Detecting Lee Yang/Fisher singularities by multi-point Padé

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In collaboration with P. Dimopoulos (Parma), K. Zambello (Pisa), G. Nicotra, C. Schmidt, S. Singh (Bielefeld), J. Goswami (RIKEN), D. Clarke (Utah)

see also talks by C. Schmidt and D. Clarke on Friday
Agenda

– An invitation (multi-point Padè)

– What we have been doing in Lattice QCD

– What we could do for the 2d Ising model: finite size scaling

– Can we do the same for QCD?
An invitation
A few words on multi-point PADÈ

Suppose you know the values of a function (and of its derivatives) at a number of points
\[ \ldots, f(z_k), f'(z_k), \ldots, f^{(s-1)}(z_k), \ldots \quad k = 1 \ldots N \]
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If you want to approximate the function with a rational function
\[
R_m^n(z) = \frac{P_m(z)}{\tilde{Q}_n(z)} = \frac{P_m(z)}{1 + Q_n(z)} = \frac{\sum_{i=0}^m a_i z^i}{1 + \sum_{j=1}^n b_j z^j}
\]
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the obvious requirement is that

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R_m^n(j)(z_k) = f^{(j)}(z_k) \quad k = 1 \ldots N, \quad j = 0 \ldots s - 1
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This is the starting point for a multi-point Padé approximation: solve the linear system

\[
\ldots
\]

\[
P_m(z_k) - f(z_k)Q_n(z_k) = f(z_k)
P'_m(z_k) - f'(z_k)Q_n(z_k) - f(z_k)Q'_n(z_k) = f'(z_k)
\]

\[
\ldots
\]

from which we want to get the unknown

\[
\{ a_i \mid i = 0 \ldots m \} \quad \{ b_j \mid j = 1 \ldots n \} \quad n + m + 1 = N s
\]
A few words on multi-point PADÈ

In principle you should require that \( \exists z_0 : P_m(z_0) = \tilde{Q}_n(z_0) = 0 \)

… but we will need to give up with this …
A few words on multi-point PADÈ

In principle you should require that \[ \forall z_0 : P_m(z_0) = \tilde{Q}_n(z_0) = 0 \]

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**Why a rational approximation instead of a polynomial?** Because you have POLES that can mimic the SINGULARITIES of your function! (at least the nearest ones ...)
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Any useful …?
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Yes! LATTICE QCD at IMAGINARY values of the baryonic chemical potential

Contribution to understanding the phase structure of strong interaction matter: Lee-Yang edge singularities from lattice QCD

P. Dimopoulos,1 L. Dini,2 F. Di Renzo,1 J. Goswami,2 G. Nicotra,2 C. Schmidt,2 S. Singh,1,3 K. Zambello,1 and F. Ziesche2

... where we computed and “multi-point Padè approximated”

\[
\chi_n^B(T, V, \mu_B) = \left( \frac{\partial}{\partial \hat{\mu}_B} \right)^n \frac{\ln Z(T, V, \mu_l, \mu_s)}{VT^3}
= \left( \frac{1}{3} \frac{\partial}{\partial \hat{\mu}_l} + \frac{1}{3} \frac{\partial}{\partial \hat{\mu}_s} \right)^n \frac{\ln Z(T, V, \mu_l, \mu_s)}{VT^3}
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In principle you should require that
\[ \# z_0 : P_m(z_0) = \tilde{Q}_n(z_0) = 0 \]
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**Why a rational approximation instead of a polynomial?** Because you have POLES that can mimic the SINGULARITIES of your function! (at least the nearest ones ...)}

**Any useful ...?**

Yes! LATTICE QCD at IMAGINARY values of the baryonic chemical potential
... a natural analytic continuation to real chemical potential!
... and not only that: singularities!

... where we computed and “multi-point Padè approximated”
\[ \chi_n^B(T, V, \mu_B) = \left( \frac{\partial}{\partial \mu_B} \right)^n \frac{\ln Z(T, V, \mu_l, \mu_s)}{V T^3} \]
\[ = \left( \frac{1}{3} \frac{\partial}{\partial \mu_l} + \frac{1}{3} \frac{\partial}{\partial \mu_s} \right)^n \frac{\ln Z(T, V, \mu_l, \mu_s)}{V T^3} \]
We present a calculation of the net baryon number density as a function of imaginary baryon number chemical potential, obtained with highly improved staggered quarks at temporal lattice extent of $N_T = 4, 6$. We construct various rational function approximations of the lattice data and discuss how poles in the complex plane can be determined from them. We compare our results of the singularities in the chemical potential plane to the theoretically expected positions of the Lee-Yang edge singularity in the vicinity of the Roberge-Weiss and chiral phase transitions. We find a temperature scaling that is in accordance with the expected power law behavior.

FIG. 5. Singularity structure in the $\hat{\mu}_B$ plane for three different temperatures (from left to right $T = 201.4, 186.3, 167.4$). Upper row: Ansatz (15); lower row: Ansatz (20).
We present a calculation of the net baryon number density as a function of imaginary baryon number chemical potential, obtained with highly improved staggered quarks at temporal lattice extent of $N_\tau = 4, 6$. We construct various rational function approximations of the lattice data and discuss how poles in the complex plane can be determined from them. We compare our results of the singularities in the chemical potential plane to the theoretically expected positions of the Lee-Yang edge singularity in the vicinity of the Roberge-Weiss and chiral phase transitions. We find a temperature scaling that is in accordance with the expected power law behavior.

![Graph showing singularity structure in the $\hat{\mu}_B$ plane for three different temperatures](image)

**FIG. 5.** Singularity structure in the $\hat{\mu}_B$ plane for three different temperatures (from left to right $T = 201.4, 186.3, 167.4$). Upper row: Ansatz (15); lower row: Ansatz (20).

![Scaling fit to the Lee-Yang edge singularities in the vicinity of the Roberge-Weiss transition](image)

**FIG. 9.** Scaling fit to the Lee-Yang edge singularities in the vicinity of the Roberge-Weiss transition to the Ansatz (22). Shown are three distinct data sets for the real parts of the $\hat{\mu}_B$ (imaginary parts of $h$) as a function of the reduced temperature $(T_{RW} - T)/T_{RW}$, as obtained from methods I–III.
Can we do *better* than this ?!?  

As reported at Lattice 2022, we tested our approach on the 2D ISING model
Let’s compare to a beautiful paper...

**ISING model**

\[ U(\sigma) = -J \sum_{\{i,j\}} \sigma_i \sigma_j - h \sum_i \sigma_i \]

\[ Z(\beta, h) = Z(0, h)e^{\beta c} \prod_k (1 - \beta / \beta_k) \]

\[ \langle U^n \rangle = (-1)^{n-1} \sum_k \frac{(n - 1)!}{(\beta_k - \beta)^n}, \quad n > 1 \]

Scaling relations are supposed to describe the approach of leading zeros to critical inverse temperature.

Dealing instead with leading zeros from magnetisation cumulants (now derive with respect to magnetic field)
The same scaling plots obtained with our multi-point PADÈ method

Real and imaginary parts of the leading (Fisher) zero as a function of (inverse) lattice size
(from the computation of specific heat at different temperatures and lattice sizes)
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Real and imaginary parts of the leading (Fisher) zero as a function of (inverse) lattice size
(from the computation of specific heat at different temperatures and lattice sizes)

Real and imaginary parts of the leading (Lee Yang) zero as a function of (inverse) lattice size
(from the computation of magnetisation at different magnetic fields and lattice sizes, sitting at $\beta_c$)
The same scaling plots obtained with our multi-point Pade method:

Real and imaginary parts of the leading (Fisher) zero as a function of (inverse) lattice size
(from the computation of specific heat at different temperatures and lattice sizes)

Real and imaginary parts of the leading (Lee Yang) zero as a function of (inverse) lattice size
(from the computation of magnetisation at different magnetic fields and lattice sizes, sitting at $\beta_c$)

Please notice: here we are following the right order! (i.e. we first get the critical temperature)
Let us focus on the second plot (i.e. we look at $m$ as a function of $h$, sitting at the critical temperature)

We compute magnetisation at different magnetic fields and lattice sizes and obtain Padè approximants

i.e.

$$ f(z) \mapsto m^{(L)}(h) \quad R_m^n(z) \mapsto R_m^n(L)(h) $$
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We compute magnetisation at different magnetic fields and lattice sizes and obtain Padè approximants i.e.

$$f(z) \mapsto m^{(L)}(h) \quad R_m^n(z) \mapsto R_m^n(L)(h)$$

We determine the leading pole (red circle) from the Padè approximants (figures are in complex $h$ plane)
Let us focus on the second plot (i.e. we look at $m$ as a function of $h$, sitting at the critical temperature).

And finally we inspect the scaling of leading poles (red circles) (figure again in complex $h$ plane)

$$h_0 \sim L^{-\frac{\beta\delta}{\nu}}$$

We compute magnetisation at different magnetic fields and lattice sizes and obtain Padè approximants i.e.

$$f(z) \mapsto m^{(L)}(h) \quad R_m^L(z) \mapsto R_m^{n(L)}(h)$$

We determine the leading pole (red circle) from the Padè approximants

Combination of the relevant critical exponents got to a few per mille
Can we repeat this for (Lattice) QCD?
We now move to the setting of QCD with baryonic chemical potential

\[ \hat{\mu}_B = \frac{\mu_B}{T} \]

\[ m^{(L)}(h) \rightarrow \chi^{B(L)}_1(\hat{\mu}_B) = \frac{\partial}{\partial \hat{\mu}_B} \ln Z \]

which we probe at \( T \sim 200 \text{ MeV} \) on a coarse lattice \( N_\tau = 4 \) with \( N_\sigma = L = 12, 16, 20, 24 \)
at imaginary baryonic chemical potential, looking for the Roberge Weiss transition.

\[ \hat{\mu}_{B \text{ cr}} = i\pi \]

and we have to look for the scaling of \( \hat{\mu}_B^R \)
We compute number density at different values of imaginary chemical potential and lattice size and obtain Padè approximants i.e.
\[ f(z) \mapsto \chi_1^B(L)(\hat{\mu}_B) \quad R_m^n(z) \mapsto R_m^n(L)(\hat{\mu}_B) \]
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We compute number density at different values of imaginary chemical potential and lattice size and obtain Padè approximants i.e.

\[ f(z) \mapsto \chi_1^{B(L)}(\hat{\mu}_B) \quad R_m^*(z) \mapsto R_m^{n(L)}(\hat{\mu}_B) \]

We determine the leading pole (red symbol) from the Padè approximants

And finally we inspect the scaling of leading poles (red circles)

(figure again in complex chem.pot. plane)

As for the combination of the relevant critical exponents we get 2.4188 vs 2.4818
You have to cheat honestly (C. Michael, private communication)
You have to cheat honestly (C. Michael, private communication)

We need to enlarge our statistics …
Something still preliminary...

(Also, again,) in view of inspecting finite size scaling, we can play the other game

\[ f(z; \cdot) \mapsto \chi_1^{B(L)}(T; \mu_B/T) \quad R_m^n(z; \cdot) \mapsto R_m^{n(L)}(T; \mu_B/T) \]
(Also, again,) in view of inspecting finite size scaling, we can play the other game

\[ f(z; -) \leftrightarrow \chi_1^B(L; \mu_B/T) \quad R_m^n(z; -) \leftrightarrow R_m^n(L; \mu_B/T) \]

Beware! Here we are *moving* in complex T plane, at different values of the imaginary chemical potential, but (at the moment) only one value (L=24) of lattice size…
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\[ f(z; -) \leftrightarrow \chi_1^{B}^{(L)}(T; \mu_B/T) \quad R_m^n(z; -) \leftrightarrow R_m^n(L)(T; \mu_B/T) \]

Beware! Here we are moving in complex T plane, at different values of the imaginary chemical potential, but (at the moment) only one value (L=24) of lattice size...

... making sense ...
CONCLUSIONS

1. The program of (multi-point) Padè analysis in the complex baryonic chemical potential plane could provide interesting informations on Lee Yang edge singularities in QCD. RW seems solid (TALK BY Christian Schmidt on Fri); we are trying to better understand other transitions… The Holy Grail (needless to say) is the critical point… **MORE ON THIS IN THE TALK BY DAVID CLARKE (Fri)!**

2. Having gained more confidence in the method (from Ising 2d) we now think we can inspect finite size scaling (also) in LQCD.

3. There is much to do for Padé analysis in the complex temperature plane. Results started making sense…