PROCEEDINGS OF SCIENCE

Taylor series coefficients at $\mu = 0$ from imaginary μ computations

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Taylor expansion at $\mu = 0$ and computations at imaginary values of the chemical potential are the two most popular approaches to tackle the sign problem in finite-density lattice QCD. The two methods are obviously related. In particular, the Taylor coefficients are often reconstructed from the data obtained at imaginary μ. In the context of the Bielefeld-Parma collaboration, we have been generating data which fed our multi-point Padé analysis of the QCD phase diagram. We report on our studies on the different techniques to compute the Taylor coefficients at $\mu = 0$.

The 41st International Symposium on Lattice Field Theory (LATTICE2024)
28 July - 3 August 2024
Liverpool, UK

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PoS(LATTICE2024)170

1. Motivations for this study: the sign problem

The QCD phase diagram is, still to this day, mostly unprobed [1]. One of the reasons is that the lattice discretization, that is the most powerful tool available to us to make non-perturbative predictions by means of Monte Carlo simulations, fails when a non-zero chemical potential is added. This is due to the so-called sign problem: the Dirac determinant becomes complex and the exponential interpreted as a Boltzmann weight, that should be real, becomes complex as well [2].

One of the most promising ways to circumvent this problem is to make simulations at purely imaginary baryon chemical potential: for such values, in fact, the Dirac determinant remains real [3, 4]. The downside of this approach is that analytic continuation in the plane $T - \mu_B$ (temperature-baryonic chemical potential) must be performed in order to make physical predictions at real values of μ_B. However, problems are expected since the data available are a finite set of points, affected by statistical errors.

The aim of this study is to illustrate the recent progress made by our group on this topic. Namely, we will review some of the possible ways to analytically continue a function known only at a finite set of points in the imaginary axis by means of a Taylor expansion at the origin. We try to assess how the statistical uncertainty is carried over the real axis of μ_B when performing such analytic continuation.

2. The algorithm: Taylor expansion

In the following section, the different ways of constructing a Taylor expansion from a given dataset will be illustrated. The function taken into account will be a generic function $f(x)$, only in the last part the baryon number density obtained through lattice simulations will be taken into account.

2.1 Taylor expansion of a generic function

Let us suppose we know a function $f(x)$ only at a finite set of N points $x_0, \dots, x_{N-1}$, *i.e.* the only known values of $f(x)$ are $f(x_0), \dots, f(x_{N-1})$. Having N conditions, one can think we can hunt for N independent parameters. For example, one could write the first N terms of the Taylor expansion of $f(x)$ around the origin

$$\begin{cases} f(x_0) = \displaystyle\sum_{k=0}^{N-1} \frac{1}{k!} f^{(k)}(0) x_0^k \\ \vdots \\ f(x_{N-1}) = \displaystyle\sum_{k=0}^{N-1} \frac{1}{k!} f^{(k)}(0) x_{N-1}^k \end{cases} \tag{1}$$

where the unknowns can be either $f^{(k)}(0)$ or $\frac{1}{k!} f^{(k)}(0)$ (that lead to different condition numbers, as it will be shown later).

Since lattice computations usually also provide the first derivative with reasonable uncertainties, the system (1) can be extended. Let us suppose to have the first derivative evaluated at M points

$f'(x_N), \dots, f'(x_{N+M-1})$. The system (1) becomes:

$$\begin{cases} f(x_i) = \displaystyle\sum_{k=0}^{N+M-1} \frac{1}{k!} f^{(k)}(0) x_i^k & i = 0, \dots, N-1 \\ \quad \vdots & \\ f'(x_j) = \displaystyle\sum_{k=1}^{N+M-1} \frac{k}{k!} f^{(k)}(0) x_j^{k-1} & j = N, \dots, N+M-1 \end{cases} \tag{2}$$

so that the derivatives up to order $N + M - 1$ can be estimated. Notice that we are systematically leaving out effects that we know are there, *i.e.* terms $O(x_l^W)$.

2.2 Taylor expansion of an odd function

Because of the charge conjugation symmetry, the baryon number density is an odd function of the chemical potential. For this reason, in order to get higher orders of derivatives from the same dataset, the truncated Taylor expansion can be written in terms of only odd powers of x. As a consequence, its first derivative will be written in terms of only even powers of x:

$$\begin{cases} f(x_i) = \displaystyle\sum_{k=0}^{N+M-1} \frac{1}{(2k+1)!} f^{(2k+1)}(0) x_i^{2k+1} & i = 0, \dots, N-1 \\ \quad \vdots & \\ f'(x_j) = \displaystyle\sum_{k=0}^{N+M-1} \frac{2k+1}{(2k+1)!} f^{(2k+1)}(0) x_j^{2k} & j = N, \dots, N+M-1 \end{cases} \tag{3}$$

We point out that neglecting the even derivatives at $x = 0$ is basically equivalent to an expansion of the function $f(x)/x$ in terms of powers of x^2. In this case, derivatives up to order $2N + 2M - 1$ can be estimated.

2.3 The linear system

As already pointed out, the system we described can be solved in two different ways. One can take the derivatives as unknowns

$$\begin{pmatrix} 1 & x_0 & \frac{x_0^2}{2!} & \cdots & \frac{x_0^{N-3}}{(N-3)!} & \frac{x_0^{N-2}}{(N-2)!} & \frac{x_0^{N-1}}{(N-1)!} \\ 1 & x_1 & \frac{x_1^2}{2!} & \cdots & \frac{x_1^{N-3}}{(N-3)!} & \frac{x_1^{N-2}}{(N-2)!} & \frac{x_1^{N-1}}{(N-1)!} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & x_{N-2} & \frac{x_{N-2}^2}{2!} & \cdots & \frac{x_{N-2}^{N-3}}{(N-3)!} & \frac{x_{N-2}^{N-2}}{(N-2)!} & \frac{x_{N-2}^{N-1}}{(N-1)!} \\ 1 & x_{N-1} & \frac{x_{N-1}^2}{2!} & \cdots & \frac{x_{N-1}^{N-3}}{(N-3)!} & \frac{x_{N-1}^{N-2}}{(N-2)!} & \frac{x_{N-1}^{N-1}}{(N-1)!} \end{pmatrix} \begin{pmatrix} f(0) \\ f^{(1)}(0) \\ f^{(2)}(0) \\ \vdots \\ f^{(N-3)}(0) \\ f^{(N-2)}(0) \\ f^{(N-1)}(0) \end{pmatrix} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{N-2}) \\ f(x_{N-1}) \end{pmatrix} \tag{4}$$

On the other hand, one can take the derivatives divided by the respective factorial as unknowns

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{N-3} & x_0^{N-2} & x_0^{N-1} \\ 1 & x_1 & x_1^2 & \dots & x_1^{N-3} & x_1^{N-2} & x_1^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & x_{N-2} & x_{N-2}^2 & \dots & x_{N-2}^{N-3} & x_{N-2}^{N-2} & x_{N-2}^{N-1} \\ 1 & x_{N-1} & x_{N-1}^2 & \dots & x_{N-1}^{N-3} & x_{N-1}^{N-2} & x_{N-1}^{N-1} \end{pmatrix} \begin{pmatrix} f(0) \\ f^{(1)}(0) \\ \frac{f^{(2)}(0)}{2!} \\ \vdots \\ \frac{f^{(N-3)}(0)}{(N-3)!} \\ \frac{f^{(N-2)}(0)}{(N-2)!} \\ \frac{f^{(N-1)}(0)}{(N-1)!} \end{pmatrix} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{N-2}) \\ f(x_{N-1}) \end{pmatrix} \tag{5}$$

As it will be shown in the following section, we will find that the system in (4) provides more accurate results (closer to the analytic ones, if applied to a known function). Still, the matrix defining the system has a higher condition number than the matrix in equation (5).

For a linear system $Ax = b$ (A is a matrix and x and b are column vectors), the condition number of A is defined as the maximum ratio of the relative error in x to the relative error in b. It can be obtained as $\mathrm{Cond}(A) = |\lambda(A)|_{\max}/|\lambda(A)|_{\min}$, where $|\lambda(A)|_{\max}$ and $|\lambda(A)|_{\min}$ are, respectively, the maximal and minimal absolute values of eigenvalues of A.

A higher condition number means a higher instability in the results under a slight change of the input; therefore, this must be taken into account when using input data affected by errors.

3. Playing with a test function

The method has been tested with a known function, $f(x) = \sin(x)$, taking as input the function evaluated at 4 equally spaced points in the interval $(0, 0.5i]$. Input data have no errors; for the moment being, we will also make no attempt at evaluating errors on results.

In Table 1, different implementations are compared: the first column presents results for derivatives of the function at the origin, taking as inputs values of the function and not taking into account parity (system (1)); the second column presents results for derivatives of the function at the origin, taking as inputs values of the function and taking into account parity (system (3); notice that (3) displays the general case in which also derivatives are taken as inputs). Two rows are there, because we can look at system (4) (first row) or system (5) (second row). Remember: the two systems differ for the factorials, which are placed either in the matrix (system (4)) or in the unknowns (system (5)). The expression $\frac{f^{(k)}(0)}{k!}k!$ means that the quantities $\frac{f^{(k)}(0)}{k!}$ are obtained from the system, then the results are multiplied by $k!$.

In Table 2 there is one single column and two rows. The meaning of the two rows is exactly the same as above. Here we use 8 input data: the same 4 points as in Table 1, plus the first derivative of the test function evaluated at the same 4 points. Notice that we have only one column: parity is always taken into account.

In both tables, the condition number of the matrix that defines the linear system is written in red at the bottom of each quadrant.

The values of successive derivatives of the function $\sin(x)$, evaluated at the origin, are expected to be alternating $+1$ and -1 for odd-order derivatives and 0 for even-order ones. This is the behavior we observe in Table 1. In the first column, we get results up to order 3 (with an error on the highest

	Points Only	Points and Parity
$f^{(k)}(0)$	$0) -9.519 \times 10^{-21} - 6.183 \times 10^{-05} i$	$1) +1.000 \times 10^{+00} + 1.205 \times 10^{-15} i$
	$1) +1.001 \times 10^{+00} + 0.000 \times 10^{+00} i$	$3) -1.000 \times 10^{+00} + 1.972 \times 10^{-13} i$
	$2) +9.660 \times 10^{-17} + 9.878 \times 10^{-03} i$	$5) +1.000 \times 10^{+00} + 2.959 \times 10^{-11} i$
	$3) -1.051 \times 10^{+00} + 3.075 \times 10^{-16} i$	$7) -1.007 \times 10^{+00} + 2.716 \times 10^{-09} i$
	Condition n.: $5.044 \times 10^{+03}$	Condition n.: $2.975 \times 10^{+07}$
$\frac{f^{(k)}(0)}{k!} k!$	$0) -1.294 \times 10^{-16} - 6.183 \times 10^{-05} i$	$1) +1.000 \times 10^{+00} + 1.150 \times 10^{-15} i$
	$1) +1.001 \times 10^{+00} - 1.554 \times 10^{-15} i$	$3) -1.000 \times 10^{+00} + 1.886 \times 10^{-13} i$
	$2) +1.130 \times 10^{-14} + 9.878 \times 10^{-03} i$	$5) +1.000 \times 10^{+00} + 2.830 \times 10^{-11} i$
	$3) -1.051 \times 10^{+00} + 4.002 \times 10^{-14} i$	$7) -1.007 \times 10^{+00} + 2.597 \times 10^{-09} i$
	Condition n.: $1.127 \times 10^{+03}$	Condition n.: $6.522 \times 10^{+03}$

Table 1: Derivatives of f (a few orders) evaluated at the origin, obtained by taking as input only the test function ($f(x) = \sin(x)$) evaluated at 4 equally spaced points in the interval $(0, 0.5i]$. Notice that results turn out to be complex.

	Points, Parity and 1st derivative	
$f^{(k)}(0)$	$1) +1.000 \times 10^{+00} + 1.858 \times 10^{-15} i$	$3) -1.000 \times 10^{+00} + 3.546 \times 10^{-13} i$
	$5) +1.000 \times 10^{+00} + 9.966 \times 10^{-11} i$	$7) -1.000 \times 10^{+00} + 2.614 \times 10^{-08} i$
	$9) +1.000 \times 10^{+00} + 5.224 \times 10^{-06} i$	$11) -1.005 \times 10^{+00} + 5.798 \times 10^{-04} i$
	$13) +5.220 \times 10^{-03} - 3.019 \times 10^{-06} i$	$15) -1.262 \times 10^{-05} + 7.304 \times 10^{-09} i$
	Condition n.: $5.658 \times 10^{+20}$	
$\frac{f^{(k)}(0)}{k!} k!$	$1) +1.000 \times 10^{+00} + 3.281 \times 10^{-15} i$	$3) -1.000 \times 10^{+00} - 4.122 \times 10^{-13} i$
	$5) +1.000 \times 10^{+00} - 1.145 \times 10^{-09} i$	$7) -1.000 \times 10^{+00} - 1.217 \times 10^{-06} i$
	$9) +1.000 \times 10^{+00} - 9.956 \times 10^{-04} i$	$11) -9.729 \times 10^{-01} - 6.334 \times 10^{-01} i$
	$13) +1.294 \times 10^{+01} - 2.826 \times 10^{+02} i$	$15) +2.789 \times 10^{+03} - 6.651 \times 10^{+04} i$
	Condition n.: $6.385 \times 10^{+08}$	

Table 2: Derivatives of f (a few orders) evaluated at the origin, obtained by taking as input the test function ($f(x) = \sin(x)$) and its first derivative ($f'(x) = cos(x)$) evaluated at 4 equally spaced points in the interval $(0, 0.5i]$. Again, results turn out to be complex

order derivative of 5%). In the second column, we get results up to order 7 (with an error on the highest order derivative of 0.7%). In Table 2, results are obtained by adding also the first derivative. The precision appears to increase: on the first row, we get an error of approximately 0.5% for a derivative as high as 11^{th} order; on the second row, we can claim an error of approximately 0.1% for the 9^{th} order derivative.

By just looking at the errors, one could conclude that with the factorials included in the matrix - see eq. (4) - we get better results. However, the condition number of the system is in this case worse. This means that we can expect more stable results for (5) once input data will be affected by errors.

4. Results with lattice QCD data

Lattice data have been taken from the Bielefeld-Parma collaboration, using Highly Improved Staggered Quarks (HISQ), with 2 light quarks and 1 heavier quark, taken at physical pion mass [5]. The number of lattice points in the time direction is $N_\tau = 6$, with an aspect ratio of 6. Simulations have been performed at the temperature $T = 157.5$ MeV, which is supposed to be close to freeze-out.

The unknown function is the baryon number density $\chi_1(\mu)$ (first cumulant). In more detail, the k-th cumulant is defined as follows:

$$\chi_k(\mu) = \frac{1}{VT^3}\frac{\partial^k}{\partial\mu^k}\ln Z(\mu, V, T) \tag{6}$$

The input data are the values of the function $\chi_1(\mu)$ and its first derivative ($\chi_2(\mu)$) at $\mu = \{+0.3928i, +0.7853i, +1.178i, +1.5709i\}$. The goal was to find the first two nonzero derivatives, evaluated at the origin, that is $\chi_2(0)$ and $\chi_4(0)$.

	$\chi_2(0)$	$\chi_4(0)$	Cond. n.
$\chi_k(0)$	0.12278	0.466	352
$\frac{\chi_k(0)}{(k-1)!}(k-1)!$	0.12278	0.466	291
$\chi_k^{odd}(0)$	0.10973 ± 0.00140	0.081 ± 0.028	$3.25e^{+5}$
$\frac{\chi_k^{odd}(0)}{(k-1)!}(k-1)!$	0.10973	0.081	489
HotQCD	0.10870 ± 0.00004	0.084 ± 0.004	

Table 3: Similar to Table 2 for the computation of $\chi_2(0)$ and $\chi_4(0)$ (see text for further details). HotQCD data in the last line for comparison.

In Table 3, we perform a comparison similar to that of the previous section. The first two lines present results coming from the systems (4) and (5), respectively, without any constraint on parity. In the third and fourth lines, parity is taken into account: because of the charge conjugation symmetry, χ_1 must be odd ($\chi_1(-\mu) = -\chi_1(\mu)$). For the moment being, results have been obtained without any estimate of systematic errors. As for the statistical ones coming from Monte Carlo errors, in all rows but the third we only take into account central values. To get a first grasp, on the third row one can inspect errors coming from a bootstrap procedure. A more careful study will ask

for an estimate of systematic errors as well. For comparison, the last line contains the results from the HotQCD collaboration [6].

As it can be seen, by including parity constraints we get results closer to the expected values, once again at the price of a larger condition number.

Of course, a more thorough study of the systematics is needed to draw better conclusions. Still, it is fair to say that we essentially got quite precise results.

5. Conclusions

Different numerical methods for the computation of Taylor series coefficients at the origin have been compared, both for a test function and for lattice QCD data.

As for the latter, through a preliminary study of statistical uncertainties, it is fair to say that we found a substantial agreement with results by the HotQCD collaboration for the first two non-null derivatives of the number density.

In the future a more thorough study of statistical errors has to be performed. Also, it will be important to compare with results coming from a new method, which is an application of the Cauchy integral formula in the form of an inverse problem [7]. Since the time of the conference, substantial progress has been achieved.

Acknowledgments

This work is supported by INFN under the research project *i.s. QCDLAT*. It is our pleasure to thank all our colleagues in the Bielefeld-Parma Collaboration: we plan to apply all this machinery in the context of our common research plans.

References

[1] M. Stephanov, *QCD Phase Diagram and the Critical Point*, *Prog. Theor. Phys. Suppl.* **153** (2004) 139 [0402115].

[2] P. de Forcrand, *Simulating QCD at finite density*, *PoS* **LATTICE2009** (2010) [1005.0539].

[3] P. de Forcrand and O. Philipsen, *The QCD phase diagram for small densities from imaginary chemical potential*, *Nucl. Phys. B* **642** (2002) 290 [hep-lat/0205016].

[4] M. D'Elia and M.-P. Lombardo, *Finite density QCD via imaginary chemical potential*, *Phys. Rev. D* **67** (2003) 014505 [hep-lat/0209146].

[5] D.A. Clarke, P. Dimopoulos, F. Di Renzo, J. Goswami, C. Schmidt, S. Singh et al., *Searching for the QCD critical endpoint using multi-point Padé approximations*, 2405.10196.

[6] HotQCD collaboration, *Taylor expansions and Padé approximants for cumulants of conserved charge fluctuations at nonvanishing chemical potentials*, *Phys. Rev. D* **105** (2022) 074511 [2202.09184].

[7] F. Di Renzo, M. Aliberti and P. Dimopoulos, *On analytic continuation from imaginary to real chemical potential in Lattice QCD*, *PoS* **LATTICE2024** (2025) 174.