

Finite density lattice QCD as an inverse problem (aka analytical continuation from imaginary to real chemical potential via Cauchy integral formula)

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Given the sign problem, many simulations of finite density lattice QCD are performed at imaginary values of the baryonic chemical potential. One is thus left with the problem of analytically continuing results to (physical) real values. We have recently introduced a new method to perform this analytical continuation, based on the Cauchy integral formula, starting from which we define and solve an inverse problem. It turns out that the method can be successfully implemented, as we show in the case of the computation of the number density. As a check, we show that results for derivatives of the number density (i.e. higher order cumulants) can be obtained, fully consistent with the values available in the literature. The method, as we will discuss, is more general than it appears in this context, having something to say about many other relevant inverse problems.

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1. Introduction

The so-called sign problem is something like a nightmare for the lattice community. When a finite baryonic chemical potential μ is in place, the lattice QCD action is complex-valued, as seen from the following property of the Dirac operator determinant ¹

$$\det(\not{D} + m + \mu\gamma_0) = (\det(\not{D} + m - \mu^*\gamma_0))^* . \quad (1)$$

As a result, the weight of the path integral is not positive definite, and thus it cannot be taken as a decent probability distribution: all in all, a direct access to Monte Carlo simulations is lost. A natural workaround can be clearly seen in Eq. (1): the sign problem is gone for imaginary chemical potential. Lattice simulation at imaginary values $\mu = i\mu_I$ ($\mu_I \in \mathbb{R}$) are in fact a popular partial solution of the sign problem [1, 2]. The solution is a partial one, since one is then left with the problem of analytically continuing results to real (physical) values of the chemical potential.

In the following we will be concerned with an approach to analytic continuation that the Parma group has recently put forward [3], which amounts to *solving the sign problem as an inverse problem*. This is basically an application of a fundamental result in complex analysis, *i.e.* the Cauchy integral formula.

2. An inverse problem from the Cauchy integral formula

We will consider the computation of a (lattice) QCD observable at imaginary values of the baryonic chemical potential and we will analytically continue results to the (physical) real- μ axis. In particular, we will be concerned with the 1-st cumulant of the net baryon density, defined for $n = 1$ by ²

$$\chi_n(T, V, \mu_B) = \left(\frac{\partial}{\partial \mu_B} \right)^n \frac{\ln \mathcal{Z}(T, V, \mu_B)}{VT^3} \quad (2)$$

Let's say we have n measurements of χ_1 , taken at (imaginary) values $\mu_k = i\mu_I^{(k)}$. Let's \mathcal{R} be a region inside which our observable is analytic (notice that we are prepared for a generic lattice QCD observable not to be analytic in the entire complex- μ plane). We will now require that (a) $\forall_{k=1\dots n} \mu_k \in \mathcal{R}$, (b) C is a closed contour entirely contained in \mathcal{R} , and (c) C is taken in such a way that all the μ_k lie inside it. Since we have taken the contour C inside the analyticity region \mathcal{R} , we know from complex analysis that the values $\chi_1(i\mu_I^{(k)})$ could be *in principle* computed via the Cauchy formula

$$\chi_1(i\mu_I^{(k)}) = \frac{1}{2\pi i} \oint_C \frac{\chi_1(\mu)}{\mu - i\mu_I^{(k)}} d\mu \quad (k = 1 \dots n) \quad (3)$$

This setting is depicted in Fig. 1. This statement is correct, but of very limited (null, actually) practical usefulness: we have no practical way of obtaining (that is, computing) $\chi_1(\mu)$ on the contour C . Notice that in Fig. 1 C has been chosen to be a circle, and so the integral can be easily

¹ \not{D} is the massless Dirac operator.

² $\mathcal{Z}(T, V, \mu_B)$ is the grand canonical partition function. Notice that this is the only formula which is correctly defined in terms of μ_B : everywhere else, to keep notation lighter, the baryonic chemical potential will be simply notated μ .

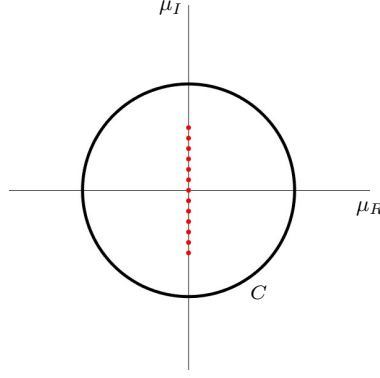


Figure 1: Provided we stay inside a region where a lattice QCD observable is analytic, its values at imaginary values of the baryonic chemical potential could be *in principle* computed from the Cauchy formula, *e.g.* integrating on a convenient close contour, let's say a circle C .

rewritten as an integral over a real interval³

$$\chi_1(i\mu_I^{(k)}) = \frac{1}{2\pi} \int_0^{2\pi} \frac{\chi_1(Re^{i\theta}) Re^{i\theta}}{Re^{i\theta} - i\mu_I^{(k)}} d\theta \quad (k = 1 \dots n) \quad (4)$$

Once the integral has been expressed as in Eq. (4), we can go numeric and *up to approximation errors* we can compute it via a quadrature formula: our choice is for Gauss-Legendre quadrature. We get

$$\chi_1(i\mu_I^{(k)}) \simeq \frac{1}{2\pi} \sum_{j=1}^n w_j \frac{Re^{i\theta_j}}{Re^{i\theta_j} - i\mu_I^{(k)}} \hat{\chi}_j \quad (k = 1 \dots n). \quad (5)$$

In Eq. (5) the θ_j are related to the roots of the Legendre polynomial of degree n ⁴ and the w_j are the associated weights, while we define $\hat{\chi}_j = \chi_1(Re^{i\theta_j})$. We now notice that Eq. (5) can be readily regarded as a linear system $Ax = b$, if we trade \simeq for $=$ and we define

$$A_{kj} = \frac{1}{2\pi} w_j \frac{Re^{i\theta_j}}{Re^{i\theta_j} - i\mu_I^{(k)}} \quad x_j = \hat{\chi}_j = \chi_1(Re^{i\theta_j}) \quad b_k = \chi_1(i\mu_I^{(k)}) \quad k, j = 1 \dots n \quad (6)$$

By switching to the linear system notation, we made it clear a new way of looking at Eq. (5): we regard our original Cauchy formula as an inverse problem, that is we want to input values $\chi_1(i\mu_I^{(k)})$ computed on the imaginary axis and get the values of χ_1 on the contour, at the quadrature points. This new setting is depicted in Fig. 2.

Finally, we are in a position to compute our observable χ_1 for physical, real values of the baryonic chemical potential: since we know χ_1 at the quadrature points, we can directly apply our (discretized) Cauchy formula and compute for any real value μ which lies inside the contour C

$$\chi_1(\mu) \simeq \frac{1}{2\pi} \sum_{j=1}^n w_j \frac{Re^{i\theta_j}}{Re^{i\theta_j} - \mu} \hat{\chi}_j \quad \mu \in \mathbb{R}. \quad (7)$$

³ R is the radius of our circle. Of course, any interval of width 2π could be as appropriate as $[0, 2\pi]$.

⁴The θ_j are not the roots themselves because we are integrating on an interval which is not $[-1, 1]$.

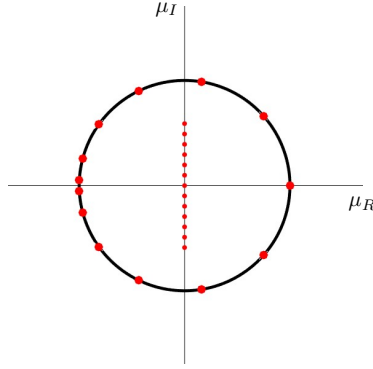


Figure 2: If we compute the integral Cauchy formula via numerical quadrature, its value is decided by the values of our observable at quadrature points on the integration contour. We cannot compute these values, but we can solve for them: once numerically discretized, a collection of several Cauchy integrals turns into a linear system in which the values of our observable at given imaginary chemical potential (which we can compute) are the known terms. A natural choice is that of having a number of imaginary chemical potentials values equal to the number of quadrature points.

The cartoon of our complete procedure is depicted in Fig. 3. *A priori*, one would be quite suspicious of trading the sign problem for an integral inverse problem: it looks like trading a difficult problem for a (possibly) even more difficult one. All in all, an integral inverse problem is always supposed

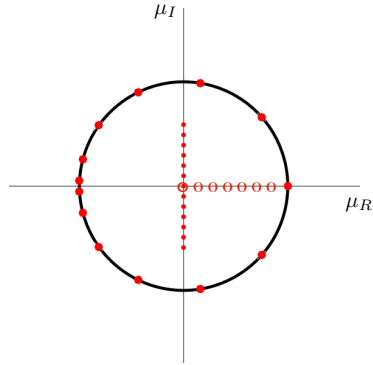


Figure 3: The cartoon of our (inverse problem) complete procedure: we input values of an observable at imaginary values of the baryonic chemical potential, which become the known terms in a linear system which encodes a collection of discretized Cauchy integral formulas; once we have solved for the values of the observable at quadrature points, a direct application of the discretized Cauchy integral formula enables us to compute the observable at real values of the chemical potential.

to be extremely hard and there are indeed very good reasons for being worried, since

- the linear system in Eq. (6) can easily be ill-conditioned;
- in our procedure we unavoidably deal with *errors*, which have a *dual nature*: (a) there are *systematic* errors, because the quadrature formulas hold true up to approximation errors; (b) there are *statistical* errors, because the observable is computed (that is, measured) with limited precision.

There is no compelling reason for being always pessimistic (and even less reasons for being always optimistic), but for sure the combination of the two issues can result in a solution which makes no sense.

Notice that the formulation of our procedure (which we got from the Cauchy formula) clearly displays the very basic difficulty of an integral inverse problem: one is trying to reconstruct a function on a contour (*i.e.* an infinite amount of information) from a limited knowledge of the function itself (*i.e.* on a discrete, finite set of points). We can at the least make one good point: since we go via a quadrature formula, we always end up with solving for n unknowns given n input pieces of information. This basic point also comes with an extra bonus (see the cartoon in Fig. 4). Suppose we first take into account n input points in our procedure: we end up with getting the values of our function at n (quadrature) contour points. If we add *one single extra point*, we gain $n + 1$ new pieces of information (quadrature points of an n -points formula are all different from those of an $n + 1$ -points formula). This allows for useful consistency checks stemming from a very general observation: we want values of our unknown function at quadrature points (on the contour) to fall on a smooth curve (in particular, if they come from different order approximations).

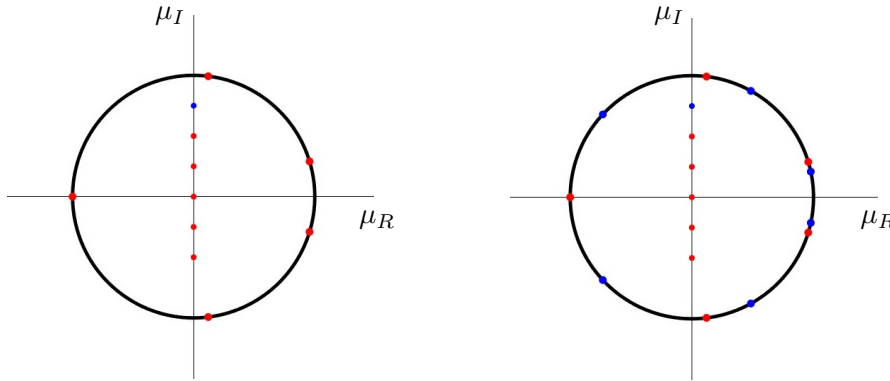


Figure 4: Suppose we set up our (inverse problem) procedure with n input points on the imaginary axis (left figure). If we add one single new input point, we get $n + 1$ brand new values of our function on the integration contour (right figure). This allows for useful consistency checks.

An example of such a consistency check is displayed in Fig. 5. In the left panel, we present the solution of our inverse problem for the \sin function: the latter is computed on the real axis starting from the knowledge of values of the function on the imaginary axis. This means that the left panel depicts the final output of our procedure. In the right panel, we plot the solution of the inverse problem itself. This means that we plot the real part of the \sin function on the integration circle C as a function of the angle θ (*i.e.* the real part of the \sin function is plotted at quadrature points). The reader will notice different colors and symbols: the plot is a collection of different computations. This means that we first completed our procedure via an n -points quadrature formula, and thus we got values at n points on the contour. Then, we repeated the procedure several times making use of n_i -points quadrature formulas ($n_i \neq n$): in this way we obtained a variety of different evaluations

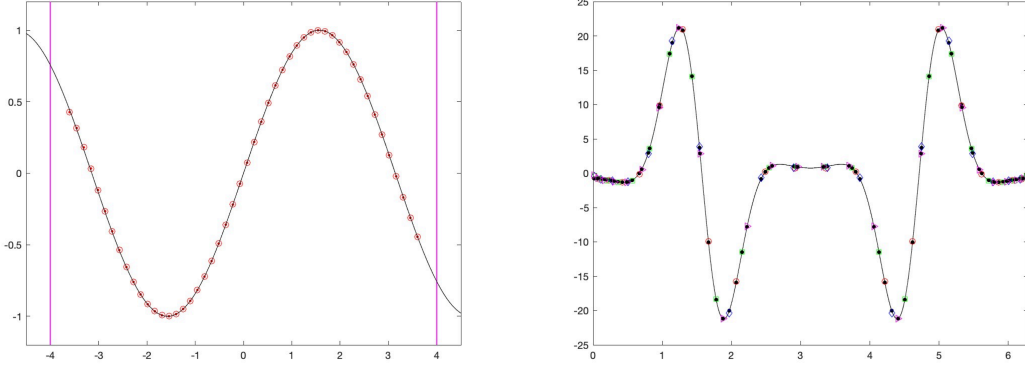


Figure 5: The \sin function on the real axis reconstructed from the knowledge of a set of values on the imaginary axis (left figure). The real part $\Re(\sin(\theta))$ at different quadrature points on the contour of the Cauchy formula, plotted as a function of the angle θ (right figure). The different symbols (and colours) make it clear that this is a collection of many computations, each obtained from a different order for the Gauss Legendre formula in Eq. (6). Even if one did not have any clue on how good was the computation of the function on the real axis, it would be nevertheless reassuring to see that all the points fall on a smooth curve (which is, by the way, the correct one, as seen by comparing to the continuous curve).

of the function at different points on the integration contour. As it is clearly seen, we end up with a smooth curve. Since we know the function we are dealing with, we can indeed check that our points fall just on top of their expected values (solid curve). Of course, in a real case one does not know the result in advance. Still, it is nice to observe that we end up with a smooth solution on the integration contour. In other terms, if we look for sanity checks (that is, how reliable the final result of the procedure is? or, can we trust what we read from the left panel of Fig. 5?), we have at least some clue on the stability of our results and this speaks in favor of the procedure.

We end this introduction to the method with an important observation. Till now we have (at least implicitly) assumed that we solve the linear system coding our inverse problem exactly as it is written in Eq. (6), that is taking n values of the function and solving an $n \times n$ system for n unknowns. This is not necessarily the case. One should keep in mind that there is a (general) Cauchy integral formula for derivatives of a function

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} dz \quad (8)$$

In case we have a function of a given parity, we can set to zero the even/odd derivatives at $z_0 = 0$ and take these relations as extra inputs (*i.e.* extra rows) in the linear system that we solve. These can be regarded as pieces of information that we get almost *for free*, meaning that they come with nothing to compute (measure from Monte Carlo, in our case) and with no error attached. It also pays to enforce a final extra input

$$0 = \oint_C f(z) dz \quad (9)$$

which is simply the Cauchy theorem, which must hold true under our analyticity assumptions. It turns out that adding both extra inputs helps, and they have been taken into account in the

computation of the *sin* function (an odd function) depicted in Fig. 5.

3. Solving the (Tychonov) regularized problem in Lattice QCD

As said since the very beginning, we applied our inverse problem procedure to the computation of $\chi_1(\mu)$, that is the number density at real values of the baryonic chemical potential. The inputs for the procedure are given by

- a few values $\chi_1^I(i\mu^I)$, that is measurements of the number density at imaginary values of the chemical potential (these are imaginary values themselves)⁵;
- a given number of constraints enforcing zero value for even derivatives of the number density at $\mu = 0$ (see Eq. (8); our target is an odd function);
- the analyticity constraint of Eq. (9).

The question is: can we hope for success, as that depicted in Fig. 5?

What we depict in Fig. 5 looks like a great success for our method, but actually we have been cheating a bit: in the computation of the *sin* function our input values had no errors. In a real case, errors are there and (not surprisingly) the smoothness of the solution appears to get lost. Again, this does not come as a surprise: the interplay between bad condition numbers and errors can result in completely unreliable results. Notice that if we had to plot again Fig. 5, this failure would show up both in the left and in the right panel. This is indeed the case when we go for the computation of $\chi_1(\mu)$.

There is a standard workaround for a ill-conditioned linear system: one has to regularize the system. A popular regularization scheme is that provided by the Tychonov approach

$$\text{In order to solve } Ax = b \text{ one minimizes } \|Ax - b\|^2 + \|\gamma x\|^2$$

This is the regularization of our choice. The problem now turns into the question: *how shall we select a proper value of γ ?*

A proper value for the parameter γ can be selected by a procedure based on *self-consistency*. Leveraging on this, we could successfully apply our method to the computation of $\chi_1(\mu)$: this can be discussed looking at Fig. 6, where we depict the values of $\chi_1^I(i\mu^I)$ coming from the computations in [4]. The *red circles* are all the measurements that we have at hand (notice the errors: they appear quite tiny, but they are enough to make the naive application of our inverse problem method fail). With *black diamonds* we highlight the values that actually entered our procedure, that is those which act as known terms in our linear system. The basic idea is now quite simple: once we have solved the inverse problem (that is, we have values of χ_1 on the integration contour), we should be able to compute $\chi_1(\mu)$ at any value of μ which lies inside our integration contour, including of

⁵These inputs are taken from computations performed by the Bielefeld-Parma Collaboration [4].

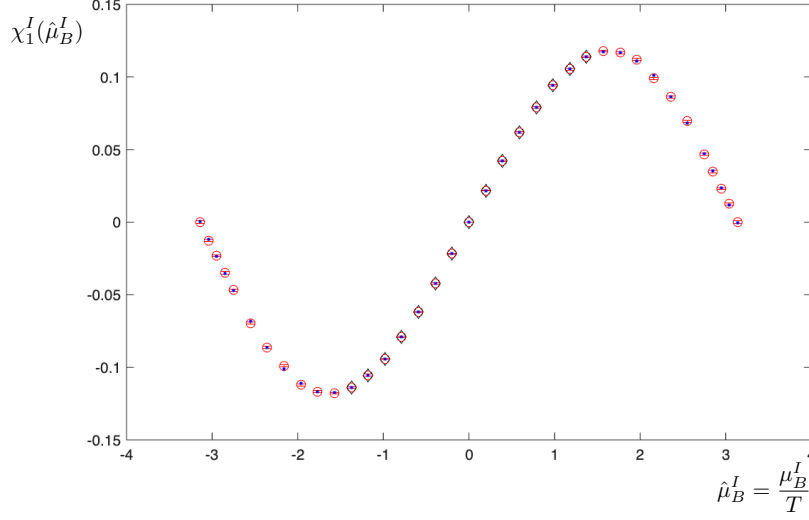


Figure 6: The imaginary part of the number density $\chi_1^I(\hat{\mu}_B^I)$ plotted as a function of the imaginary chemical potential $\hat{\mu}_B^I = \frac{\mu_B^I}{T}$. The red circles are the values we computed by Monte Carlo. Black diamonds highlight the points which entered our (inverse problem) procedure. The (tiny) blue dots are the values of the function as reconstructed by our procedure. The Tychonov parameter has been set in such a way that values computed by our procedure fall on top of values computed by Monte Carlo.

course imaginary values for which we plot $\chi_1^I(i\mu^I)$ in Fig. 6⁶. For a *generic* value of the Tychonov parameter γ one correctly gets the values $\chi_1^I(i\mu^I)$ at the *black diamonds points*, but *misses the values outside that interval*. If instead we *tune the value of γ* , we can select a value for which *all the red points* are correctly got, that is the values computed by our procedure fall on top of the measurements: these values (the outcome of our procedure) are depicted as *blue dots* in Fig. 6. Once this has been accomplished, we claim success for the method since

- we obtain a smooth $\chi_1(\mu)$ for real μ ;
- via Eq. (8) we can compute the values of other cumulants at $\mu = 0$ (namely $\chi_2(0)$, $\chi_4(0)$, $\chi_6(0)$, $\chi_8(0)$) and these can be nicely compared with values from the literature [5];
- we can even pin down a value for $\chi_{10}(0)$, a quantity that has never been computed before.

Numerical results (together with other computational details) can be found in another contribution from our group [6].

4. Conclusions and outlook

We discussed a recently proposed technique to analytically continue lattice QCD results from imaginary to real values of the baryonic chemical potential, based on an inverse problem that we

⁶For given values of the radius of the circle C , we can compute our function for all those points.

derive from the Cauchy integral formula. The method has been successfully applied to the computation of the number density $\chi_1(\mu)$.

As a final remark, we stress that the approach to (integral) inverse problems that we discussed can have other applications. Along these lines, one can approach the inversion of Laplace transforms (which are *e.g.* relevant in the context of the extraction of spectral functions from lattice correlators); for our first steps along this direction, see [7].

Acknowledgments

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