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Detecting Lee-Yang/Fisher singularities by multi-point Padè

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The Bielefeld Parma Collaboration has in recent years put forward a method to probe finite density QCD by the detection of Lee-Yang singularities. The location of the latter is obtained by multi-point Padè approximants, which are in turn calculated matching Taylor series results obtained from Monte Carlo computations at (a variety of values of) imaginary baryonic chemical potential. The method has been successfully applied to probe the Roberge Weiss phase transition and preliminary, interesting results are showing up in the vicinity of a possible QCD critical endpoint candidate. In this talk we will be concerned with a couple of significant aspects in view of a more powerful application of the method. First, we will discuss the possibility of detecting finite size scaling of Lee-Yang/Fisher singularities in finite density (lattice) QCD. Second, we will briefly mention our attempts at detecting both singularities in the complex chemical potential plane and singularities in the complex temperature plane. The former are obtained from rational approximations which are functions of the chemical potential at given values of the temperature; the latter are obtained from rational approximations which are functions of the temperature at given values of the chemical potential.

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1. Our workhorse: multi-point Padè

Since a few years [1] the Bielefeld Parma collaboration has started a project aiming to probe the QCD phase diagram by reconstructing the singularity structure of the theory in the complex chemical potential plane. The method is based on the approximation of the relevant observables by a rational function via the so-called multi-point Padè method.
The method works as follows. Suppose we know a few Taylor expansion coefficients of a given function $f(z)$ at different points

$$\ldots,\ f(z_k),\ f'(z_k),\ldots,f^{(s-1)}(z_k),\ \ldots\quad k=1\ldots N \tag{1}$$

The basic idea of our multi-point Padé approach is to approximate (interpolate, actually) $f(z)$ by a convenient function. While a polynomial approximation would be a natural choice with many respects, that is not what we are interested in, because it would leave us with no singularity pattern for $|z|\neq\infty$. Since we want instead to guess the singularity structure of our $f(z)$, we consider the rational function $R_n^m(z)$

$$R_n^m(z)=\frac{P_m(z)}{\tilde{Q}_n(z)}=\frac{P_m(z)}{1+Q_n(z)}=\frac{\sum\limits_{i=0}^{m}a_i\,z^i}{1+\sum\limits_{j=1}^{n}b_j\,z^j} \tag{2}$$

with m and n being the degrees of the polynomials at numerator and denominator respectively. We make a couple of preliminary observations which will be useful in the following. First of all, writing $\tilde{Q}_n(z)=1+Q_n(z)$ ensures that the rational function depends essentially on $n+m+1$ parameters. Having said that, we stress that *a priori* we should naturally demand that there is no point z_0 such that $P_m(z_0)=\tilde{Q}_n(z_0)=0$. The latter request seems indeed natural: we should in principle exclude any (common) zero of both numerator and denominator. Strictly speaking, if this were not the case, we would have rather essentially defined the rational function $R_{n'}^{m'}(z)$ with $n=n'+l$ and $m=m'+l$ for some integer $l>0$. We will nevertheless not exclude the possibility of common zeros, and we will instead live with that: as will see, the fact that common zeros do show up will be a very frequent event. We also make it clear that the number of coefficients we know can be different at different points. For the sake of simplicity we will however assume that $f^{(s-1)}$ is the highest order derivative which is known at each point (together with all derivatives of degree $0\leq g<s-1$).
Now remember: we want $R_n^m(z)$ to be a good interpolation for $f(z)$. It is quite obvious that we want the rational function to account for all the information available from (1). In order for this to hold true, the somehow simplest case is that of having $n+m+1=Ns$. If that is the case, we will have

$$\left(\frac{d}{dz}\right)^g R_n^m(z)|_{z=z_k}=f^{(g)}(z_k)$$

if we solve a system of equations, that is

$$\begin{aligned}
&\vdots \\
P_m(z_k) - f(z_k)Q_n(z_k) &= f(z_k) \\
P'_m(z_k) - f'(z_k)Q_n(z_k) - f(z_k)Q'_n(z_k) &= f'(z_k) \\
&\vdots \\
P_m^{(s-1)}(z_k) - f^{(s-1)}(z_k)Q_n(z_k) - \ldots - f(z_k)Q_n^{(s-1)}(z_k) & \\
= f^{(s-1)}(z_k) & \\
&\vdots
\end{aligned} \tag{3}$$

This is our recipe: by solving this system of linear equations we determine the coefficients of the polynomials P_m and Q_n. In order to estimate the coefficients of the rational functions we could of course rely on different methods, all somehow related to the idea of minimizing a generalized χ^2, *i.e.* we could want to minimize the distance between the input Taylor coefficients and the relevant rational function, weighted by the errors available on the input coefficients (the latter will in the end come from Monte Carlo measurements). Notice that this is equivalent to solving an over-constrained system ($n + m + 1 < Ns$) in a least squares sense. This has been compared to the linear solver method in [2].

Let us pause and inspect where we stand with respect to what we could be interested in. A first observation is that the method leaves us with an *interpolation* of $f(z)$, but of course we could be interested in *extrapolating*, that is we could want to get some information on $f(z)$ outside the interval where we collected the information encoded in (1). This is actually the case for lattice QCD. As a matter of fact, this was for us a strong motivation for introducing the method. This has to do with the (in)famous sign problem: for real values of the baryonic chemical potential, lattice QCD computations by Monte Carlo methods are hampered. The problem disappears for imaginary values, and this has been largely relied on [3, 4]: one performs computations where the latter are viable and then has to continue results for real (*i.e.* physical) values of the chemical potential. By our method we can compute a rational approximation interpolating results obtained for imaginary values of the baryonic chemical potential. The analytic continuation (that's what we need) of the results is in our approach a most natural one: simply compute our $R_n^m(\mu)$ for real μ. Although important, this is not the only thing we could be interested in. As already pointed out, having a $R_n^m(z)$ as an interpolation for the function $f(z)$ enables us to guess the singularity structure of $f(z)$: simply look at the poles of the rational function. Actually, in the following this is what we are interested in.

2. The best case playground for the method: 2D Ising model

In [2] we applied for the first time the method to lattice QCD. Namely, we were able to probe the Roberge Weiss transition. By studying the number density at various temperatures and for different imaginary values of $\hat{\mu}_B = \frac{\mu_B}{T}$ (μ_B being the baryonic chemical potential), for a given value of the temperature one should recognise a phase transition taking place at $\hat{\mu}_B = i\pi$. By studying our

rational approximants, we were able to inspect singularities at $\mathrm{Im}\hat{\mu}_B = \pi$. At different values of the temperature, the singularities take place closer and closer to the imaginary axis as temperature gets closer and closer to T_{RW}, the critical temperature of the Roberge Weiss transition. At each temperature we registered $\mathrm{Re}\hat{\mu}_{B0}$, to be read as the real part of the singularity with minimum real part. This quantity was shown to verify the expected scaling in T as the temperature was approaching T_{RW}. An updated account on our study of the Roberge Weiss transition has been presented in [5]. The singularities we have been talking about are known as *Lee-Yang singularities*, simply related to zeros of the partition function of the theory.
While the result in [2] was a success, we can notice that our result was obtained for a single scaling variable. Given our setting, there are in principle finite size errors in the procedure, which appeared to be quite well under control. One would nevertheless like to apply the method in a cleaner setting, in particular having the finite size effects acting as main characters and not as minor ones.

This is what we did in [6, 7], to which we refer the interested reader for more details: in the following we will mainly sketch the conceptual path, to set the stage for the experiments in lattice QCD. The theory which we probed is the well-known Ising model in $D = 2$

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i \qquad (\sigma_i = \pm 1) \tag{4}$$

We were able to probe both the *thermal singularities*, related to the so-called *Fisher zeros* and the *magnetic singularities*, related to the so-called *Lee-Yang zeros*. Roughly speaking, Fisher zeros are values of β at which the partition function at $h = 0$ is zero, while Lee-Yang zeros are values of h at which the partition function at $\beta = \beta_c$ is zero, β_c being singled out by studying Fisher zeros. All this is associated to the phase transition taking place (at the critical temperature, *i.e.* at $\beta = \beta_c$) at $h = 0$ and separating the paramagnetic phase from the ferromagnetic one. Here we recap what is going on with Lee-Yang zeros. For the case at hand, the $f(z)$ of (1) is the magnetization $m^{(L)}(h)$, which is computed at various values of the lattice size L as a function of the magnetic field h, at $\beta = \beta_c$. The rational function in (2) now reads $R_n^{m(L)}(h)$. All in all, we can recap

$$f(z) \to m^{(L)}(h) \qquad R_n^m(z) \to R_n^{m(L)}(h)$$

The dependence on the lattice size L here is crucial. We first of all compute the magnetization $m^{(L)}(h)$ at $\beta = \beta_c$ and various values of external magnetic field h and lattice size L. At each value of L, these results are interpolated by the $R_n^{m(L)}(h)$, which display singularities which are the candidate Lee-Yang zeros $h_0^{(L)}$, *i.e.* the singularity of the rational approximant for the magnetisation which is the closest to the real axis. As a matter of fact, $h_0^{(L)}$ always sits at $\mathrm{Re}(h_0^{(L)}) = 0$, but with an imaginary part $\mathrm{Im}(h_0^{(L)})$ scaling in L as

$$\mathrm{Im}(h_0^{(L)}) \sim L^{\mathcal{D}} \tag{5}$$

$\mathcal{D}$ being a combination of critical exponents of the 2D Ising model reading $\mathcal{D} = \frac{1}{8} - 2$. Fig. 1 displays how our determinations of $\mathrm{Im}(h_0^{(L)})$ indeed turn out to get closer to the real axis as L increases. Notice that a few zeros of the denominator are canceled by corresponding zeros of the numerator. These are not genuine pieces of information: actually their location vary if we vary *e.g.*

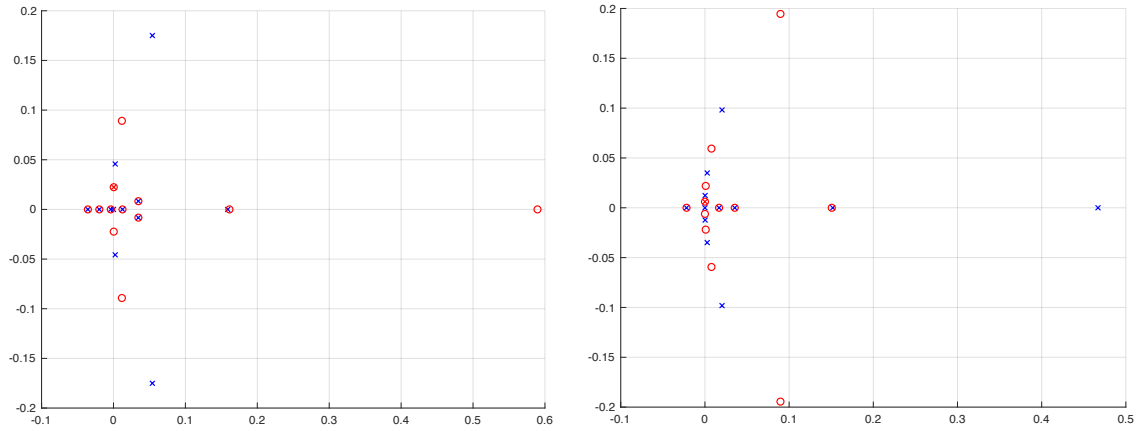

Figure 1: In the left panel we plot as blue crosses the zeros of the numerator of the rational approximant $R_n^{m(L)}(h)$ for the magnetisation on $L = 15$; red circles are the zeros of the denominator. In the right panel we plot the same for $L = 30$. In both cases we highlight the closest singularity to the real axis. Plots are in the complex h plane.

the order of the Padé approximant $[m, n]$. This is a consequence of numerical errors in our data. But the key point is that genuine pieces of information (*i.e.* actual zeros and poles) stay constant to a very good precision. In Fig. 2 we depict the scaling of $\mathrm{Im}(h_0^{(L)})$: to guide the eye, the horizontal axis is $L^{\frac{1}{8}-2}$ (*i.e.* the theoretically expected power of L), but the value we got (1.88) is indeed quite accurate. All in all, the method is working beautifully.

Of course, we were not at all the first to study phase transitions by Fisher/Lee-Yang zeros. For example, our method can be compared to [8]: the good piece of information is that our method is competitive.

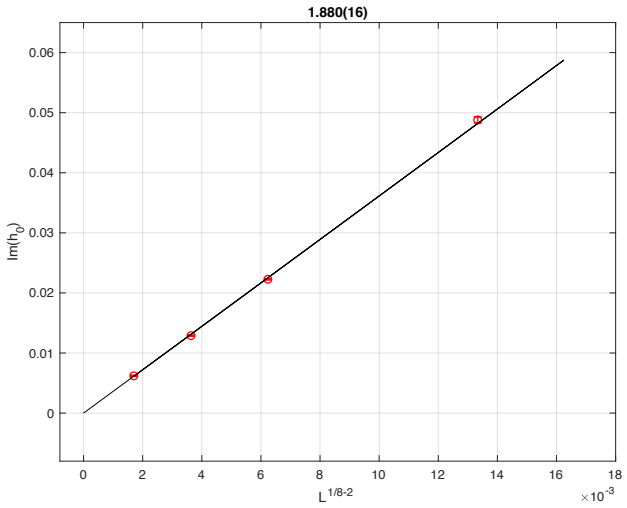

Figure 2: As got from the rational approximants $R_n^{m(L)}(h)$, we plot the finite size scaling of the imaginary part of the singularity which is the closest to the real axis, $\mathrm{Im}(h_0^{(L)})$. As expected, the phase transition appears to take place at $h = 0$.

3. Can we do the same for Lattice QCD?

The obvious question is: can we repeat the procedure for QCD? Now that we have established a dictionary, what to do is pretty simple to describe

$$m^{(L)}(h) \to \chi_1^{B(L)}(\hat{\mu}_B) = \frac{\partial}{\partial \hat{\mu}_B} \frac{\ln Z}{VT^3} \qquad R_n^{m(L)}(h) \to R_n^{m(L)}(\hat{\mu}_B) \tag{6}$$

where we have adopted for the number density the notation is terms of its definition as a susceptibility (χ_1^B). All the measurements are here taken at $T = T_{RW} \sim 200MeV$ on lattices whose sizes are fixed by the spatial volume $(aN_s)^3$ (we adhere to the usual notation of finite temperature QCD for the spatial size, *i.e.* $L = aN_s$, where a is the lattice spacing). We notice that our lattice regularization is a coarse one, given the value $N_T = 4$ for the (inverse) temperature in units of the lattice spacing. As for spatial sizes, these were dictated by our choice $N_s = 12, 16, 20, 24$.

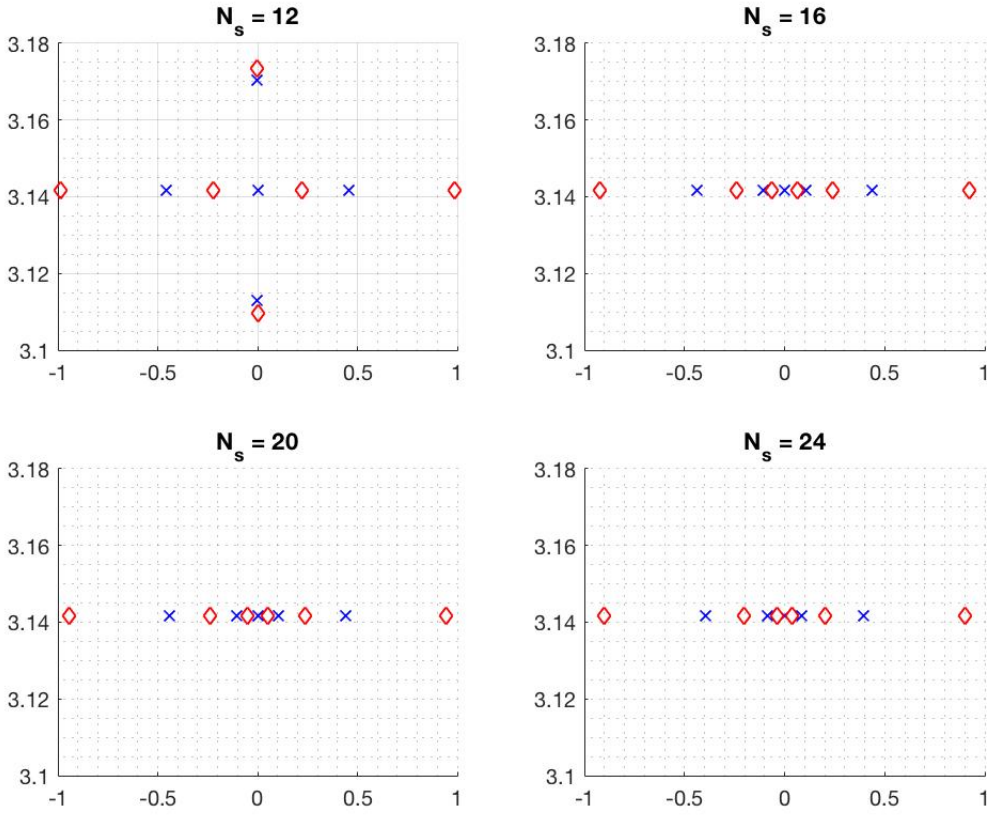

Figure 3: In the complex-$\hat{\mu}_B$ plane, we plot as blue crosses the zeros of the numerator of the rational approximant $R_n^{m(L)}(\hat{\mu}_B)$ for the number density of QCD computed at $T = T_{RW} \sim 200MeV$; red circles are the zeros of the denominator. The various panels are for different values of $L = aN_s$. As expected, the singularities which are the closest to the imaginary axis get closer and closer to the expected Roberge Weiss transition point, *i.e.* $\hat{\mu}_B = i\pi$.

Fig. 3 depicts the singularities which we find for the rational approximation of our observable (the plot is in the complex-$\hat{\mu}_B$ plane). In particular, one can inspect the location of $\mathrm{Re}(\mu_{B0}^{(L)})$, which is the real part of the singularity that at a given value of L has real part that is the closest to zero. Notice that, as for imaginary parts, we always find that they sit at π, that is to say that $\mathrm{Im}(\mu_{B0}^{(L)}) = \pi$. As $L = aN_S$ gets larger and larger, $\mathrm{Re}(\mu_{B0}^{(L)})$ gets closer and closer to zero: this means that the method is doing a good job, at least at a qualitative level. To make all this quantitative, we have (as in the case of the Ising model) to look at the scaling with the lattice size L. Also in this case we should find a power law

$$\mathrm{Re}(\mu_{B0}^{(L)}) \sim L^{\mathcal{D}'} \tag{7}$$

with $\mathcal{D}' = 2.4818\ldots$, once again fixed by a combination of relevant critical exponents. As seen in Fig. 4, our analysis does not work that badly. The power is very close to the exact one, with a reasonable value for the χ^2. Error-bars are quite important (and, by the way, they look quite funny in the figure, due to the log-log plot), and thus we can conclude that, while the picture is making sense, as in the case of the Ising model, we need to refine the statistics and collect more measurements in order to fully trust the procedure as effective.

4. Outlook

We reported on a first attempt at the study of finite size scaling in the study of Lee-Yang zeros in QCD. This is not the only new application of the multi-point Padè method we are developing.

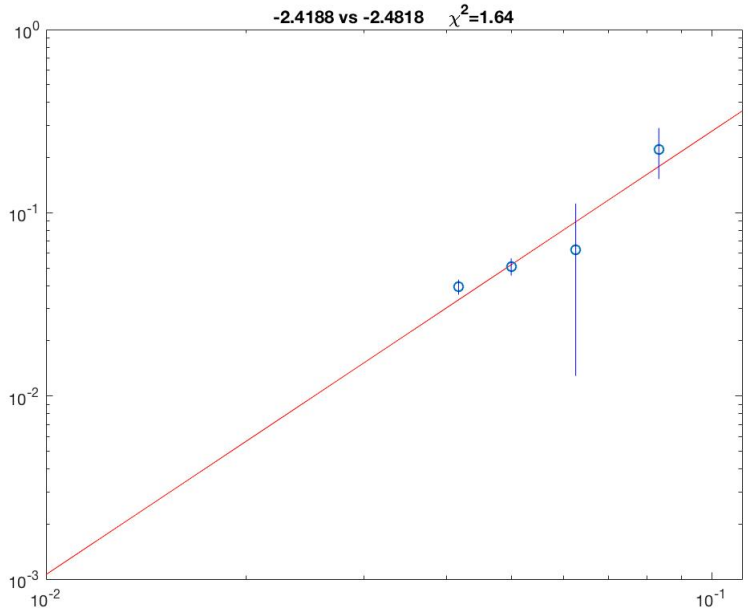

Figure 4: For the rational approximants $R_n^{m(L)}(\hat{\mu}_B)$, we plot the real part of the singularity which is the closest to the imaginary axis, $\mathrm{Re}(\hat{\mu}_{B0})$ (vertical axis) versus $L^{-1} \sim N_S^{-1}$ (horizontal axis). Notice how the error-bars are deformed in the log-log plot. The slope of the (finite size scaling) curve is very close to the expected one (but we are living with quite sizeable errors).

One can actually study rational approximations of the form $R_n^m(T;\hat{\mu}_B)$. Here the notation explicitly accounts for the measurements being taken at different values of the temperature T for fixed values of $\hat{\mu}_B$. The approach is like that of [2], *i.e.* in terms of a single scaling variable, but this time singularities show up in the complex-T plane. While we presented very preliminary results at this year conference, we are looking forward to reporting on a more precise analysis in a not that long time. In a quite near future, we hope we will also be able to confirm preliminary, interesting results showing up in the vicinity of a possible QCD critical endpoint candidate [9].

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