Detecting Lee Yang/Fisher singularities by multi-point Padé

Francesco Di Renzo (University of Parma and INFN)

LATTICE 2023

Fermilab, 07/31/2023

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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

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

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If you want to approximate the function with a rational function

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

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This is the starting point for a ***multi-point Padè 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

$$\{a_i\,|\,i = 0\ldots m\} \quad \{b_j\,|\,j = 1\ldots n\} \qquad n + m + 1 = N\,s$$

A few words on multi-point PADÈ

In principle you should require that $\nexists\, z_0 \;:\; P_m(z_0) = \tilde{Q}_n(z_0) = 0$

… but we will need to give up with this …

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Yes! LATTICE QCD at IMAGINARY values of the baryonic chemical potential

PHYSICAL REVIEW D **105,** 034513 (2022)

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,*] K. Zambello,[1] and F. Ziesché[2]

… where we computed and "multi-point Padè approximated"

$$\chi_n^B(T,V,\mu_B) = \left(\frac{\partial}{\partial\hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$
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… a natural analytic continuation to real chemical potential!

… and not only that: singularities!

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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.

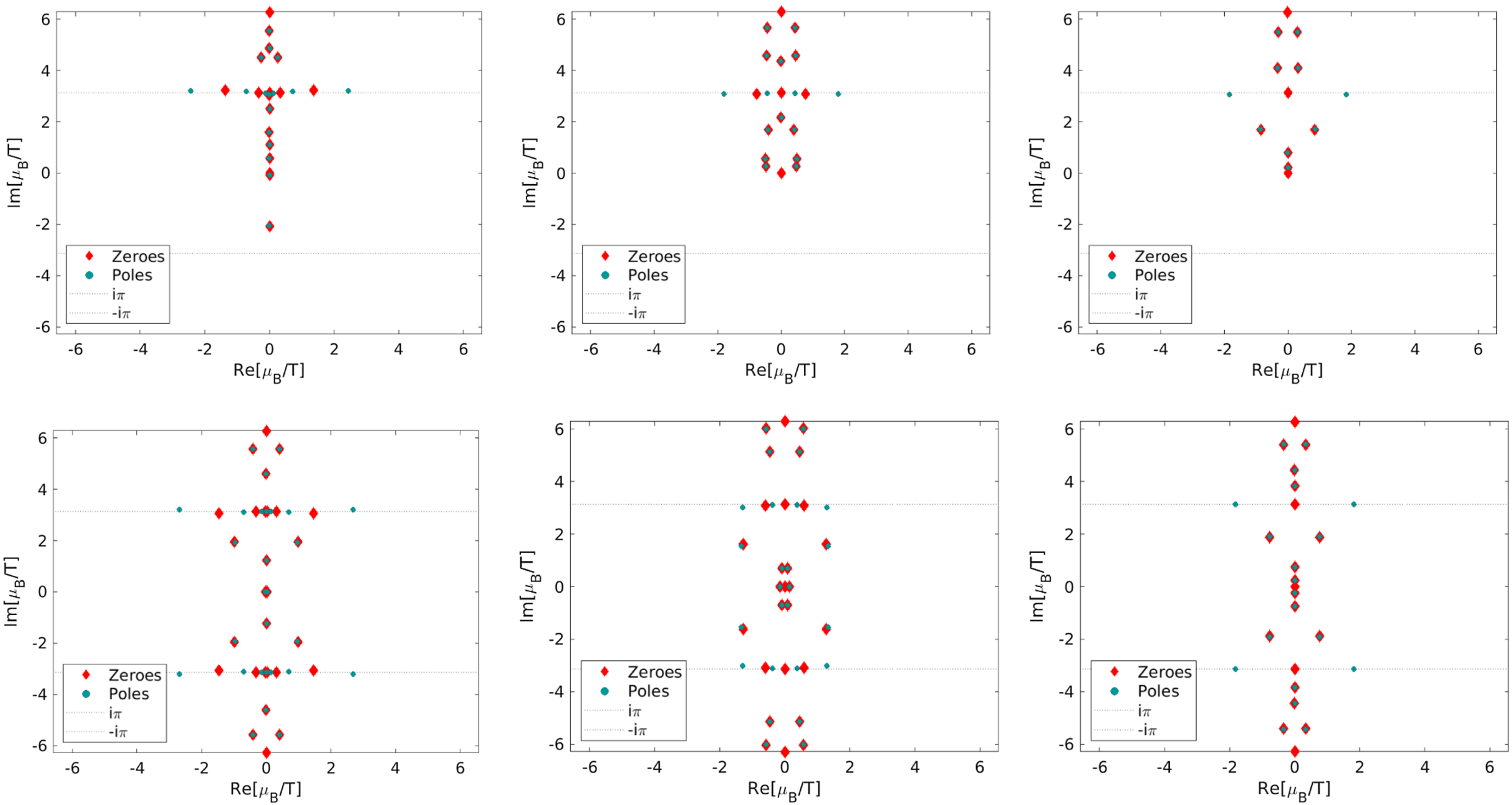

FIG. 5. Singularity structure in the $\hat{\mu}_B$ plane for three different temperatures (from left to right $T = 201.4, 186.3, 167.4$). Upper row: *Ansatz* (15); lower row: *Ansatz* (20).

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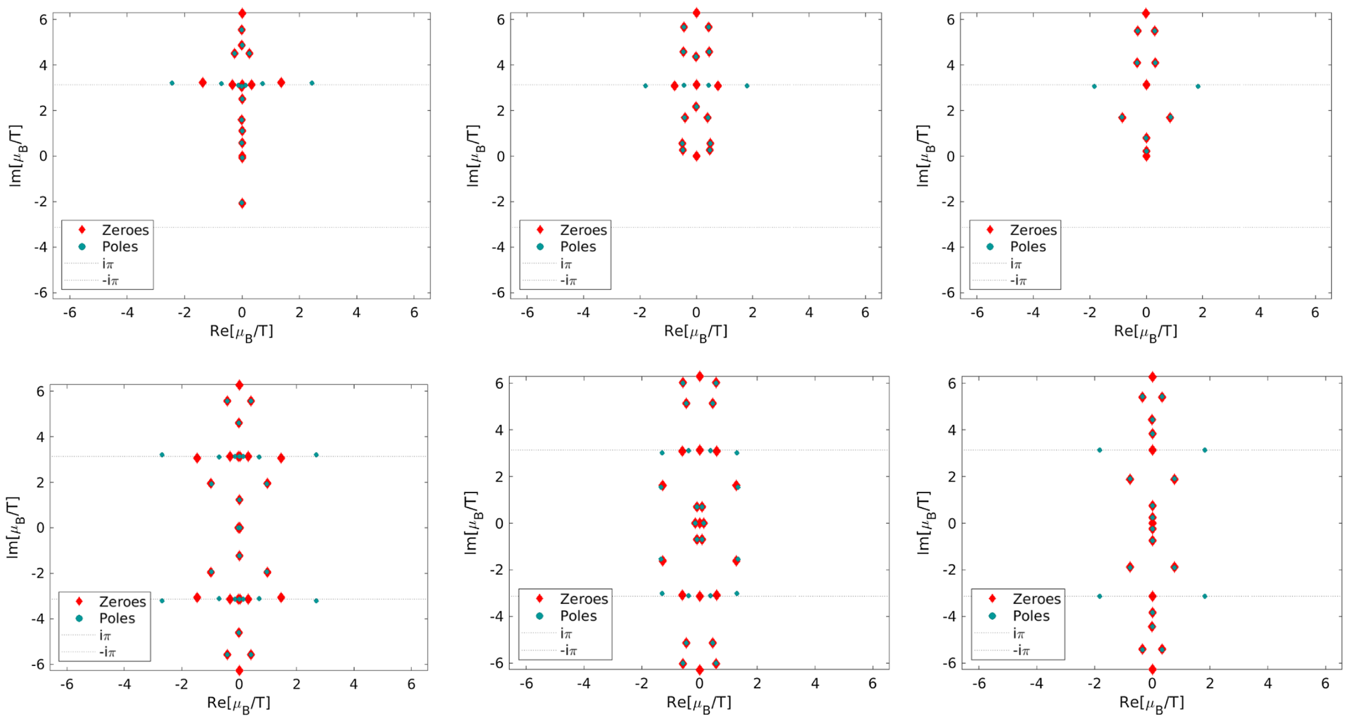

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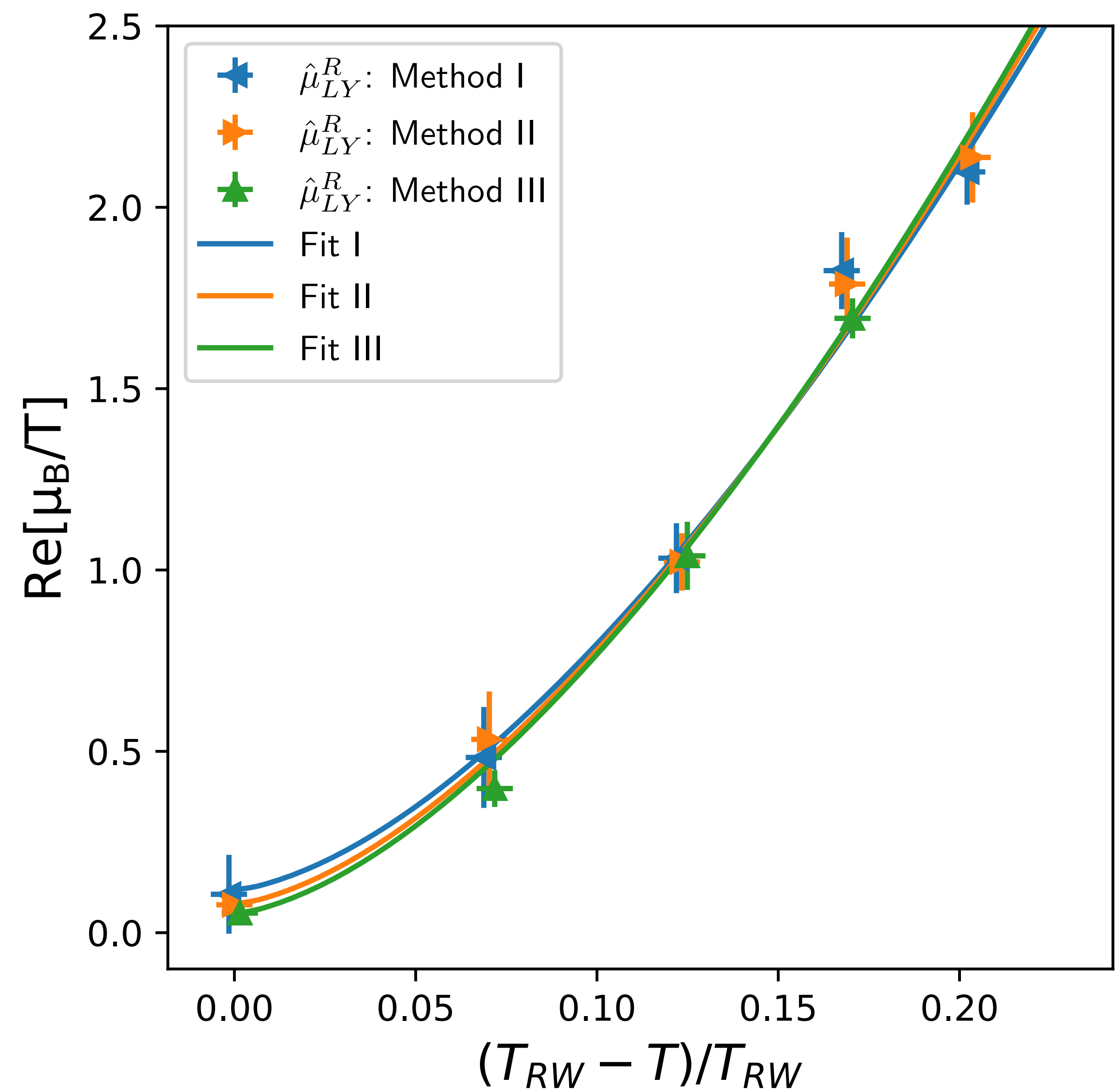


FIG. 9. Scaling fit to the Lee-Yang edge singularities in the vicinity of the Roberge-Weiss transition to the *Ansatz* (22). Shown are three distinct data sets for the real parts of the $\hat{\mu}_B$ (imaginary parts of h) as a function of the reduced temperature $(T_{\rm RW} - T)/T_{\rm RW}$, as obtained 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…

PHYSICAL REVIEW RESEARCH **1**, 023004 (2019)

Determination of universal critical exponents using Lee-Yang theory

Aydin Deger and Christian Flindt
Department of Applied Physics, Aalto University, 00076 Aalto, Finland

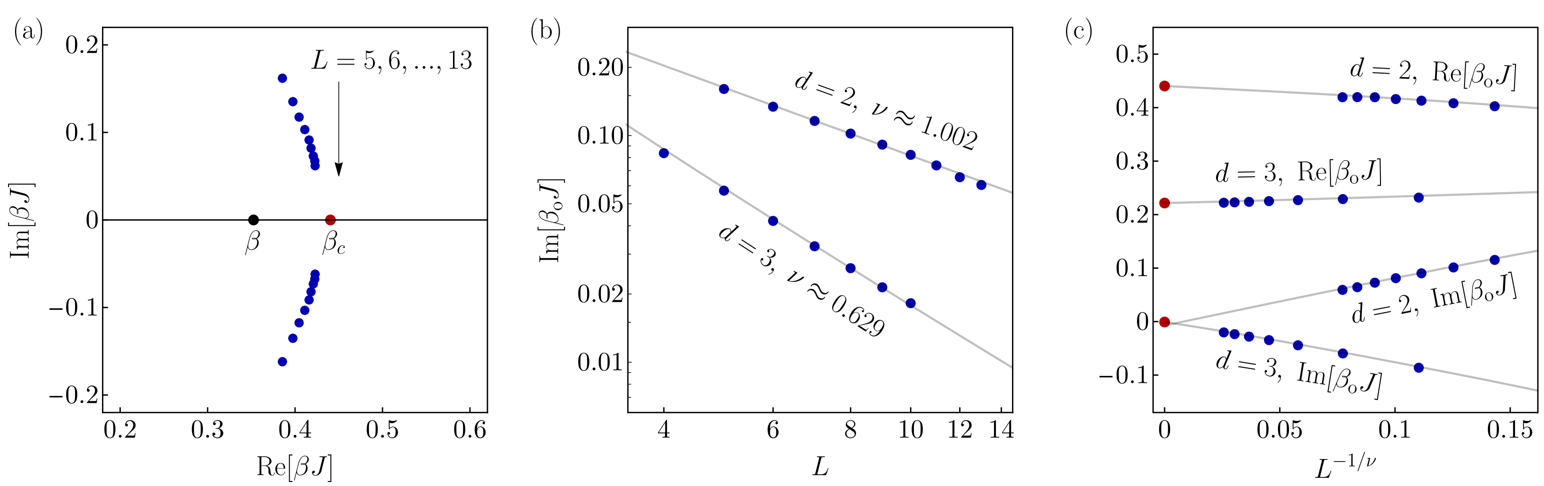
ISING model $U(\boldsymbol{\sigma}) = -J \sum_{\langle i,j\rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$

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

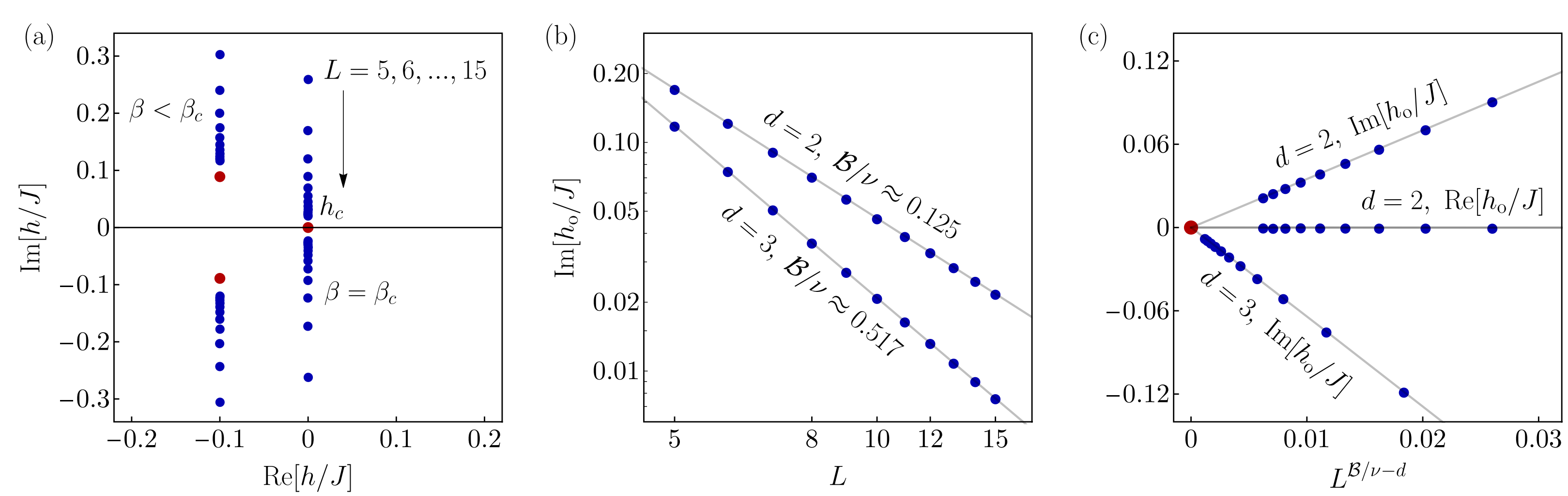
$$\langle\langle U^n \rangle\rangle = (-1)^{(n-1)} \sum_k \frac{(n-1)!}{(\beta_k - \beta)^n}, \quad n > 1$$

Zeros of the partition function determined via computations of cumulants (derivatives of *log(Z)* with respect to inverse temperature)

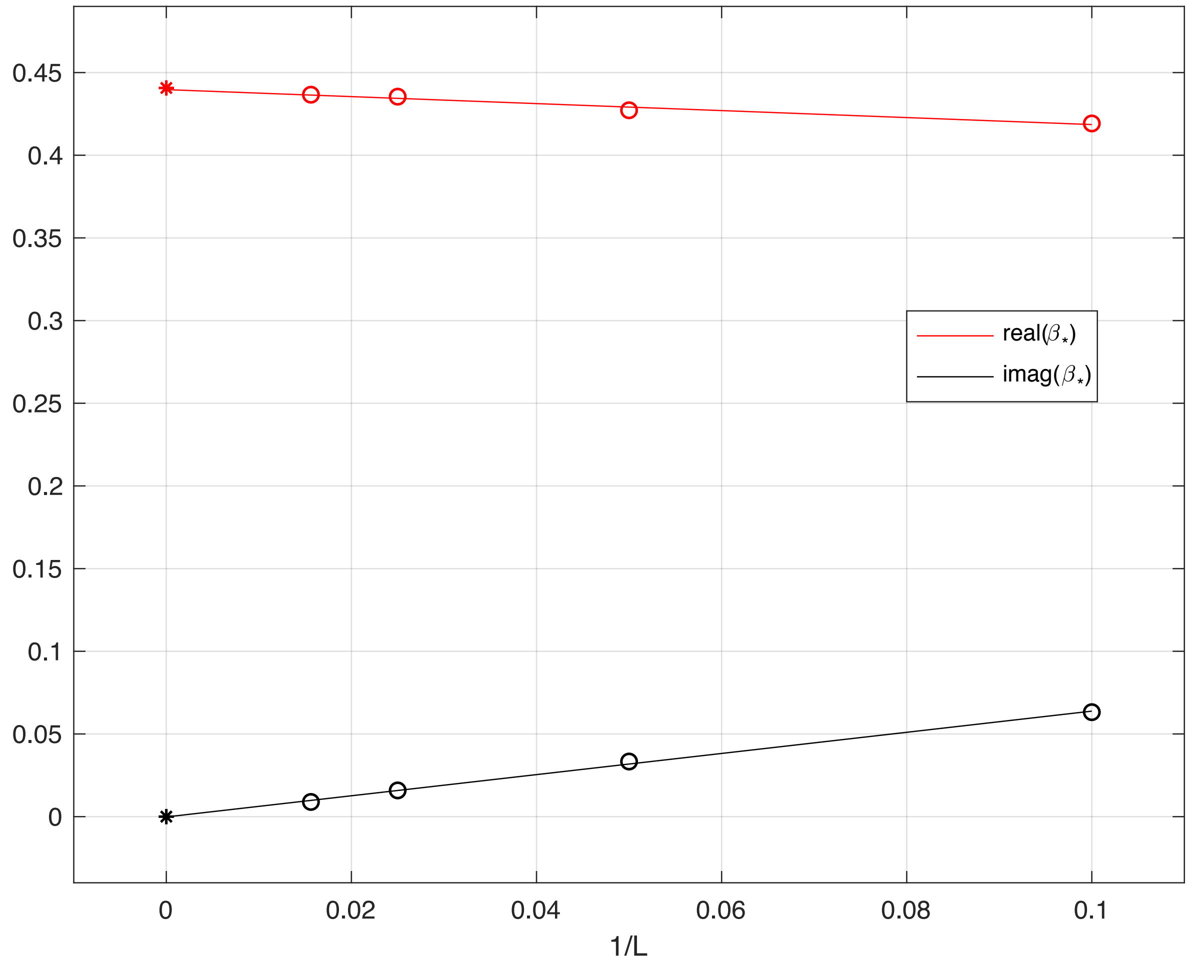
Scaling relations are supposed to describe the approach of leading zeros to critical inverse temperature.



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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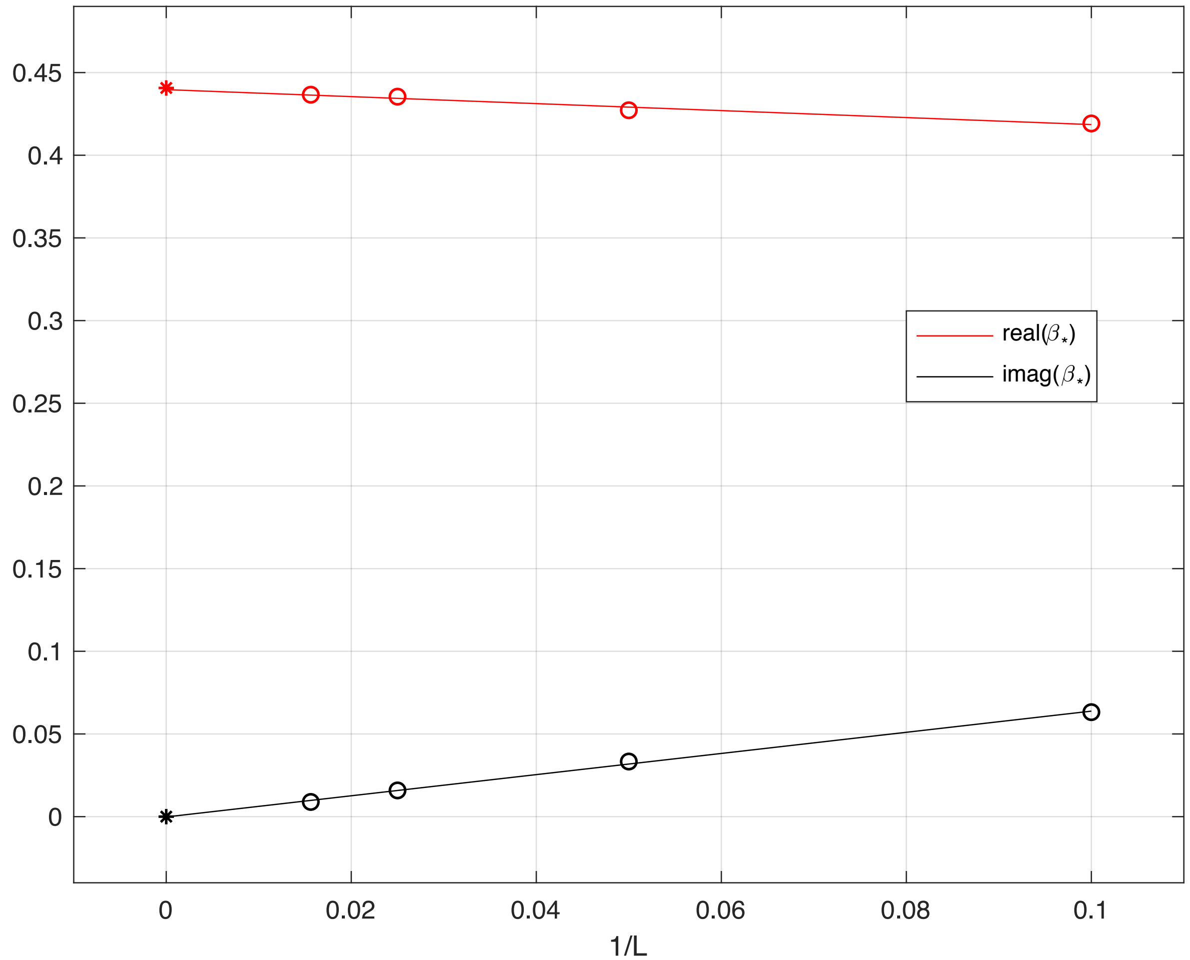

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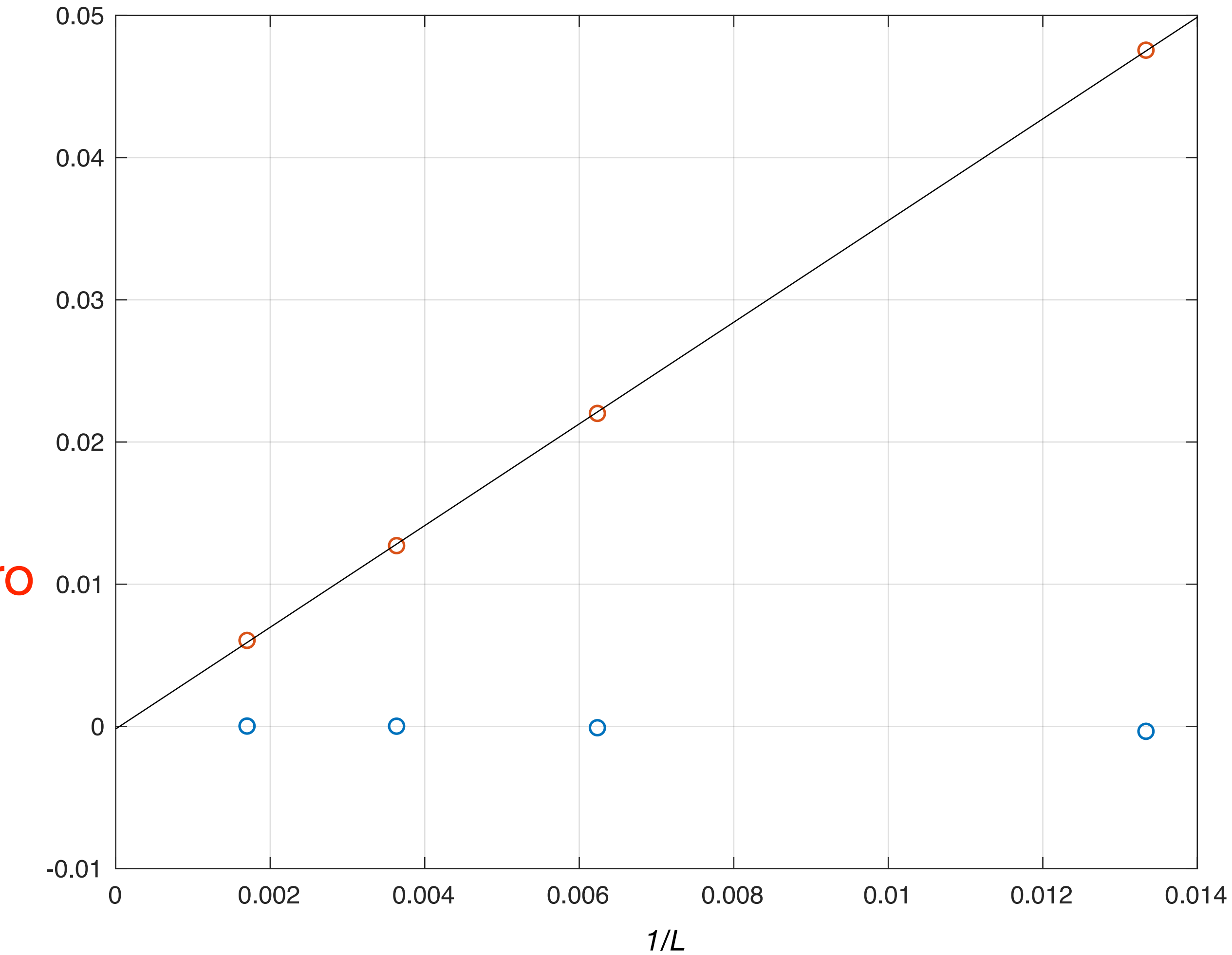

Real and imaginary parts of the leading (Lee Yang) zero as a function of (inverse) lattice size

(*from the computation of magnetisation at different magnetic fields and lattice sizes, sitting at* β_c)

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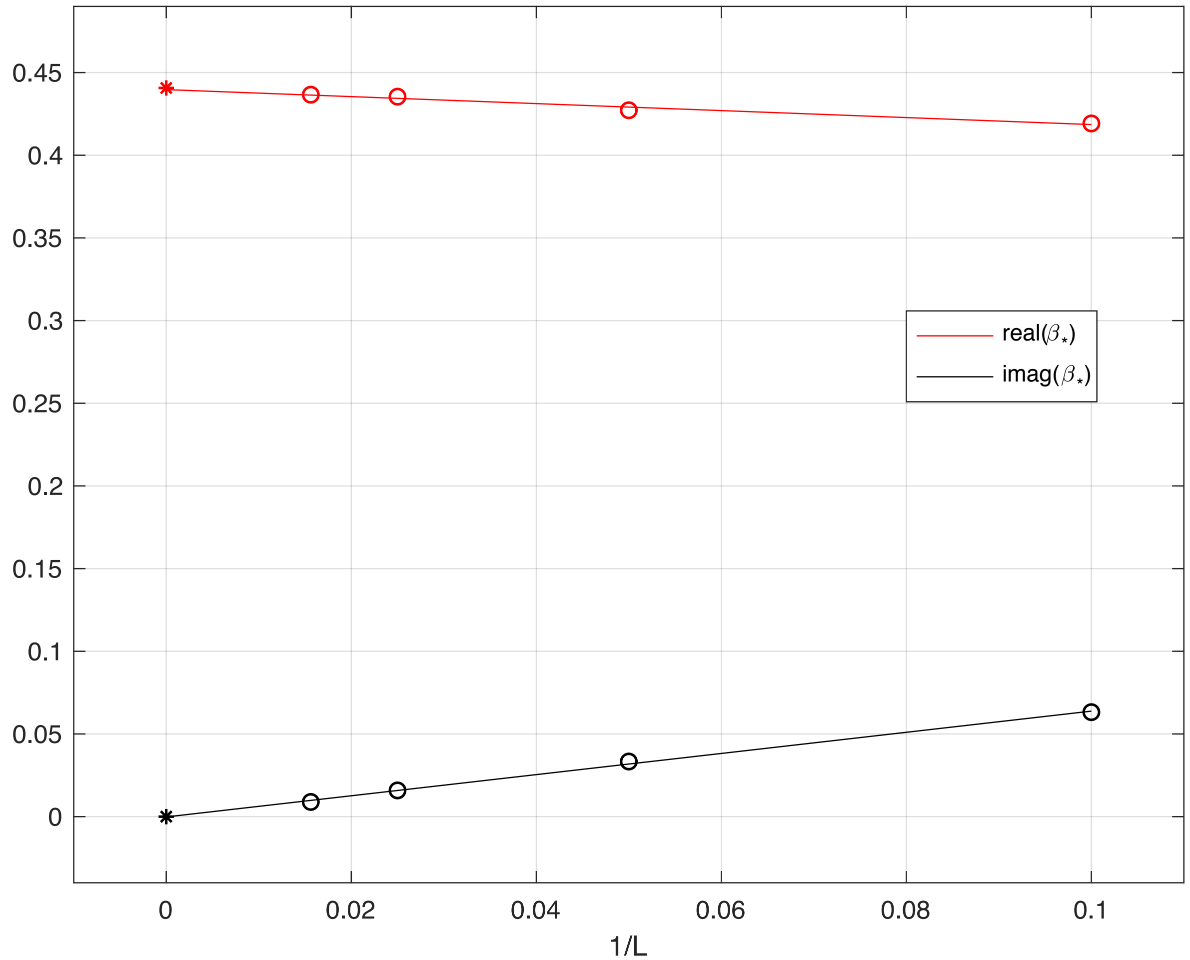

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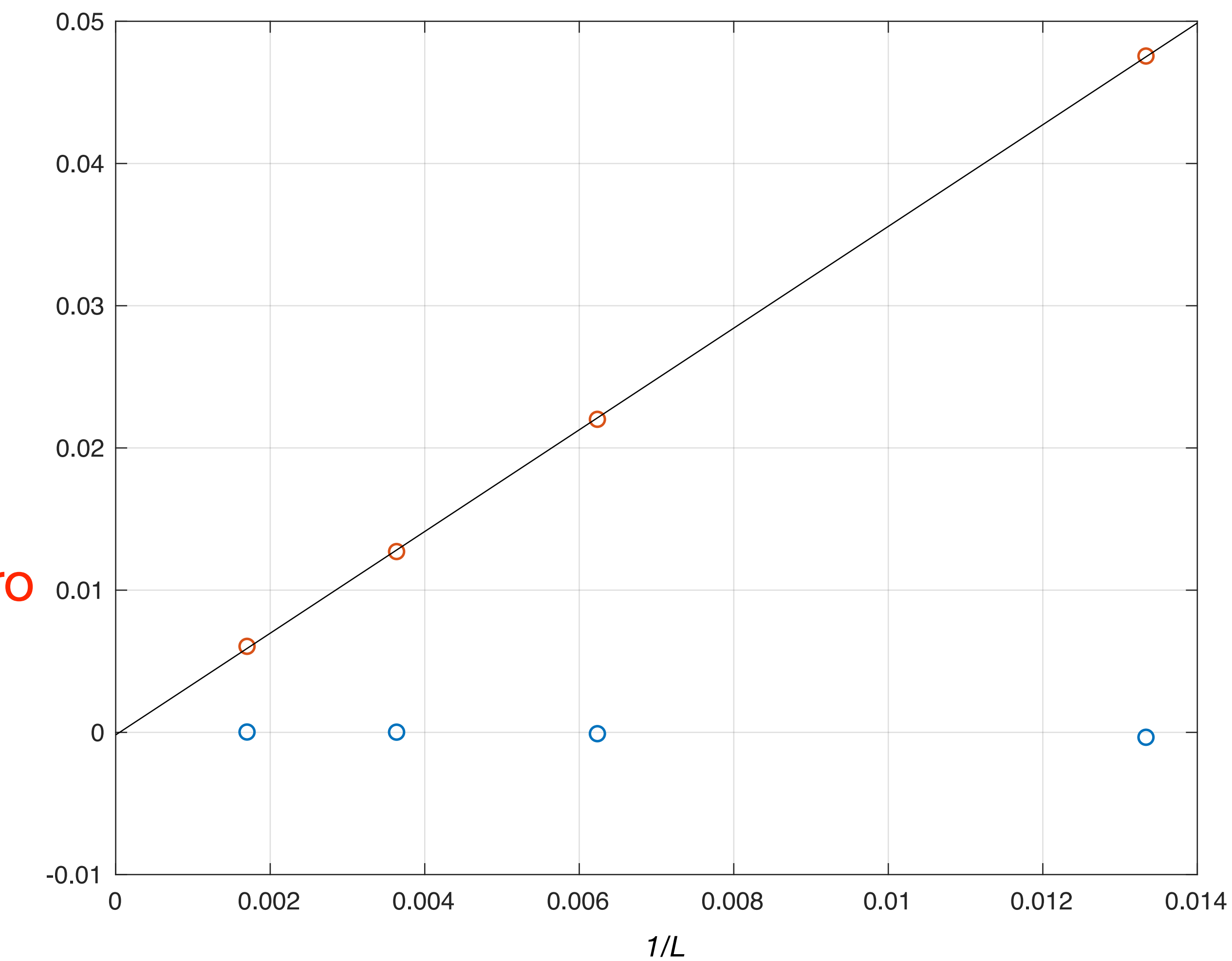

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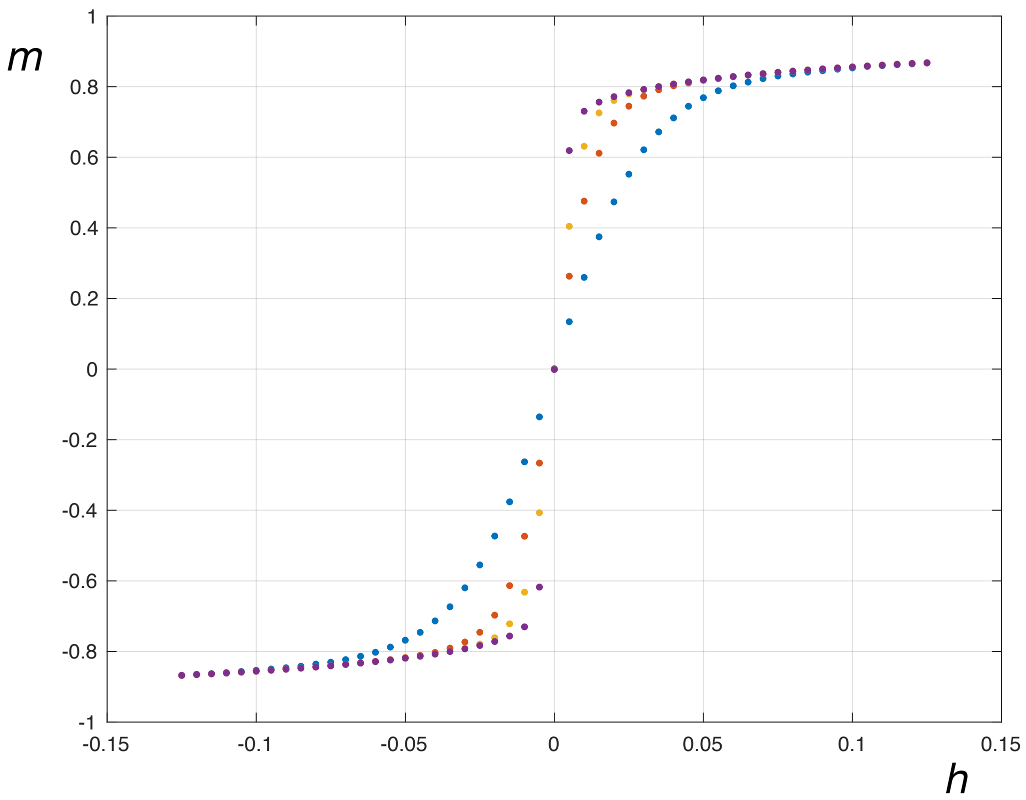
Please notice: here we are following the right order! (i.e. we first get the critical temperature)

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.

$$f(z) \mapsto m^{(L)}(h) \qquad R^n_m(z) \mapsto R^{n\,(L)}_m(h)$$

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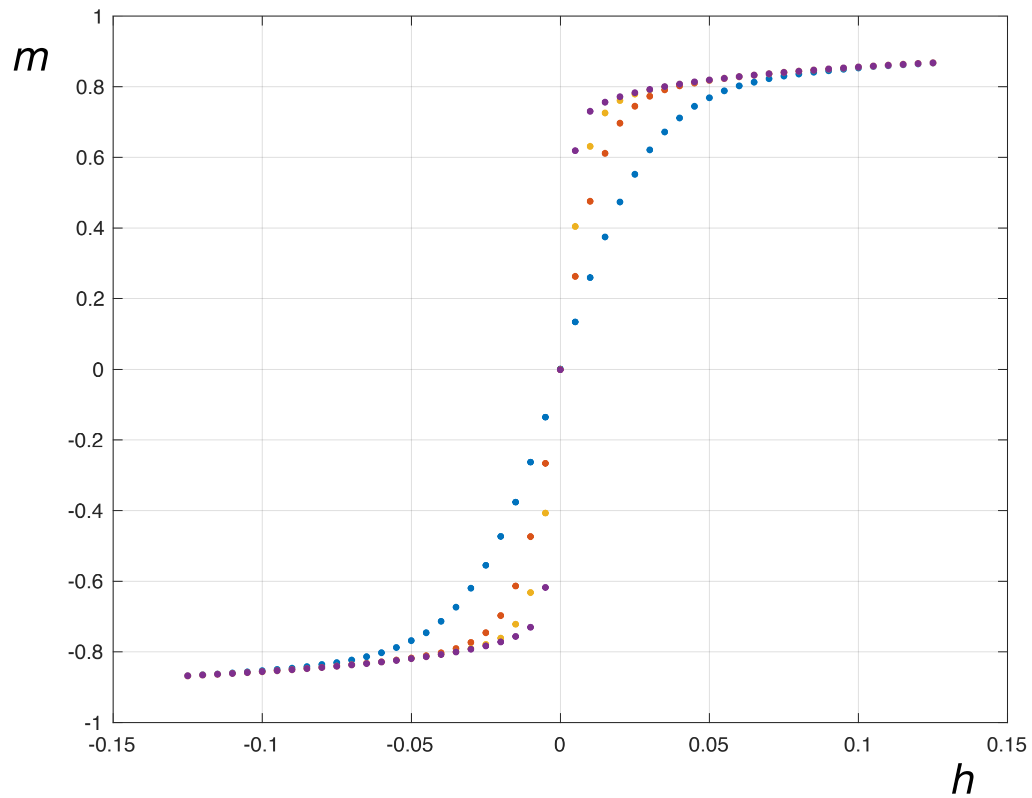

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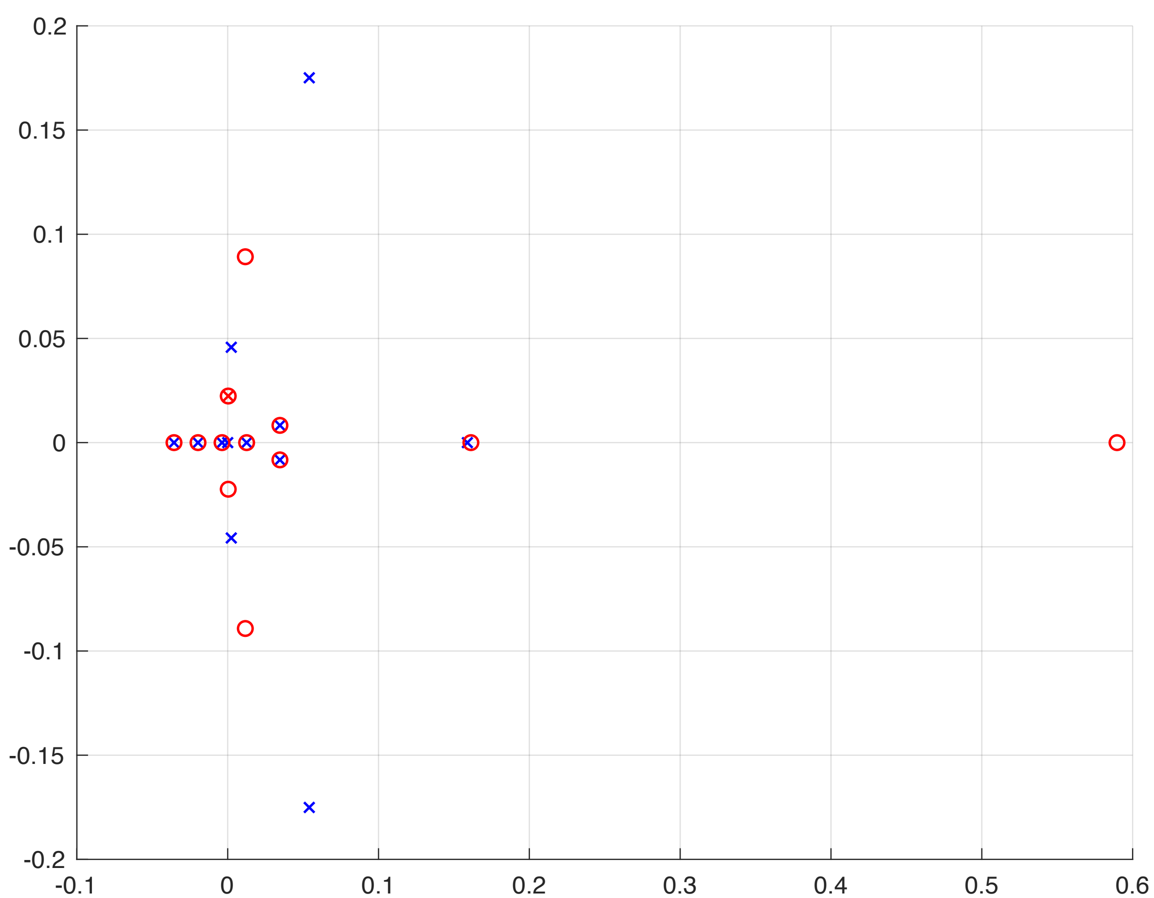
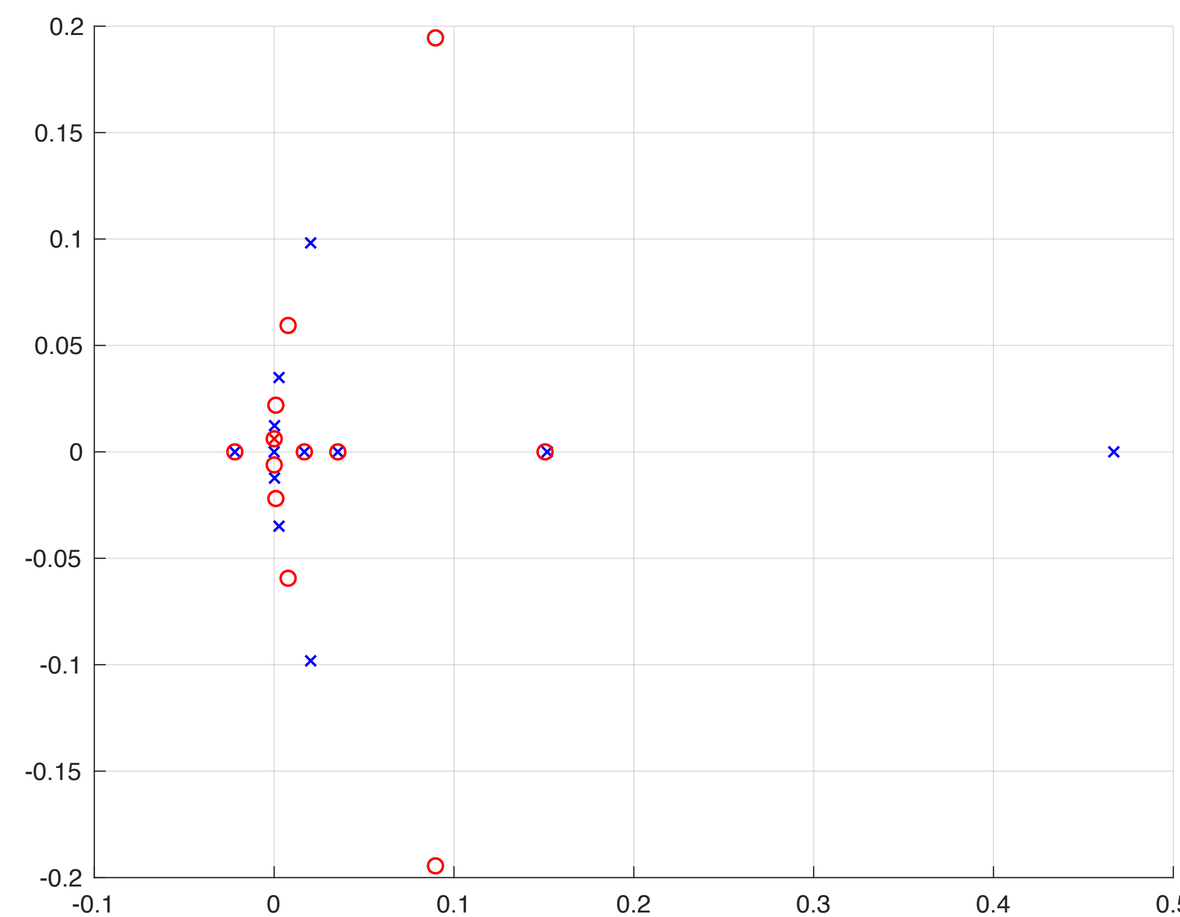
We determine the leading pole (red circle)
from the Padè approximants

(figures are in complex *h* plane)





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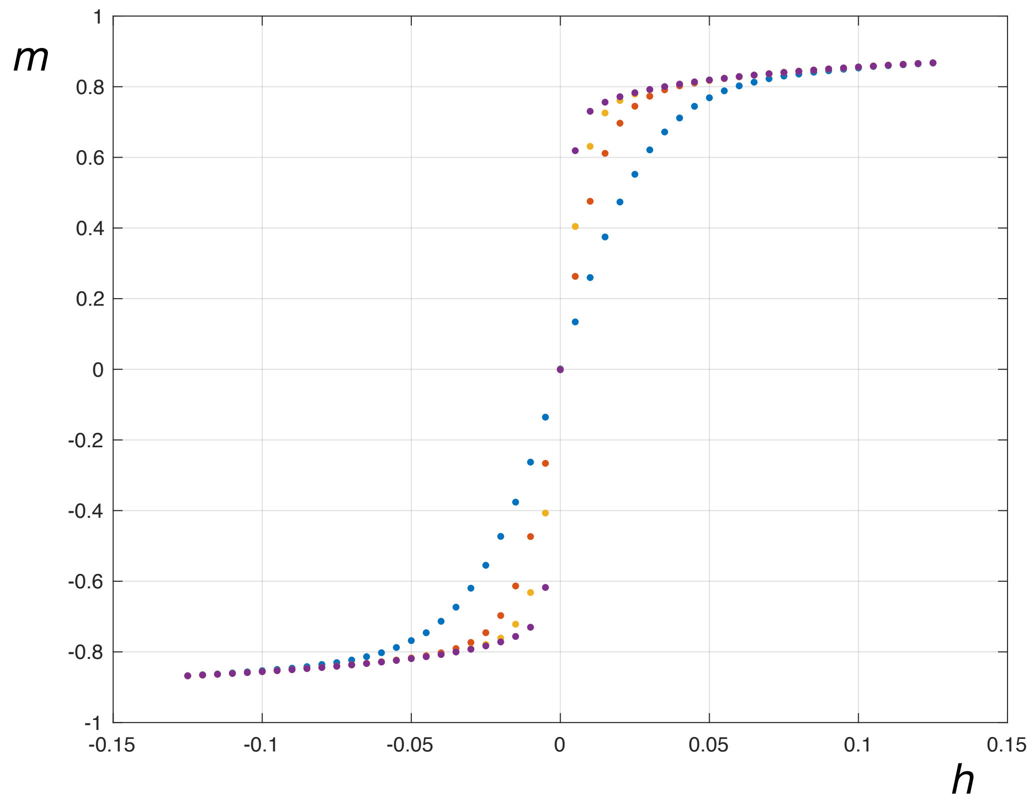

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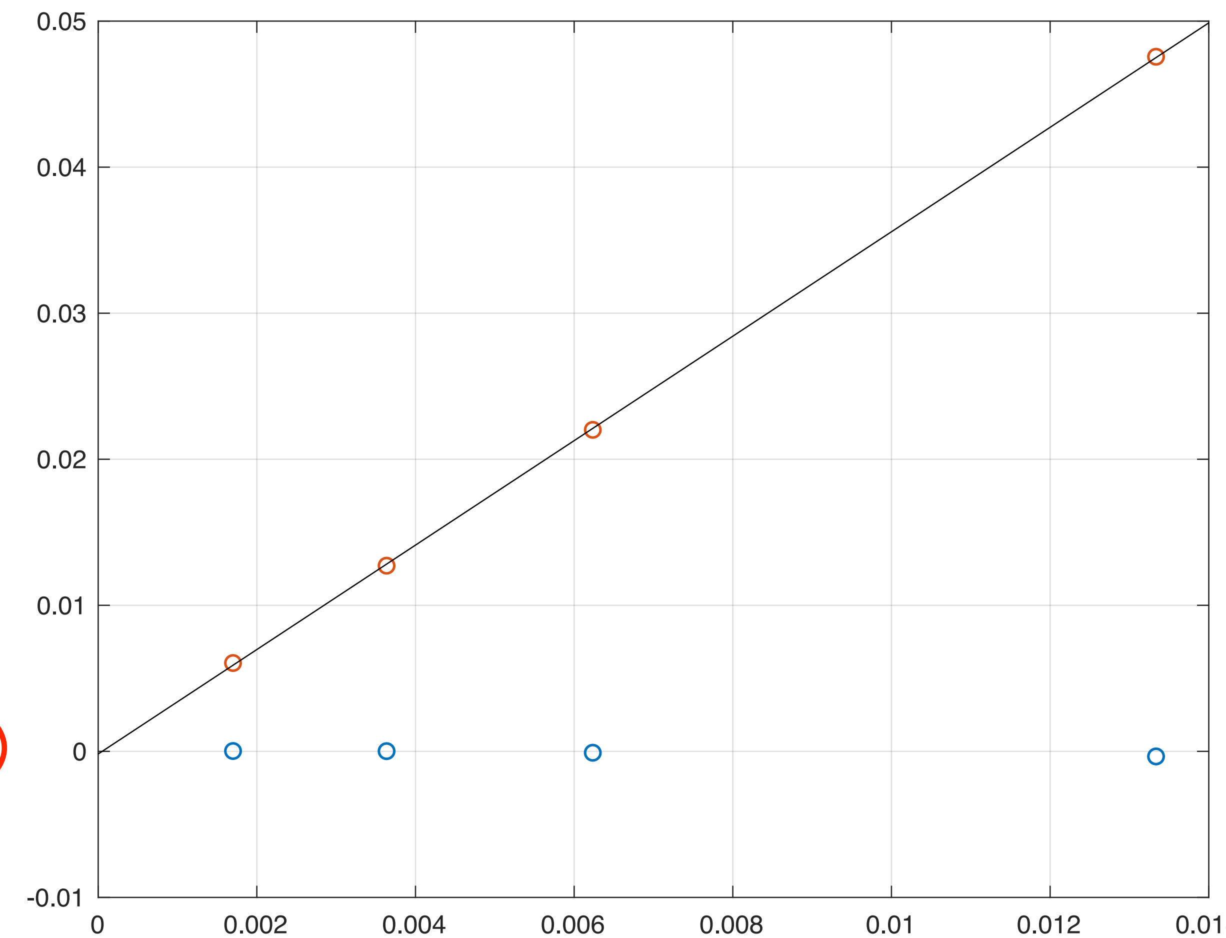
And finally we inspect the scaling of
leading poles (red circles)

(figure again in complex h plane)

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



Combination of the relevant critical exponents
got to a few per mille

Can we repeat this
for (Lattice) QCD?

Who is who …

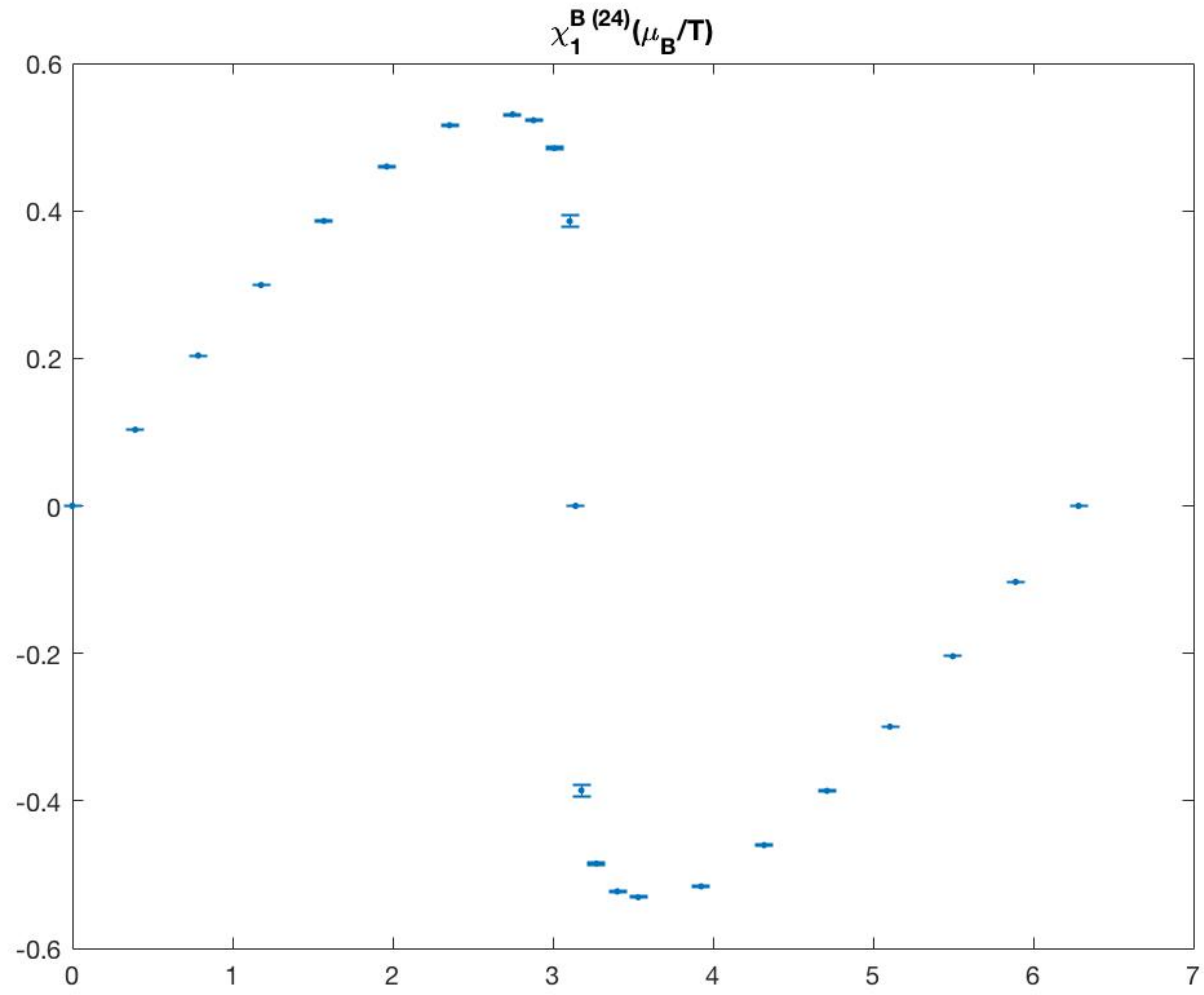
We now move to the setting of QCD with baryonic chemical potential

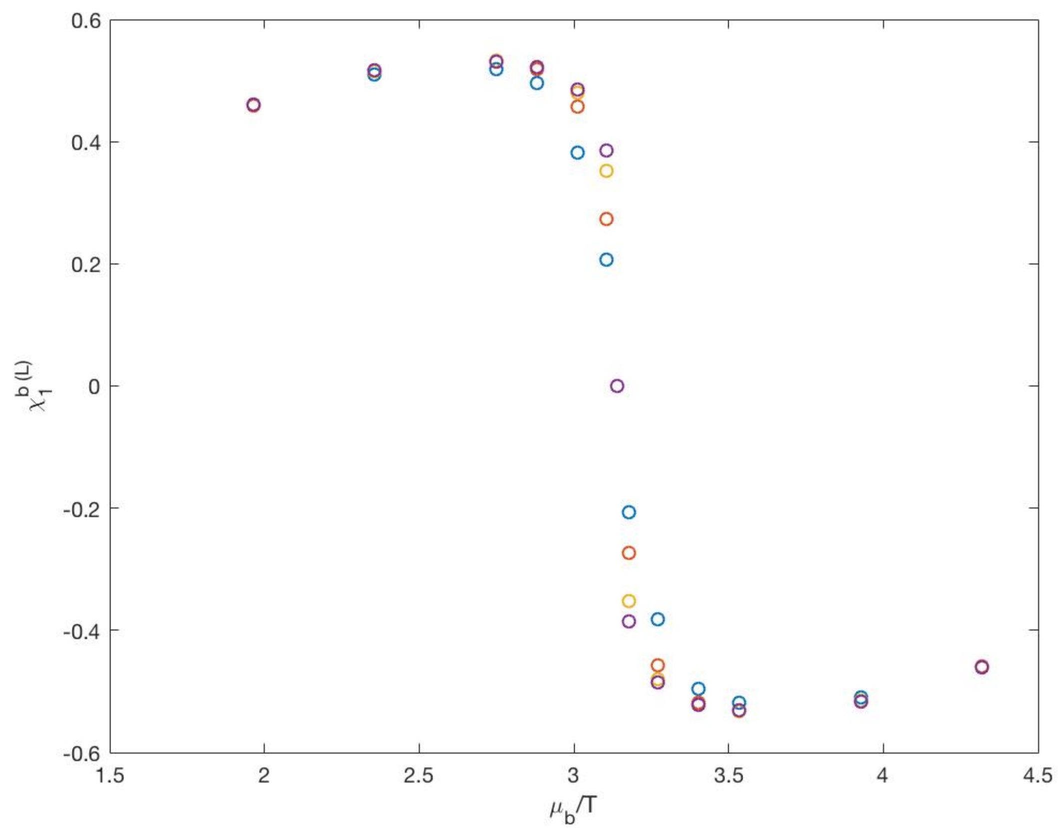
$$h \;\mapsto\; \hat{\mu}_B = \frac{\mu_B}{T} \qquad\qquad m^{(L)}(h) \;\mapsto\; \chi_1^{B\,(L)}(\hat{\mu}_B) = \frac{\partial}{\partial \hat{\mu}_B} \frac{\ln Z}{V T^3}$$

which we probe at $T \sim 200\,\mathrm{MeV}$ 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.

$$\hat{\mu}_{B\,cr} = i\pi$$

and we have to look for the scaling of $\hat{\mu}_{B\,0}^{(R)}$





We compute number density
at different values of imaginary chemical potential and lattice size
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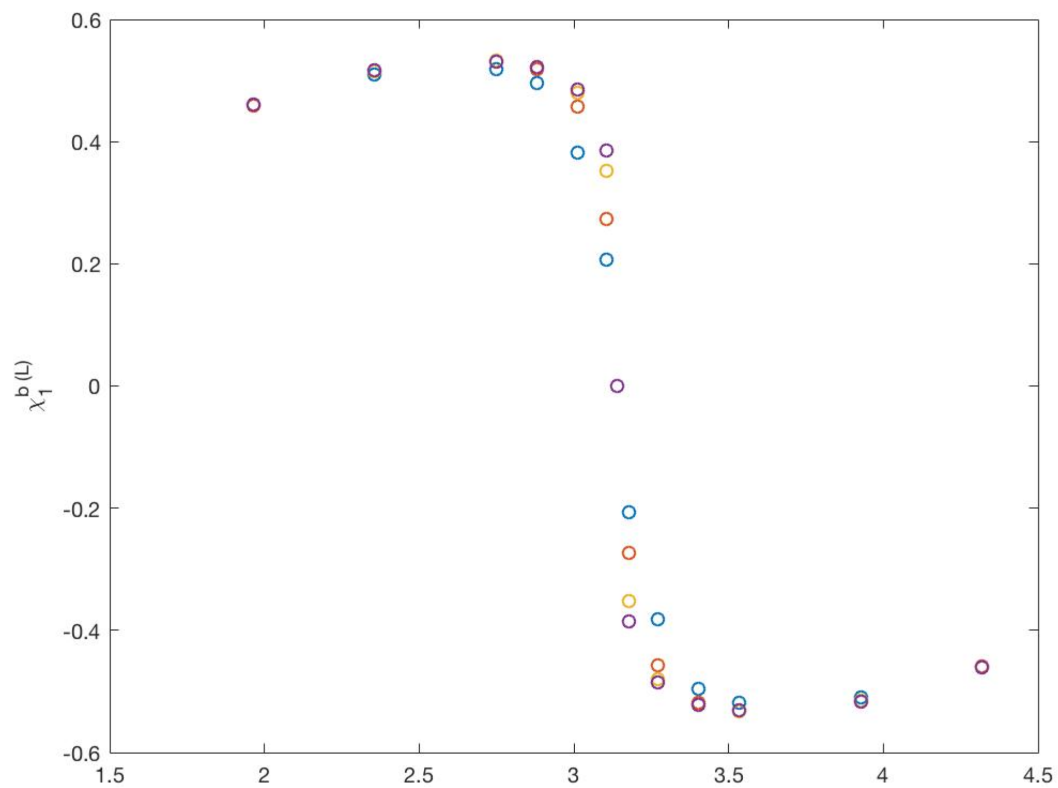

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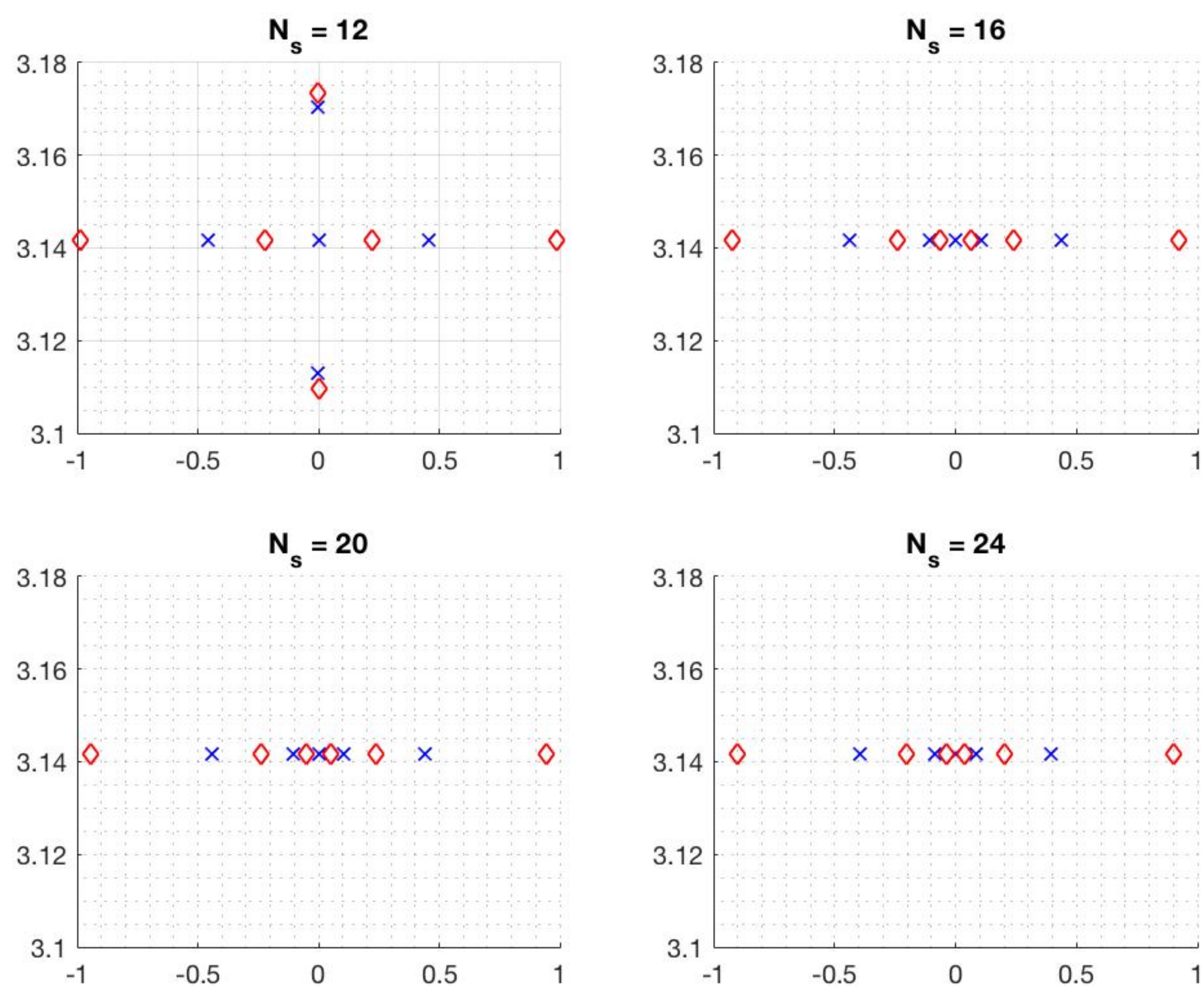
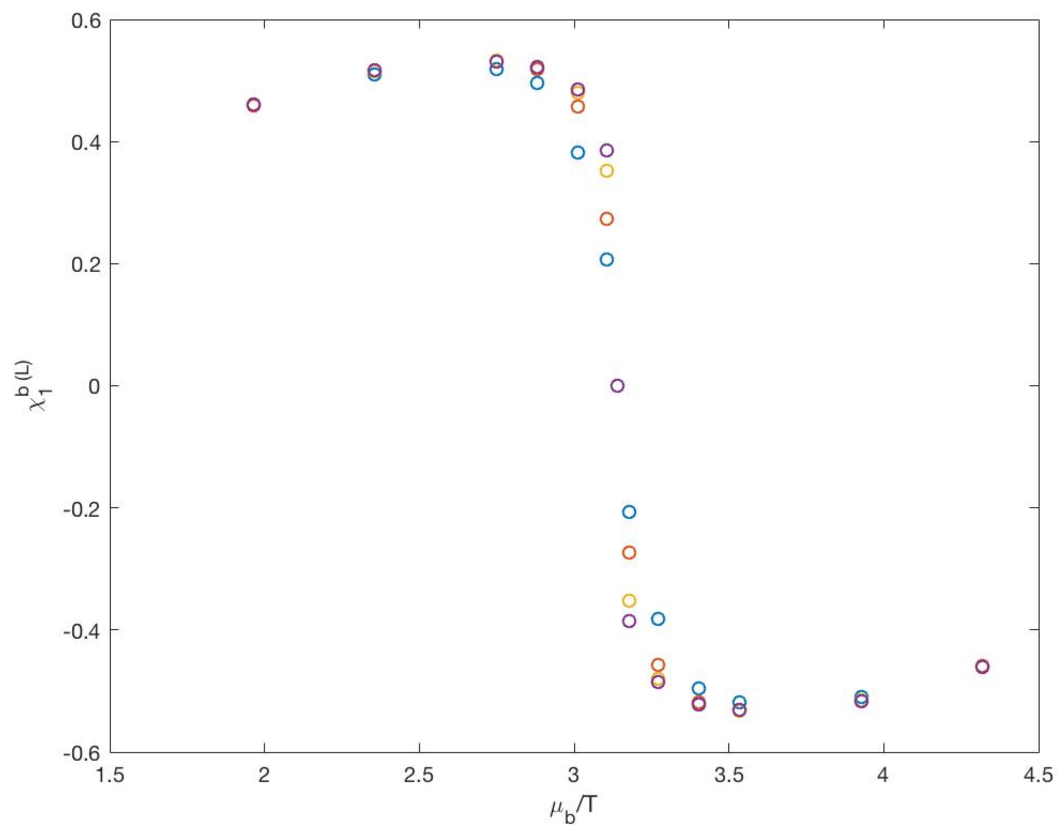
We determine the leading pole (red symbol) from the Padè approximants

(figures are in complex *chem.pot.* plane)





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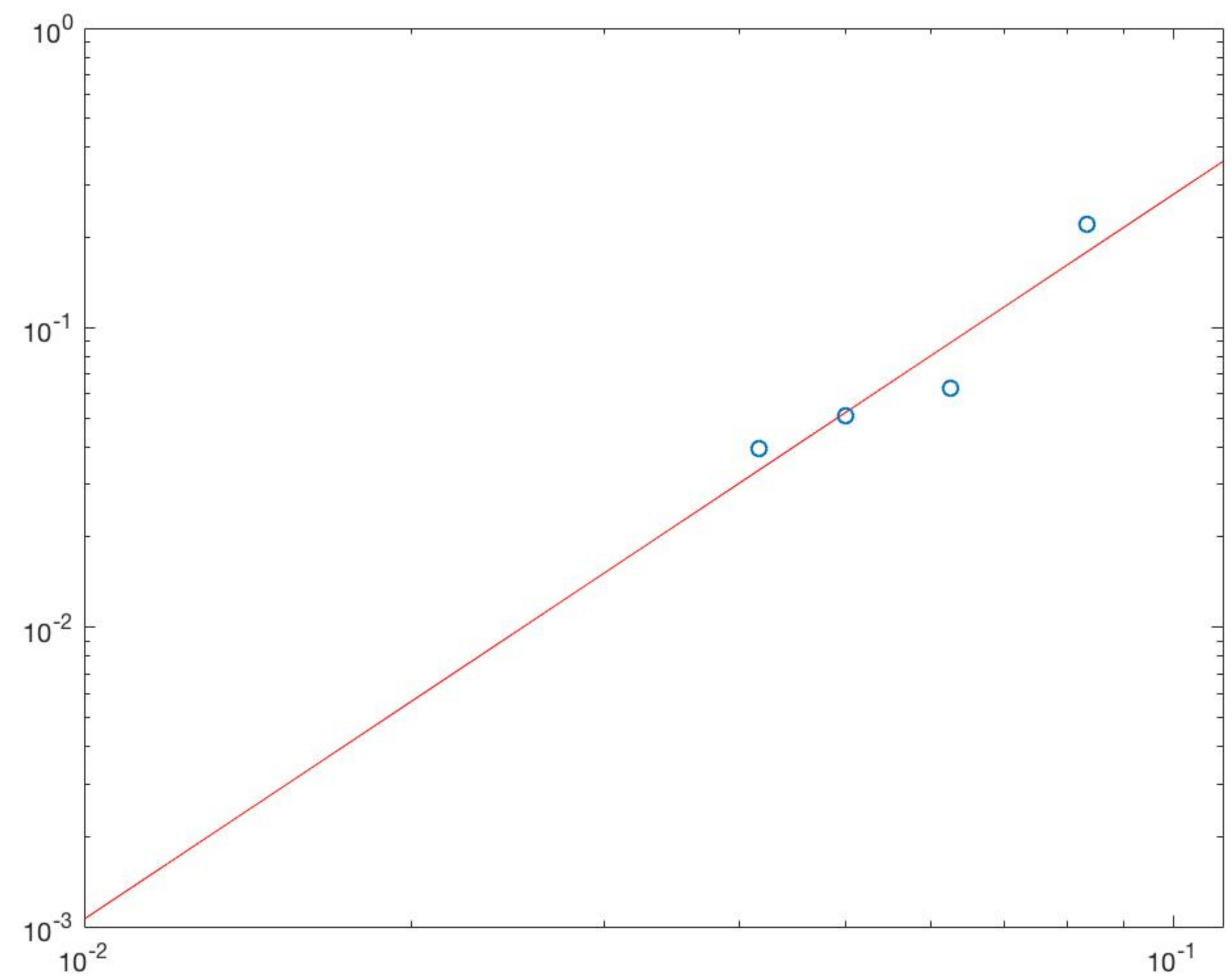
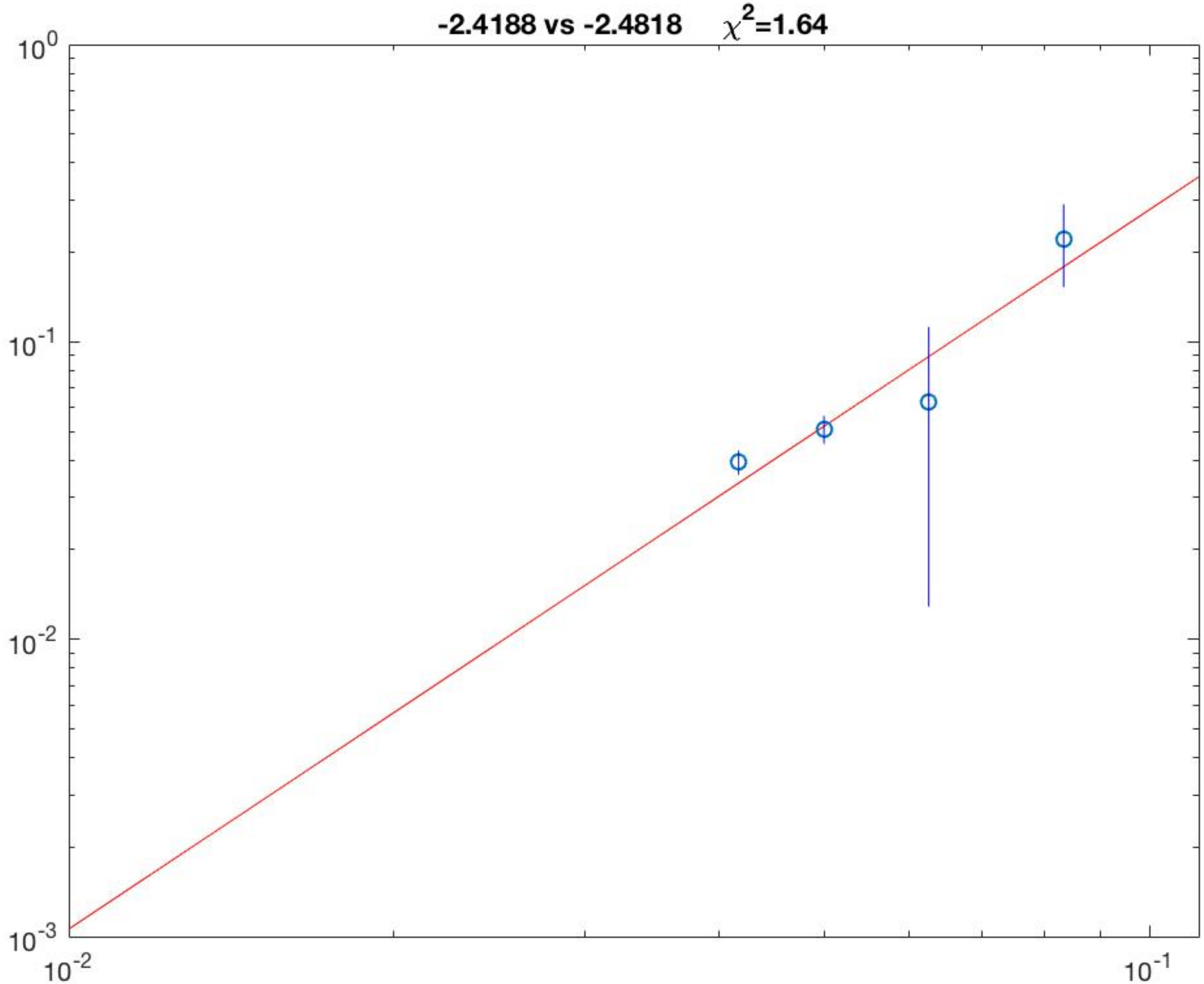
$$\hat{\mu}_{B\,0}^{(R)} \sim L^{-\frac{\beta\delta}{\nu}}$$

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)



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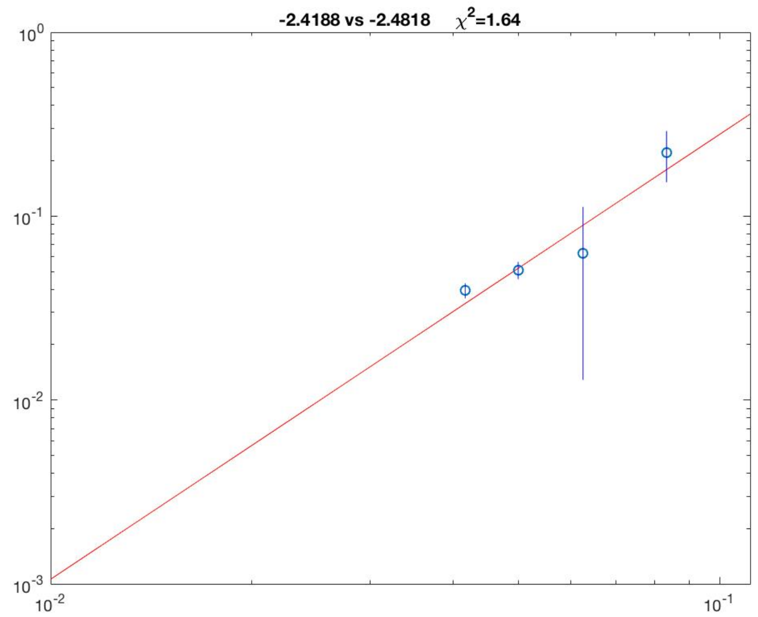

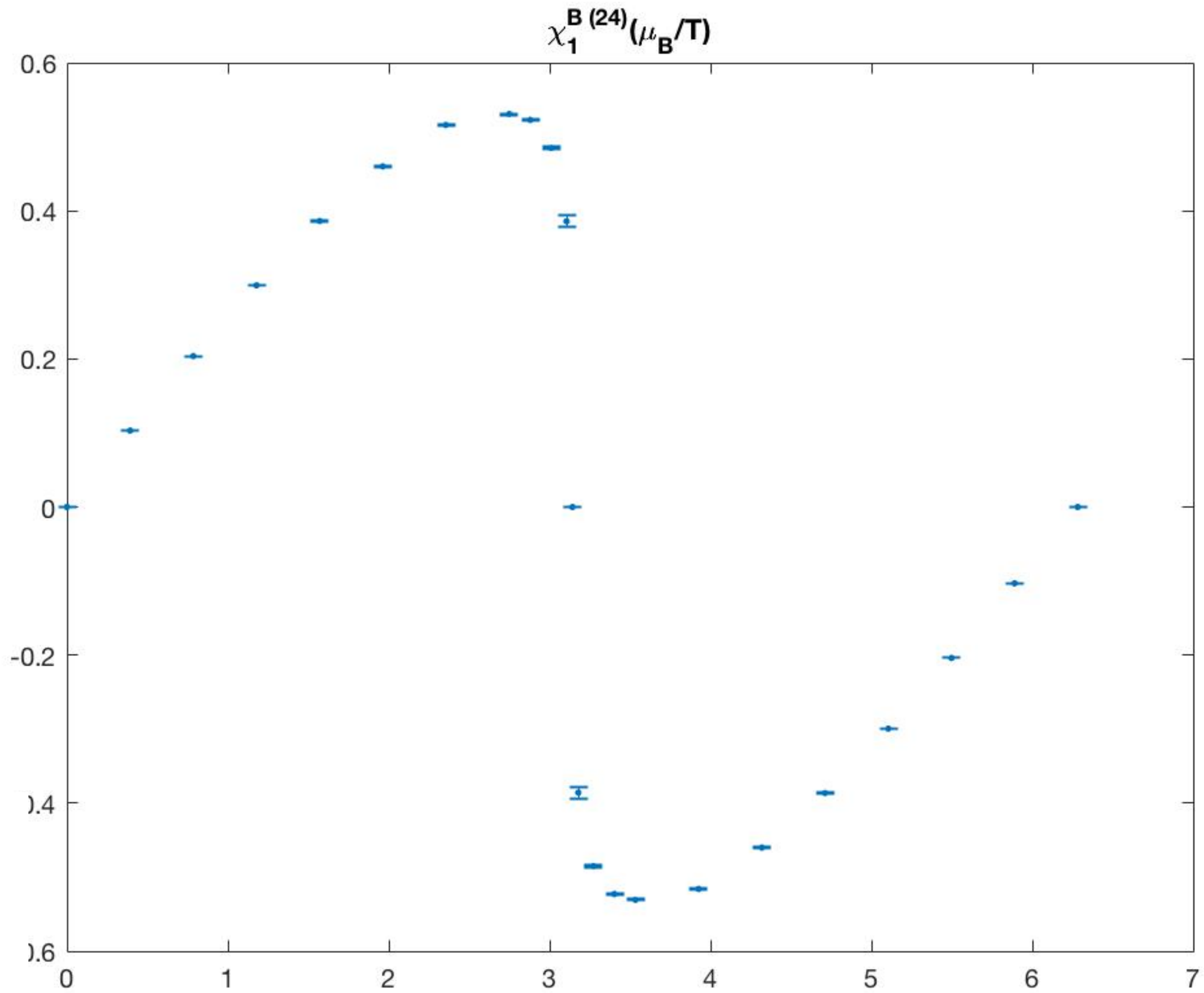

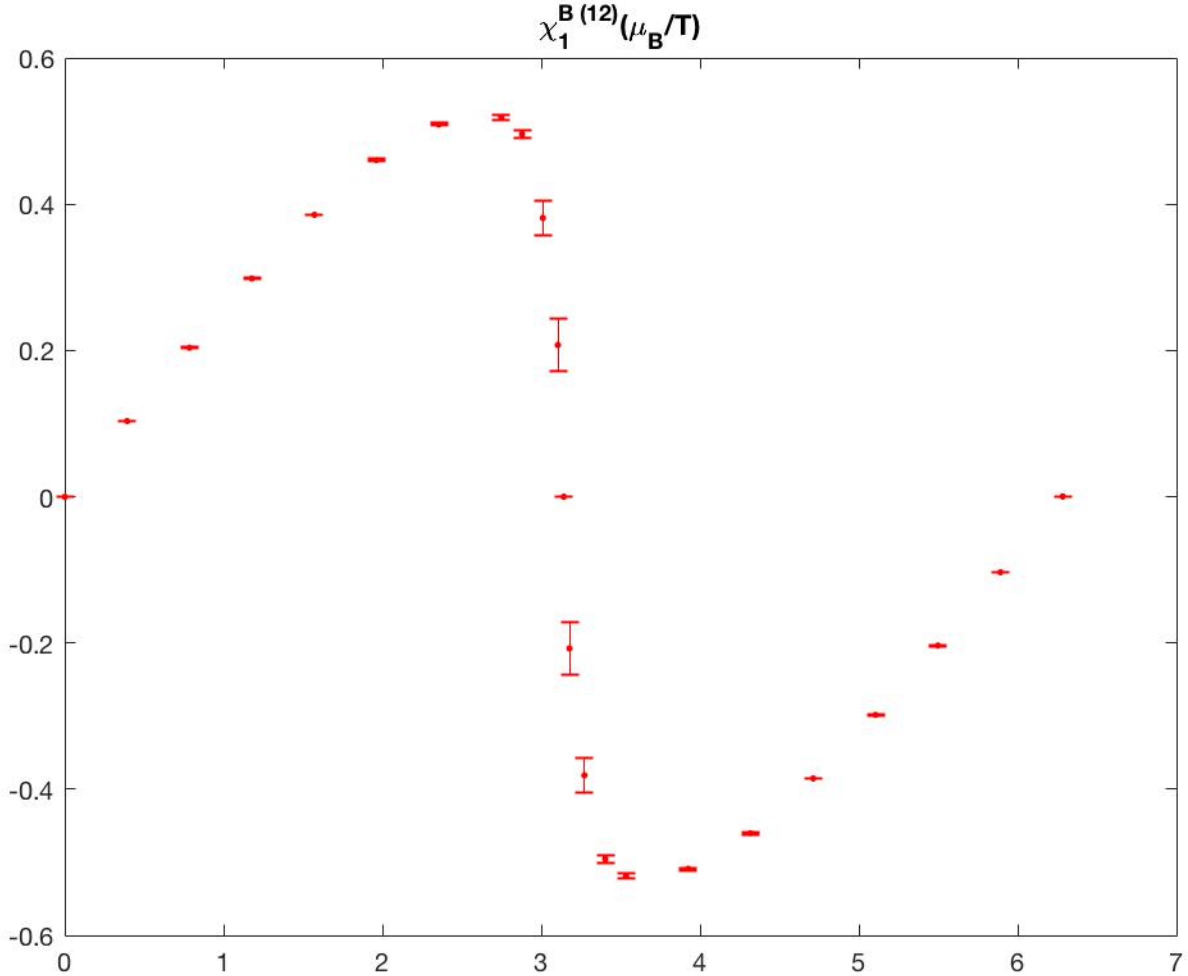

We need to enlarge our statistics …

Something still preliminary...

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

$$f(z; \_) \mapsto \chi_1^{B\,(L)}(T; \mu_B/T) \qquad R_m^n(z; \_) \mapsto R_m^{n\,(L)}(T; \mu_B/T)$$

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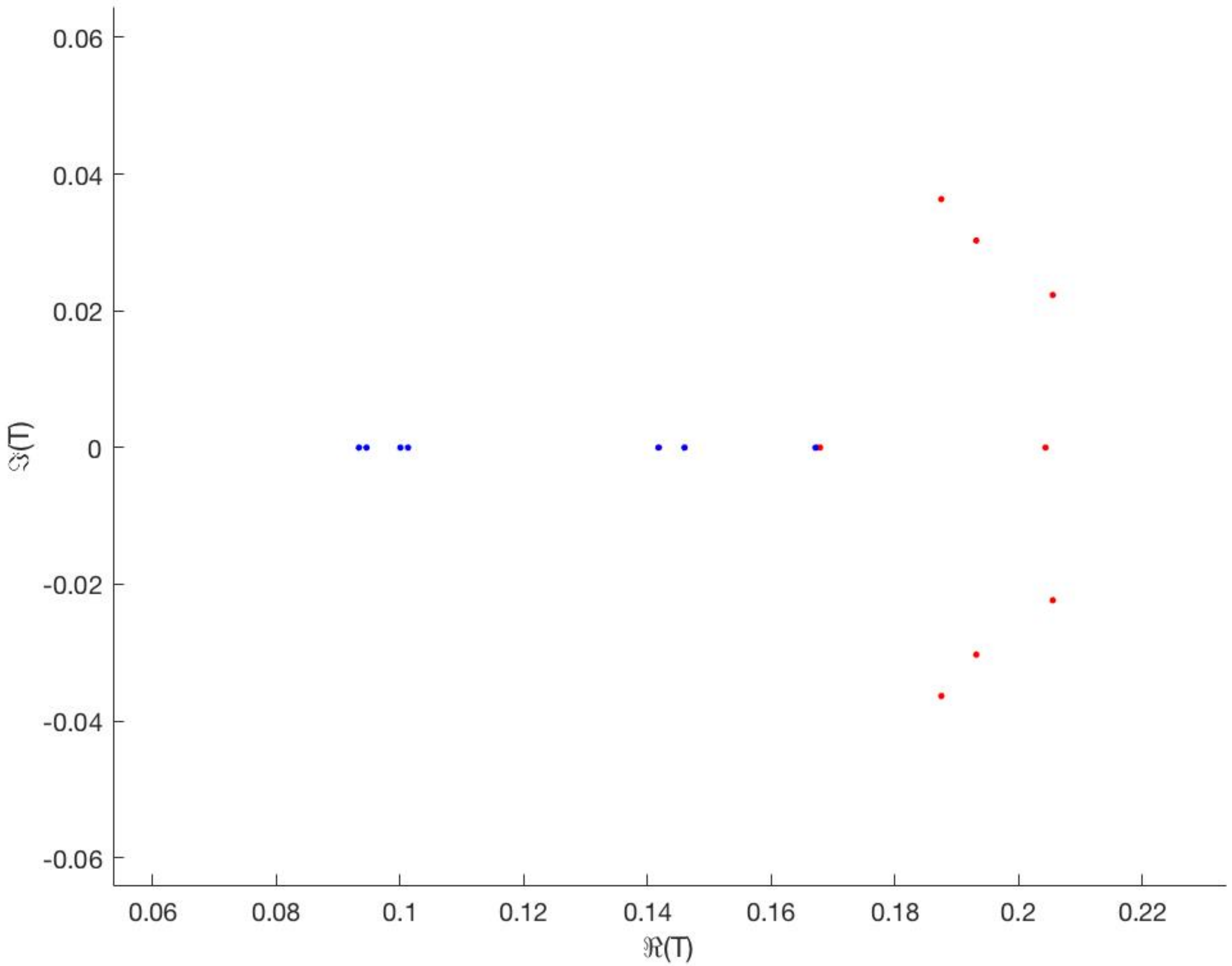
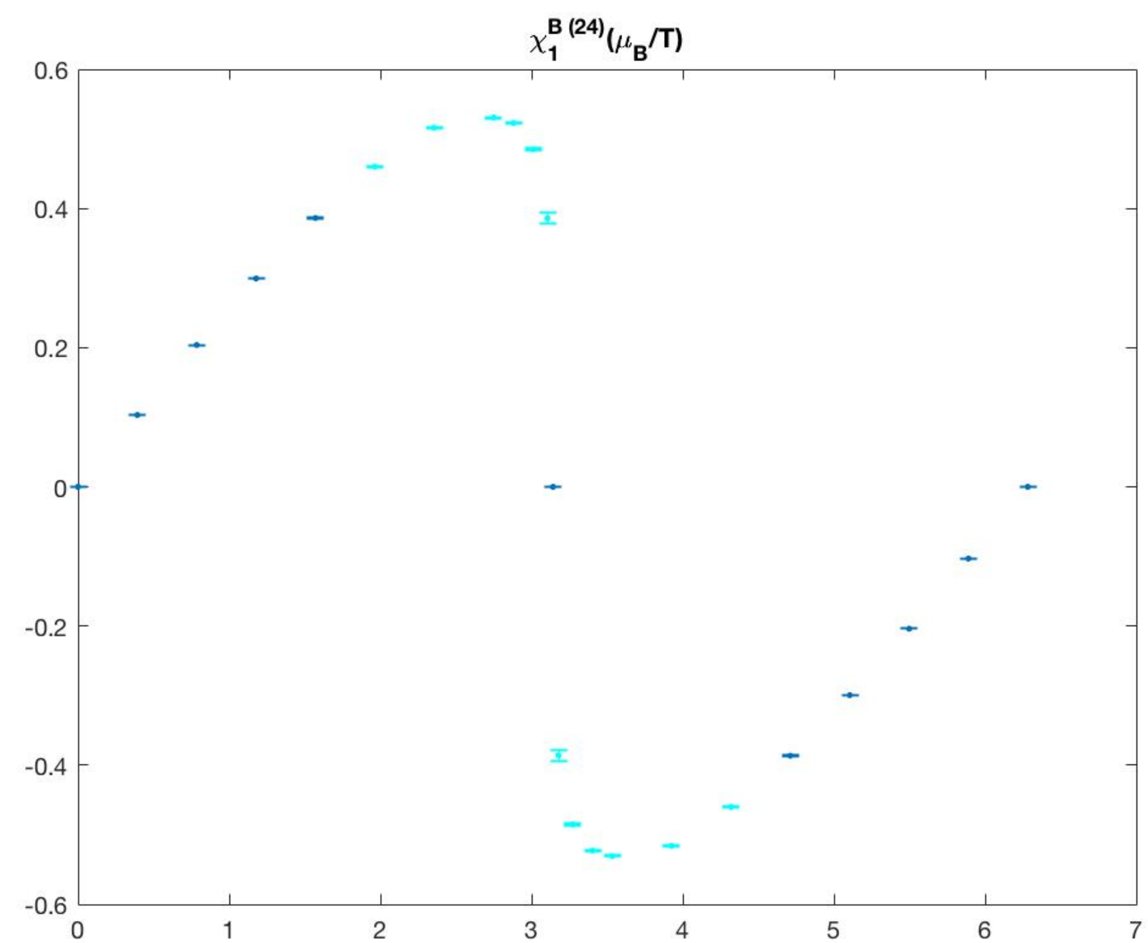


Beware! Here we are *moving* in complex T plane, at different values of the imaginary chemical potential, but (at the moment) only one value (L=24) of lattice size…



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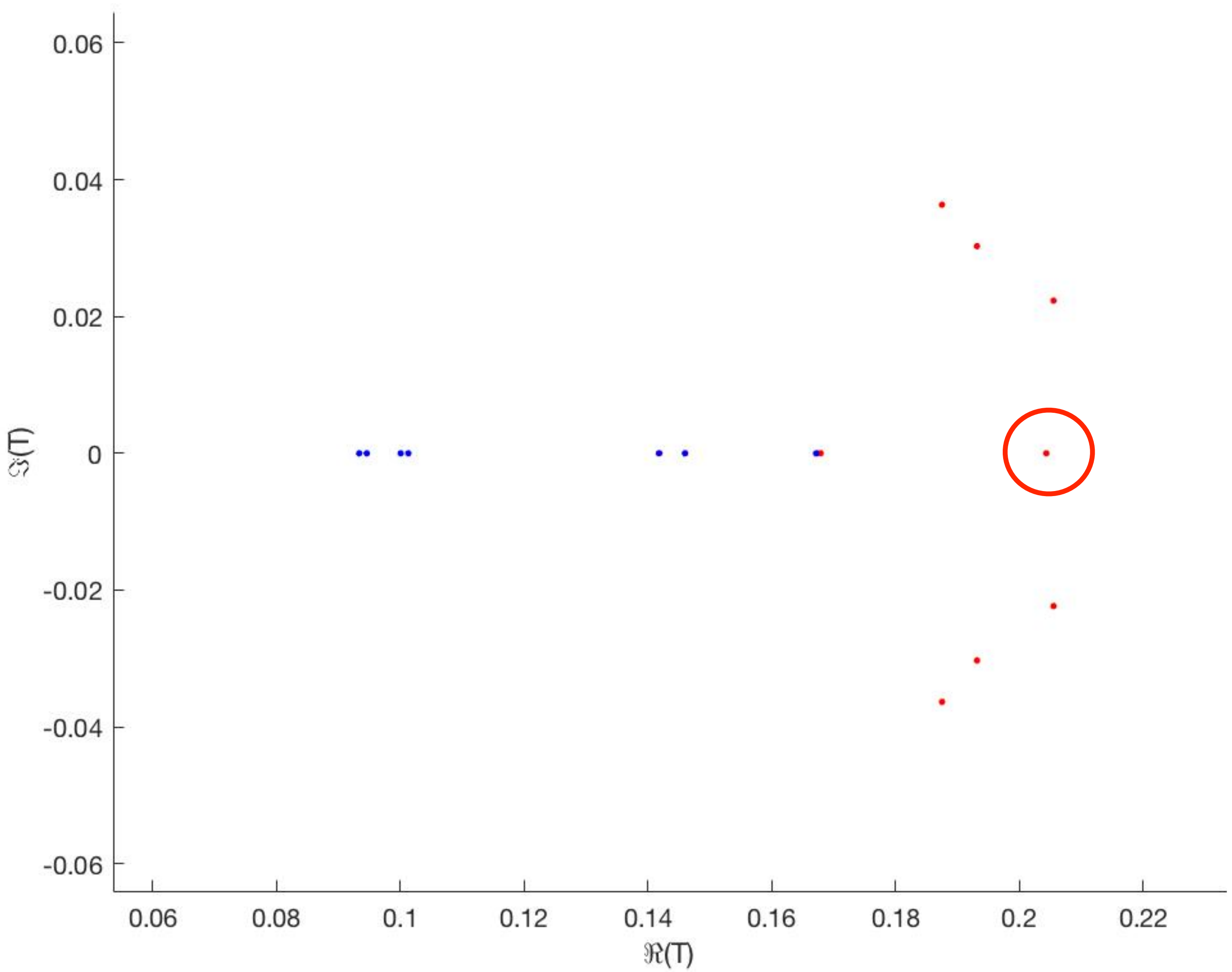
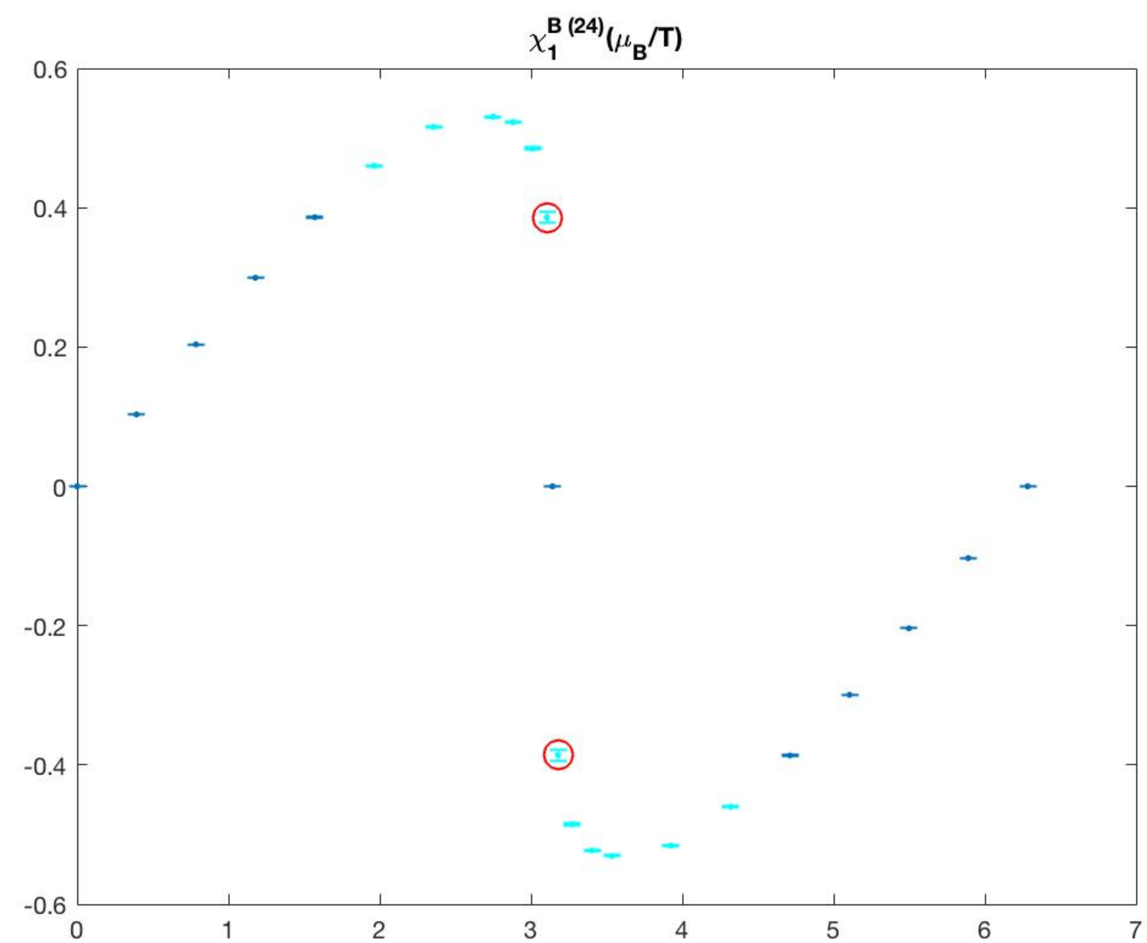


Beware! Here we are *moving* in complex T plane, at different values of the imaginary chemical potential, but (at the moment) only one value (L=24) of lattice size…



… 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…