$ will be computed for a discrete set of values of ν and then integrated numerically. The precision attained for $\langle e^{i2\theta}\rangle_{i\mu}$ will depend both on the statistical errors of the single determinations and on the systematic uncertainty linked to numerical integration; the last can be estimated, for instance, by varying the chosen interpolation procedure. In principle it is also possible to determine further derivatives of ρ in order to improve the integration accuracy.

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

$$\langle e^{i2\theta}\rangle_{i\mu} = \frac{Z(i\mu, i\mu)}{Z(i\mu, -i\mu)} = \frac{Z_N}{Z_{N-1}}\frac{Z_{N-1}}{Z_{N-2}}\ldots\frac{Z_1}{Z_0} \equiv \prod_{k=1}^{N} r_k, \tag{9}$$

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

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

with $\delta\nu = 2\mu/N$. The idea is to compute each single ratio r_k by a different Monte Carlo simulation. This is not conceptually different from the first approach: finite differences of a free energy are computed in this case instead of its derivative. However the numerical procedure is different and it is not clear *a priori* which approach is more convenient.

In the second case the improvement comes from the increased overlap between each couple of partition functions and from the simple form in which the observable appearing in each ratio r_k can be rewritten, for large enough N. Indeed we have

$$\begin{aligned} r_k &= \langle \det M(i(\nu + \delta\nu)) / \det M(i\nu)\rangle_{(i\mu,i\nu)} \\ &= \langle \exp(\mathrm{Tr} \ln A(\nu, \delta\nu))\rangle_{(i\mu,i\nu)},\end{aligned} \tag{11}$$

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

$$A[U, \nu, \delta\nu] \equiv M[U, i\nu]^{-1} M[U, i(\nu + \delta\nu)]. \tag{12}$$

If $\delta\nu$ is small, the matrix $A[U, \nu, \delta\nu]$ is very close to the identity matrix Id for each gauge configuration U, hence r_k can be easily computed by a variety of methods. One possibility could be, for instance, the use of unbiased estimators of $\det A$ [28,29], which would involve the computation of the square root of A.

Our choice is instead that of expanding the logarithm in Eq. (11), thus rewriting the following approximate expression for r_k:

$$r_k \simeq \langle \exp(\mathrm{Tr}(A - \mathrm{Id}) - \tfrac{1}{2}\mathrm{Tr}(A - \mathrm{Id})^2 + \ldots)\rangle. \tag{13}$$

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

$$\mathrm{Tr}\,(A[U] - \mathrm{Id})^n \simeq \frac{1}{K}\sum_{j=1}^{K} \eta^{(j)\dagger}(A[U] - \mathrm{Id})^n \eta^{(j)}, \tag{14}$$

where $\eta^{(j)}$ is a random vector satisfying $\langle \eta_{i_1}^{(j)\dagger} \eta_{i_2}^{(j)} \rangle_\eta = \delta_{i_1, i_2}$. 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 $\eta^{(j)}$ (or to $(A[U] - \mathrm{Id})^{n-1} \eta^{(j)}$ at higher orders), $\eta^{(j)}$ itself is taken as a starting tentative solution for the inverter giving $M[U, i\nu]^{-1}(M[U, i(\nu + \delta\nu)]\eta^{(j)})$: the guess is better and better as $\delta\nu \to 0$. In this case the estimator is biased, hence the final result must be checked to be independent of the number K of random vectors used. Moreover the systematic error involved in the truncation of the logarithm expansion, Eq. (13), must be properly estimated and kept under control. As we will show in the following, in all the examined cases (parameter sets and values of $\delta\nu$) the bias can be made negligible with very few random vectors, while corrections beyond the second order in the logarithm expansion are irrelevant.

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 phase of the determinant. Numerical simulations have been performed mostly on the APEmille facility in Pisa. The INFN apeNEXT facility in Rome has been used for the largest lattice. The standard exact HMC algorithm [30] has been used with trajectories of length 1.

TABLE I. Collection of determinations of the average phase factor continued to imaginary values of μ 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 ρ 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 for the smallest lattice also a direct determination of the expectation value in Eq. (4) is reported for comparison.

L_s	β	Im(μ)	Method	$\langle e^{i2\theta} \rangle_{i\mu}$	HMC trajs
4	4.8	0.025	DER(10)	1.003 22(42)	700 k
4	4.8	0.025	RAT(5)	1.0030(18)	150 k
4	4.8	0.025	RAT(10)	1.0028(11)	300 k
4	4.8	0.025	direct	1.0033(11)	40 k
4	4.8	0.05	DER(20)	1.0108(11)	800 k
4	4.8	0.05	RAT(10)	1.0122(16)	500 k
4	4.8	0.075	DER(15)	1.0266(17)	350 k
4	4.8	0.10	DER(20)	1.0454(16)	700 k
4	4.8	0.20	DER(16)	1.283(8)	700 k
8	4.8	0.025	DER(10)	1.0164(19)	150 k
8	4.8	0.025	RAT(5)	1.0200(50)	50 k
16	4.8	0.025	DER(10)	1.0732(85)	60 k
16	4.8	0.025	RAT(5)	1.053(33)	40 k
16	4.8	0.05	DER(10)	1.368(30)	40 k
4	4.6	0.025	DER(5)	1.0061(10)	200 k
4	4.6	0.05	DER(10)	1.0270(15)	350 k

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

A. Systematic errors and comparison of the methods

In Figs. 1–3 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 ν in all cases, independently of the lattice size and of the explored phase (confined or deconfined) [31]. 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 Sec. II, we have adopted a standard trick [25] in order to reduce systematic effects. Each partial ratio r_k in Eq. (9) has been rewritten as

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

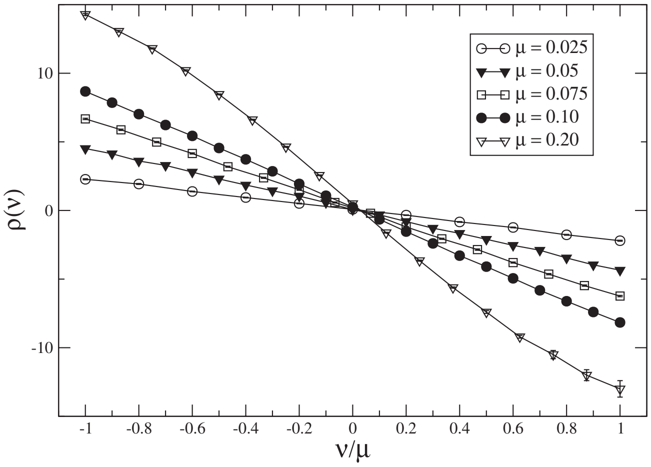

FIG. 1. $\rho(\nu)$ for various values of μ at $\beta = 4.8$ and $L_s = 4$.

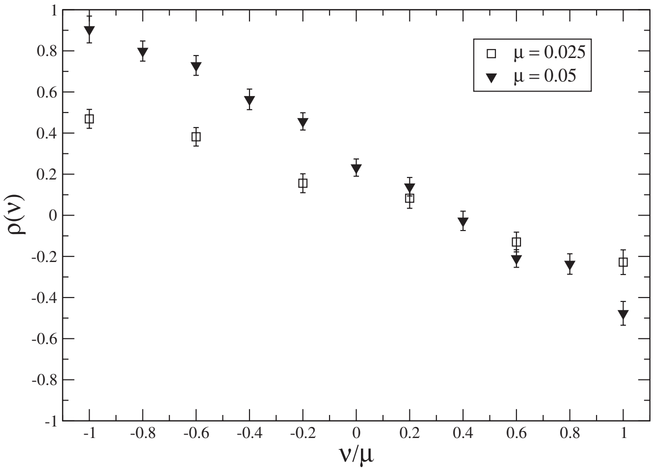

FIG. 2. $\rho(\nu)$ for various values of μ at $\beta = 4.6$ and $L_s = 4$.

r_k can again be evaluated by 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. (15), 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, which roughly optimizes the precision obtained on r_k at constant numerical effort.

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 1 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 $\langle e^{i2\theta}\rangle_{i\mu}$ is stable against the variation of the number of intermediate ratios.

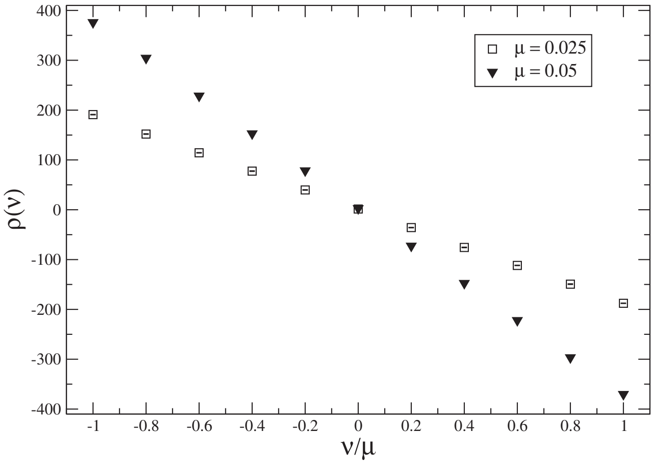

FIG. 3. $\rho(\nu)$ for various values of μ at $\beta = 4.8$ and $L_s = 16$.

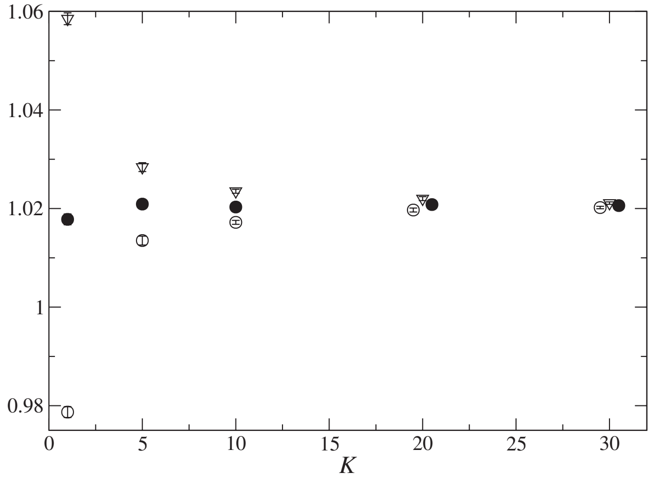

FIG. 4. r_k^+ (blank triangles) and the inverse of r_k^- (blank circles) defined in Eq. (15), together with their geometric mean, i.e. $\sqrt{r_k}$ (filled circles). Data are showed for $L_s = 4$, $\mu = 0.05$, $\nu = -0.045$, and $\delta\nu = 0.005$.

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; this is especially true on the largest lattice. We have therefore chosen this method in order to perform more extensive studies of $\langle e^{i2\theta}\rangle_{i\mu}$.

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 [20,21] to be an analytic function of μ^2 around $\mu^2 = 0$ [32]. We can test analytic continuation by comparing our results with direct determinations of $\langle e^{i2\theta}\rangle$ performed at real chemical potentials: this is done only for the smallest lattice ($L_s = 4$), where the second determination is easily affordable.

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 behavior

$$\langle e^{i2\theta}\rangle = 1 + A\mu^2 \tag{16}$$

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

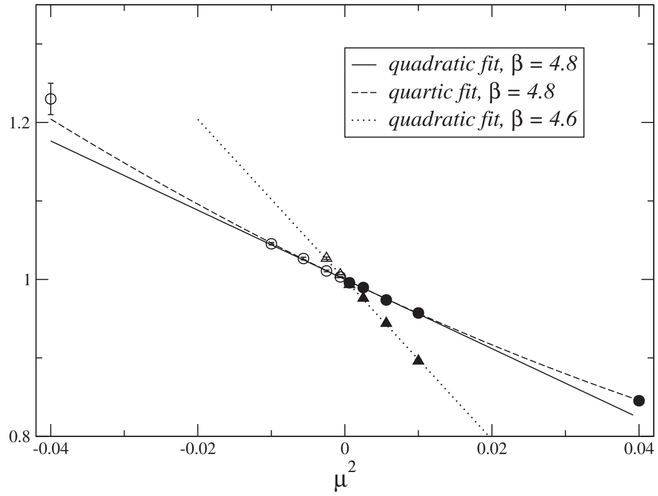

FIG. 5. $\langle e^{i2\theta}\rangle$ computed for different values of μ^2 at $\beta = 4.8$ and $\beta = 4.6$ on a 4^4 lattice. Best-fit quadratic and quartic functions in μ^2 are displayed, showing the validity of analytic continuation around $\mu^2 = 0$.

tended a quartic term is necessary

$$\langle e^{i2\theta}\rangle = 1 + A\mu^2 + B\mu^4 \tag{17}$$

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

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 taking place at $\text{Im}(\mu) = \pi/(3L_t)$, hence within the expected range of validity of analytic continuation for $\mu^2 < 0$ at high temperatures.

C. Large volume scaling

We have performed numerical simulations at different values of L_s in order to test both the behavior of $\langle e^{i2\theta}\rangle$ 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 behavior

$$\langle e^{i2\theta}\rangle = 1 + CL_s^{\gamma} \tag{18}$$

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

Concerning the numerical efficiency, we notice that to obtain a comparable precision (of the order of 10%) for $(\langle e^{i2\theta}\rangle - 1)$, on the largest lattice ($16^3 \times 4$) we needed a CPU time which is less than 1 order of magnitude bigger than what we needed on the smallest lattice (4^4). 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.

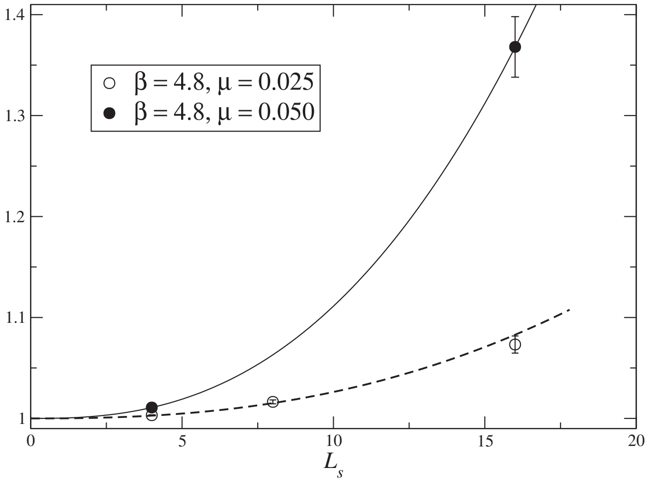

FIG. 6. $\langle e^{i2\theta}\rangle_{i\mu}$ as a function of the spatial lattice size L_s for two values of $i\mu$. A best-fit according to Eq. (18) is reported in both cases.

IV. CONCLUSIONS

We have presented two different techniques, described, respectively, by Eqs. (8) and (9), 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. (8), 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 can be used to perform more extensive studies of the average phase factor continued to imaginary chemical potentials, with more physical quark masses and number of flavors.

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[31] Clearly one expects a nonsmooth behavior if $Z(i\mu, i\mu)$ and $Z(i\mu, -i\mu)$ belong to two different phases, so that some transition is met when ν goes from $-\mu$ to μ, however in these cases analytic continuation itself is not applicable.

[32] It is even in μ for symmetry reasons.