PROCEEDINGS OF SCIENCE

Analytic continuation of the phase of the fermionic determinant

Simone Conradi*
Dipartimento di Fisica dell'Università di Genova and INFN, Sezione di Genova, Via Dodecaneso 33, I-16146 Genova, Italy
E-mail: conradi@ge.infn.it

Massimo D'Elia
Dipartimento di Fisica dell'Università di Genova and INFN, Sezione di Genova, Via Dodecaneso 33, I-16146 Genova, Italy
E-mail: delia@ge.infn.it

The numerical simulation of QCD at finite baryonic density is made difficult by the complex nature of the fermionic determinant. We study the severeness of the problem as a function of the chemical potential by determining the average phase factor of the determinant at imaginary chemical potentials.

The XXV International Symposium on Lattice Field Theory
July 30-4 August 2007
Regensburg, Germany

*Speaker.

PoS(LATTICE 2007)176

1. The sign problem and the phase of the fermionic determinant

The QCD partition function with two flavours of quarks (or eight flavours of staggered quarks), which are given the same chemical potential μ, is:

$$\begin{aligned} Z(\mu,\mu) &\equiv \int \mathscr{D}U e^{-S_G[U]} (\det M[U,\mu])^2 \\ &= \int \mathscr{D}U e^{-S_G[U]} |\det M[U,\mu]|^2 e^{i2\theta} \,, \end{aligned} \tag{1.1}$$

where θ is the phase of the complex determinant. When $\mu \neq 0$ then $\theta \neq 0$ and Monte Carlo simulations are not feasible: this is the notorious sign problem.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].

If the two flavours have opposite chemical potentials, the problem is solved because $\det M[U,-\mu] = \det M[U,\mu]^*$, and:

$$Z(\mu,-\mu) = \int \mathscr{D}U e^{-S_G[U]} |\det M[U,\mu]|^2 \,. \tag{1.2}$$

An indicator of the severness of the sign problem ([20, 21]) is $\langle e^{i2\theta} \rangle$. When $\langle e^{i2\theta} \rangle \sim 0$ the problem is relevant and there is a significant difference between finite isospin density simulations and finite baryon density ones. It's easy to see that:

$$\langle e^{i2\theta} \rangle_\mu \equiv \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle_{(\mu,-\mu)} = \frac{Z(\mu,\mu)}{Z(\mu,-\mu)} \,. \tag{1.3}$$

Recently it has been proposed [20, 21] to study the analytic continuation of the average phase factor to imaginary chemical potentials:

$$\begin{aligned} \langle e^{i2\theta} \rangle_{i\mu} &\equiv \left\langle \frac{\det M(i\mu)}{\det M(-i\mu)} \right\rangle_{(i\mu,-i\mu)} = \frac{Z(i\mu,i\mu)}{Z(i\mu,-i\mu)} \\ &= \frac{\int \mathscr{D}U e^{-S_G[U]} \det M[U,i\mu] \det M[U,i\mu]}{\int \mathscr{D}U e^{-S_G[U]} \det M[U,i\mu] \det M[U,-i\mu]} \end{aligned} \tag{1.4}$$

Notice that in Eq. (1.4) both partition functions are suitable for numerical simulations because $\det M[U,\pm i\mu]$ is real. In the present work we propose and test new strategies for an efficient numerical determination of $\langle e^{i2\theta} \rangle$ which fully exploit the fact of working at imaginary values of μ.

2. The method

In evaluating $\langle e^{i2\theta} \rangle_{i\mu}$, there are some numerical difficulties. First, fermionic determinants are very expensive to calculate; second, the statistical distributions generated by $Z(i\mu,i\mu)$ and $Z(i\mu,-i\mu)$ could have poor overlap. Similar problems happen in the evaluation of disorder parameters in lattice gauge theories; in this case, powerful techniques have been developed [22, 23, 24, 25, 26, 27]. We have introduced two methods to overcome these problems [28].

2.1 Derivatives method

It is useful to define:

$$R_\mu(\nu) = \frac{Z(i\mu, i\nu)}{Z(i\mu, -i\mu)} \tag{2.1}$$

where $R_\mu(\mu)$ is the ratio we want to evaluate and $R_\mu(-\mu) = 1$. The partition function $Z(i\mu, i\nu)$ in Eq. (2.1) is suitable for numerical Monte Carlo simulations for generic values of $i\mu, i\nu$. It is obvious that:

$$\begin{aligned} \rho(\nu) &\equiv \frac{d}{d\nu} \ln R_\mu(\nu) = \frac{d}{d\nu} \ln Z(i\mu, i\nu) \\ &= \left\langle i \,\mathrm{Tr}\left(M^{-1}(i\nu) \frac{d}{d(i\nu)} M(i\nu) \right) \right\rangle_{(i\mu, i\nu)} . \end{aligned} \tag{2.2}$$

The trace in equation (2.2) is the number (imaginary) of quark coupled to the chemical potential $i\nu$: it can be computed easily by an unbiased noisy estimator. The average phase factor is then

$$\langle e^{i2\theta} \rangle_{i\mu} = \exp\left(\int_{-\mu}^{\mu} \rho(\nu) d\nu \right) \tag{2.3}$$

i.e. it can be obtained without any determinant calculation. In practice we compute the derivative $\rho(\nu)$ for a discrete set of ν and then we integrate them numerically. In principle it is also possible to determine further derivatives of ρ in order to improve the computation accuracy.

2.2 Factorization method

We rewrite the average phase factor as a product of intermediate ratios:

$$\langle e^{i2\theta} \rangle_{i\mu} = \frac{Z(i\mu, i\mu)}{Z(i\mu, -i\mu)} = \frac{Z_N}{Z_{N-1}} \frac{Z_{N-1}}{Z_{N-2}} \cdots \frac{Z_1}{Z_0} \equiv \prod_{k=1}^{N} r_k \tag{2.4}$$

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

$$Z_k \equiv \int \mathscr{D}U e^{-S_G[U]} \det M[U, i\mu] \det M[U, i(-\mu + k\delta\nu)] \tag{2.5}$$

with $\delta\nu = 2\mu/N$. We compute each single ratio r_k which is not affected by overlap problems. We note that:

$$\begin{aligned} r_k &= \langle \det M(i(\nu + \delta\nu)) / \det M(i\nu) \rangle_{(i\mu, i\nu)} \\ &= \langle \exp(\mathrm{Tr} \ln A(\nu, \delta\nu)) \rangle_{(i\mu, i\nu)} \end{aligned} \tag{2.6}$$

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

$$A[U, \nu, \delta\nu] \equiv M[U, i\nu]^{-1} M[U, i(\nu + \delta\nu)] . \tag{2.7}$$

The calculation of each r_k is easy: for large N (and small $\delta\nu$), $A[U, \nu, \delta\nu]$ is very close to the identity matrix Id, for each configuration U. So we can expand the logarithm obtaining:

$$r_k \simeq \left\langle \exp\left(\mathrm{Tr}(A - \mathrm{Id}) - \frac{1}{2} \mathrm{Tr}(A - \mathrm{Id})^2 + \ldots \right) \right\rangle \tag{2.8}$$

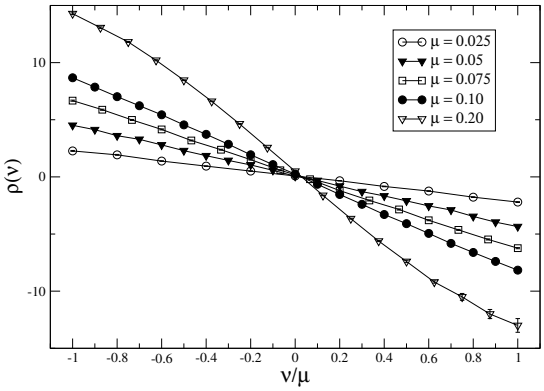

Figure 1: $\rho(\nu)$ for various values of μ at $\beta = 4.8$ and $L_s = 4$.

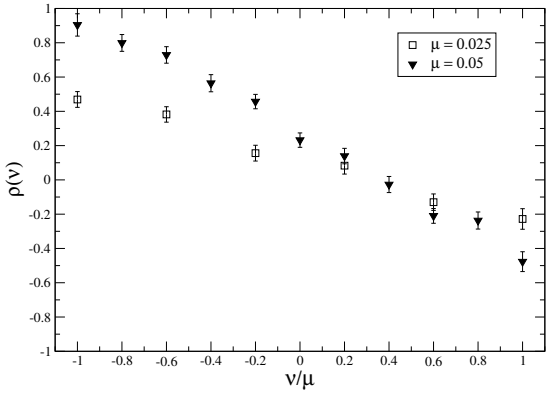

Figure 2: $\rho(\nu)$ for various values of μ at $\beta = 4.6$ and $L_s = 4$.

Each trace is evaluated by a noisy estimator as follows:

$$\mathrm{Tr}(A[U]-\mathrm{Id})^n \simeq \frac{1}{K}\sum_{j=1}^{K} \eta^{(j)\dagger}(A[U]-\mathrm{Id})^n \eta^{(j)} \tag{2.9}$$

where $\eta^{(j)}$ is a random vector satisfying $\langle \eta_{i_1}^{(j)\dagger} \eta_{i_2}^{(j)} \rangle_\eta = \delta_{i_1,i_2}$ and K is sufficently large; in our simulations we always use $K = 30$ and we adopt a third order expansion for the logarithm.

3. Numerical Results

We have tested our methods for the theory with 8 staggered flavors of mass $am = 0.1$ and we will present results obtained on $L_s^3 \times L_t$ lattices with $L_t = 4$ and $L_s = 4, 8, 16$. At $\mu = 0$ the theory presents a strong first order deconfinement/chiral transition for $\beta_c \cong 4.7$ and $L_t = 4$. On the smallest lattice ($L_s = 4$) we will compare our results directly with those obtained at real isospin chemical potential, by a direct evualuation of the determinant phase based on LU factorization. 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. We have adopted the standard exact HMC algorithm with trajectories of length 1. A full account of our results is reported in Ref. [28].

In table (1) we put the average phase factor continued to imaginary values of μ for various parameter sets and computation methods. In the fourth column we put data obtained with derivatives method DER(N) or with factorization method RAT(N). Finally on the smallest lattices also a direct determination of the expectation value in Eq. (1.4) is reported for comparison (direct). It is clear that, with a comparable numerical effort, the derivative method furnishes more accurate determinations. We have therefore chosen this method for most of our analysis.

In figures (1), (2) and (3) we show $\rho(\nu)$, for various μ β and L_S. It is apparent that $\rho(\nu)$ is always a very smooth function, so that the systematic errors involved in its numerical integration, hence in the determination of $\langle e^{i2\theta} \rangle_{i\mu}$ through equation (2.3), are negligible.

The average phase factor computed at finite isospin chemical potential, at variance with that computed in the quenched theory, is expected to be an analytic function of μ^2 around $\mu^2 = 0$. We

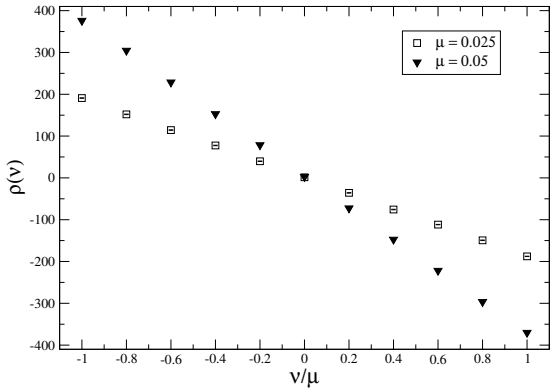

Figure 3: $\rho(\nu)$ for various values of μ at $\beta = 4.8$ and $L_s = 16$.

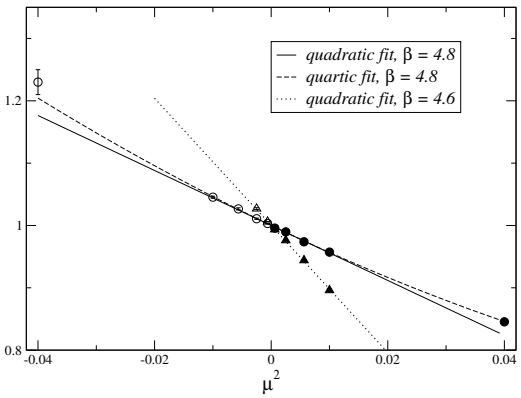

Figure 4: $\langle e^{i2\theta} \rangle$ computed for different values of μ^2 at $\beta = 4.8$ and $\beta = 4.6$ on a 4^4 lattice. Best fit quadratic and quartic functions in μ^2 are displayed, showing good validity of analytic continuation.

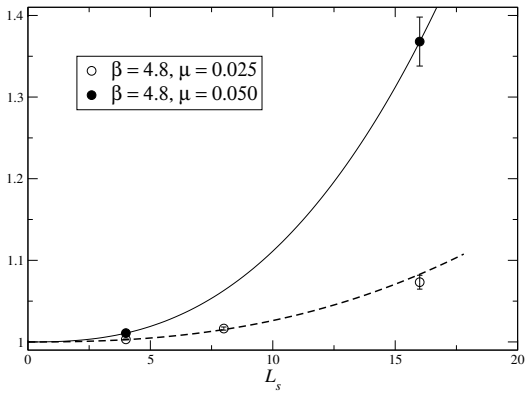

Figure 5: $\langle e^{i2\theta} \rangle_{i\mu}$ as a function of the spatial lattice size L_s for two values of $i\mu$. A best fit according to $1 + CL_s^{\gamma}$ is reported in both cases.We obtain $\gamma \approx 2.5$ for both values of μ. Therefore the numerical effort scales in an affordable way with the lattice size.

have tested analytic continuation by comparing our results with direct determinations of $\langle e^{i2\theta} \rangle_{i\mu}$ performed at real chemical potentials: this has been done only for the smallest lattice ($L_s = 4$), where the second determination is easily affordable. In our biggest range of values we have:

$$\langle e^{i2\theta} \rangle = 1 + A\mu^2 + B\mu^4 \tag{3.1}$$

as shown in the figure (4). 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 have also performed numerical simulations at different values of L_s in order to test both the behaviour of $\langle e^{i2\theta} \rangle$ and the efficiency of our method as the lattice volume is increased. In Fig. (5) we report determinations performed at fixed values of $i\mu$ and variable L_s at $\beta = 4.8$. A behaviour

$$\langle e^{i2\theta} \rangle = 1 + CL_s^{\gamma} \tag{3.2}$$

well describes the data with $\gamma \sim 2.5$ for both values of $i\mu$. From the data in table 1 we also learn that the numerical effort scales in an affordable way with the lattice size L_s: to obtain comparable

uncertainties (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 one order of magnitude bigger than what needed on the smallest lattice (4^4).

4. Conclusions

We have presented two techniques for an efficient numerical determination of the average phase factor of the fermionic determinant continued to imaginary values of the chemical potential and we have applied both methods to QCD with 8 dynamical staggered flavors. In our simulations we have verified the absence of uncontrolled systematic effects and performed a comparison of the efficiencies, with the conclusion that the method based on the integration of the imaginary part of the baryon density, Eq. (2.3), is numerically more convenient.

We have also directly tested, on small lattices, the analiticity of the average phase factor around $\mu^2 = 0$. The method proposed and tested in the present paper will be used to perform more extensive studies, with more physical quark masses and number of flavors, of the average phase factor continued to imaginary chemical potential.

L_s	β	Im(μ)	method	$\langle e^{i2\theta}\rangle_{i\mu}$	HMC trajs
4	4.8	0.025	DER(10)	1.00322(42)	700k
4	4.8	0.025	RAT(5)	1.0030(18)	150k
4	4.8	0.025	RAT(10)	1.0028(11)	300k
4	4.8	0.025	direct	1.0033(11)	40k
4	4.8	0.05	DER(20)	1.0108(11)	800k
4	4.8	0.05	RAT(10)	1.0122(16)	500k
4	4.8	0.075	DER(15)	1.0266(17)	350k
4	4.8	0.10	DER(20)	1.0454(16)	700k
4	4.8	0.20	DER(16)	1.283(8)	700k
8	4.8	0.025	DER(10)	1.0164(19)	150k
8	4.8	0.025	RAT(5)	1.0200(50)	50k
16	4.8	0.025	DER(10)	1.0732(85)	60k
16	4.8	0.025	RAT(5)	1.053(33)	40k
16	4.8	0.05	DER(10)	1.368(30)	40k
4	4.6	0.025	DER(5)	1.0061(10)	200k
4	4.6	0.05	DER(10)	1.0270(15)	350k

Table 1: Determinations of the average phase factor continued to imaginary μ's for various parameters and computation methods. In the fourth column we report the method used to obtain the determination: DER(N) stands for the integration of the first derivative ρ determined on (N+1) points, Eq. (2.3); RAT(N) stands for the evaluation of N intermediate ratios r_k, Eq. (2.4). On the smallest lattices also a direct determination of the expectation value in Eq. (1.4) is reported for comparison.

References

[1] I. M. Barbour, S. E. Morrison, E. G. Klepfish, J. B. Kogut and M. P. Lombardo, Nucl. Phys. Proc. Suppl. **60A** (1998) 220.

[2] Z. Fodor, S. D. Katz, Phys. Lett. B **534** (2002) 87; JHEP **0203** (2002) 14.

[3] Z. Fodor, S. D. Katz and C. Schmidt, JHEP **0703** (2007) 121.

[4] Ph. de Forcrand and O. Philipsen, Nucl. Phys. B **642** (2002) 290; Nucl. Phys. B **673** (2003) 170.

[5] M. D'Elia and M.P. Lombardo, Phys. Rev. D **67** (2003) 014505; Phys. Rev. D **70** (2004) 074509 .

[6] V. Azcoiti, G. Di Carlo, A. Galante and V. Laliena, Nucl. Phys. B **723** (2005) 77.

[7] H. S. Chen and X. Q. Luo, Phys. Rev. D **72** (2005) 034504.

[8] P. Giudice and A. Papa, Phys. Rev. D **69** (2004) 094509

[9] P. Cea, L. Cosmai, M. D'Elia and A. Papa, JHEP **0702** (2007) 066.

[10] M. D'Elia, F. Di Renzo, M.P. Lombardo, arXiv:0705.3814 [hep-lat].

[11] A. Roberge and N. Weiss, Nucl. Phys. B **275** (1986) 734.

[12] S. Kratochvila and P. de Forcrand, PoS **LAT2005** (2006).

[13] A. Alexandru, M. Faber, I. Horvath and K. F. Liu, Phys. Rev. D **72** (2005) 114513.

[14] C. R. Allton et al., Phys. Rev. D **66**, 074507 (2002); Phys. Rev. D **71** (2005) 054508 .

[15] R. V. Gavai and S. Gupta, Phys. Rev. D **68** (2003) 034506; Phys. Rev. D **73** (2006) 014004.

[16] T. C. Blum, J. E. Hetrick and D. Toussaint, Phys. Rev. Lett. **76** (1996) 1019.

[17] J. Engels, O. Kaczmarek, F. Karsch and E. Laermann, Nucl. Phys. B **558** (1999) 307.

[18] R. De Pietri, A. Feo, E. Seiler and I. O. Stamatescu, arXiv:0705.3420 [hep-lat].

[19] K. Splittorff, PoS **LAT2006** (2006) 023 [arXiv:hep-lat/0610072].

[20] K. Splittorff and J. J. M. Verbaarschot, Phys. Rev. D **75** (2007) 116003.

[21] K. Splittorff and B. Svetitsky, Phys. Rev. D **75** (2007) 114504.

[22] L. Del Debbio, A. Di Giacomo and G. Paffuti, Phys. Lett. B **349** (1995) 513.

[23] P. Cea, L. Cosmai and A. D. Polosa, Phys. Lett. B **392** (1997) 177

[24] L. Del Debbio, A. Di Giacomo, B. Lucini, Nucl. Phys. **B594** (2001) 287; Phys. Lett. **B500** (2001) 326.

[25] Ph. de Forcrand, M. D'Elia, M. Pepe, Phys. Rev. Lett. **86** (2001) 1438.

[26] Ph. de Forcrand and M. Vettorazzo, Nucl. Phys. **B686** (2004) 85.

[27] M. D'Elia and L. Tagliacozzo, Phys. Rev. D **74** (2006) 114510.

[28] S. Conradi and M. D'Elia, arXiv:0707.1987 [hep-lat].

[29] S.A. Gottlieb, W. Liu, D. Toussaint, R.L. Renken and R.L. Sugar, Phys. Rev. D **35** (1987) 2531.