Multi-point Padé for the study of phase transitions: from the Ising model to lattice QCD.

Francesco Di Renzo (University of Parma and INFN)

LATTICE 2022

Bonn, 08/08/2022

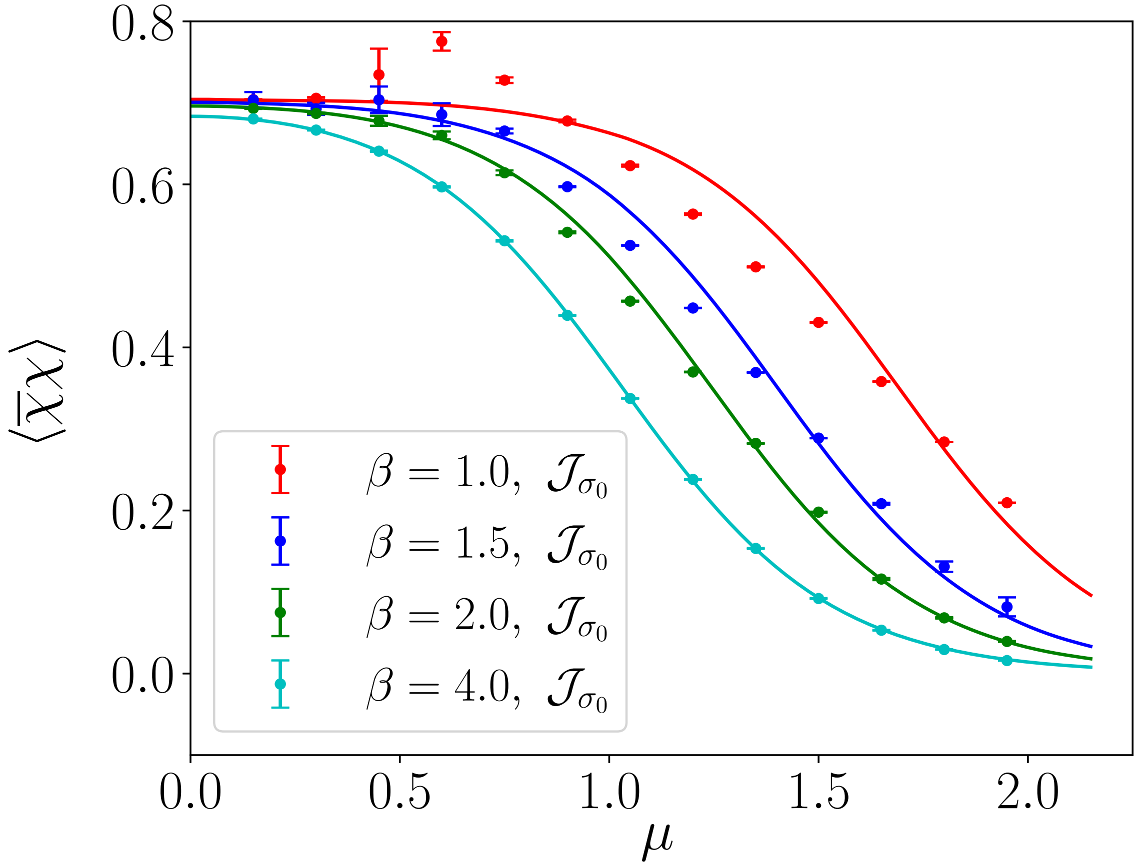
In collaboration with P. Dimopoulos, S. Singh (Parma), K. Zambello (Parma -> Pisa),
J. Goswami, D. Clarke, G. Nicotra, C. Schmidt (Bielefeld)

see also next talks by K. Zambello and C. Schmidt

An invitation

How it all began: Thirring model in Thimble Regularisation (from a failure to a new opportunity)

$$S = \beta \sum_{n=1\dots L} (1 - \cos(\phi_n)) - \log \ \det \ D$$



Those who know a little bit about thimbles should remember the single thimble dominance hypothesis (and all that …)

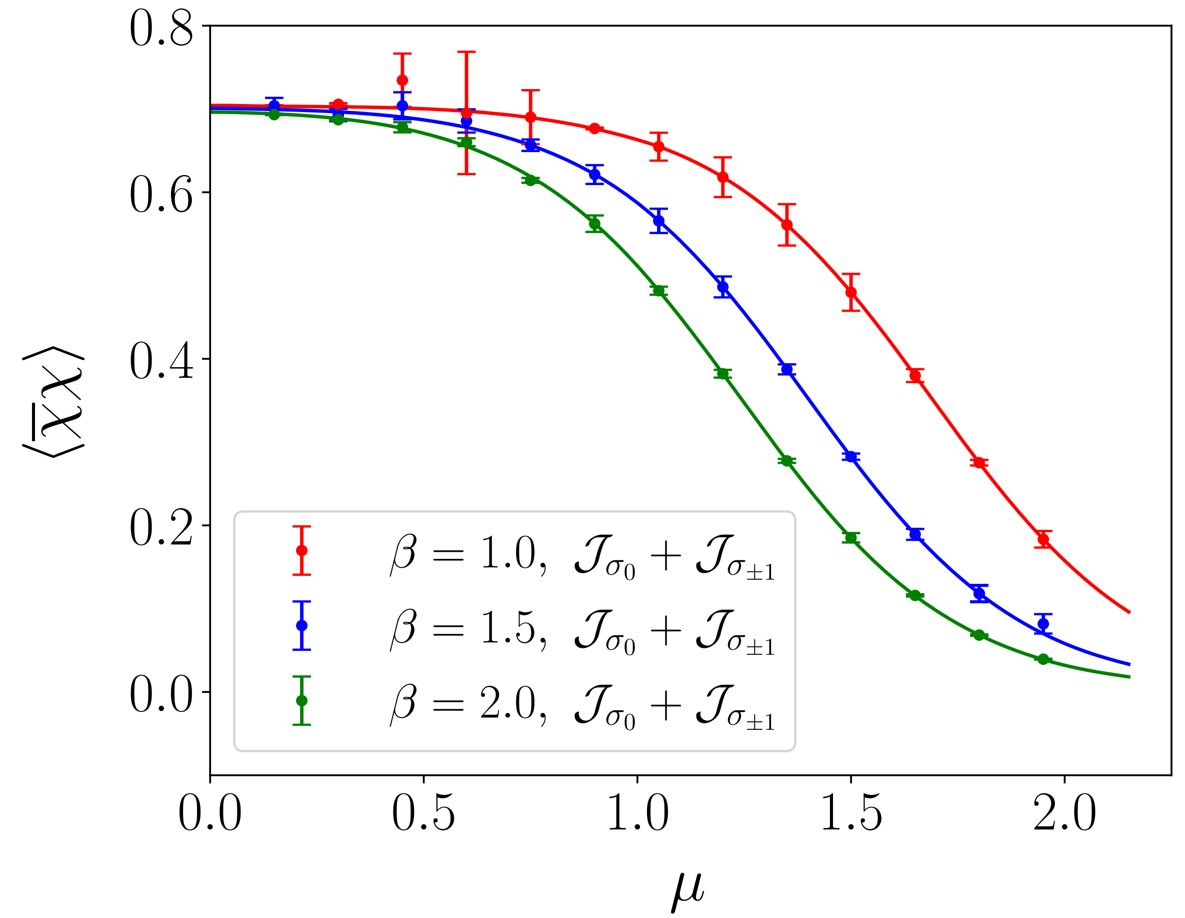
Single thimble fails …

Y. Kikukawa et al (2016), A. Alexandru et al (2016)

… which is a pain in the neck …

(even if two can be enough …)

F. Di Renzo, K. Zambello (2022)



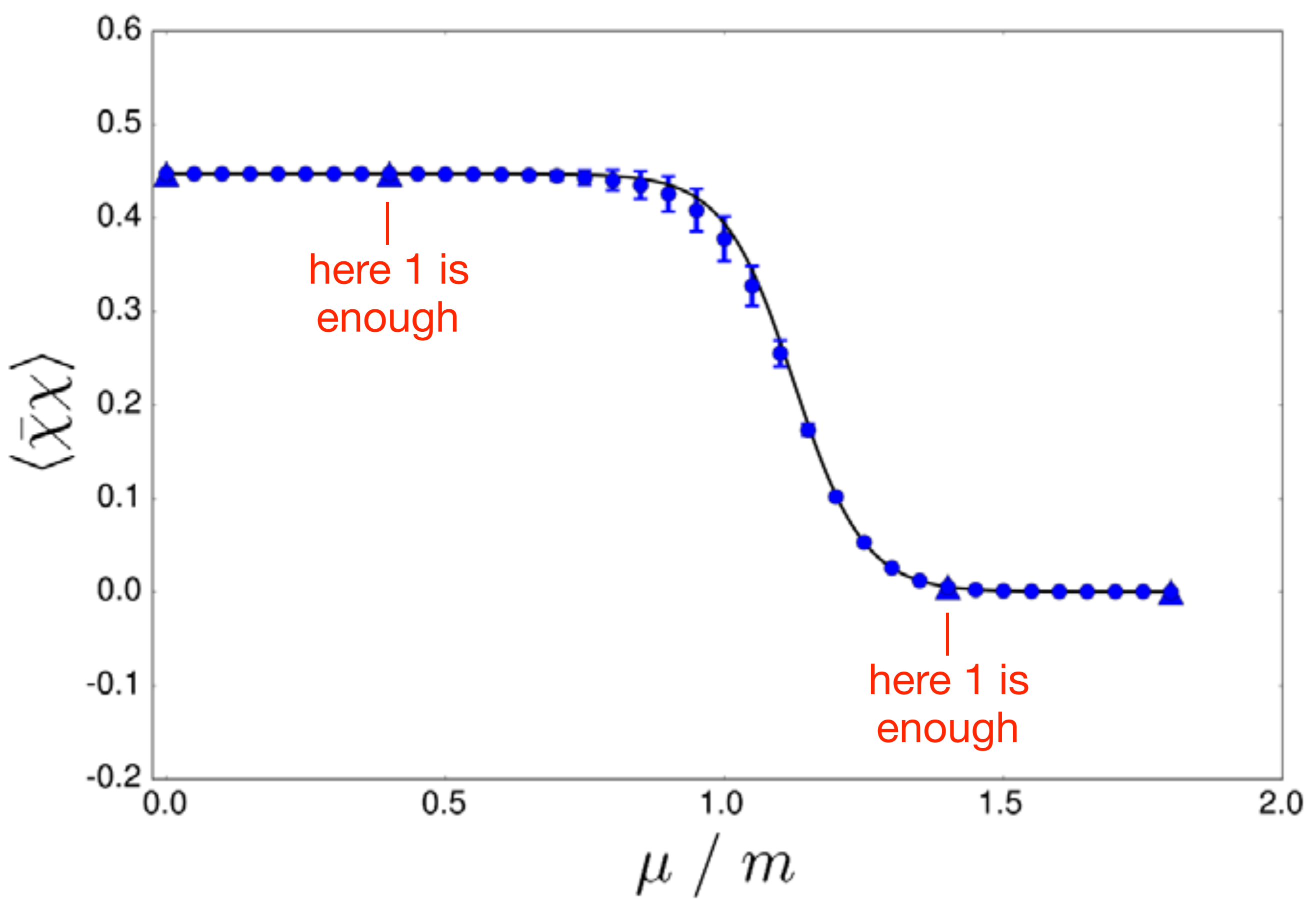
From Taylor expansions to Padé approximates (on Lefschetz thimbles)

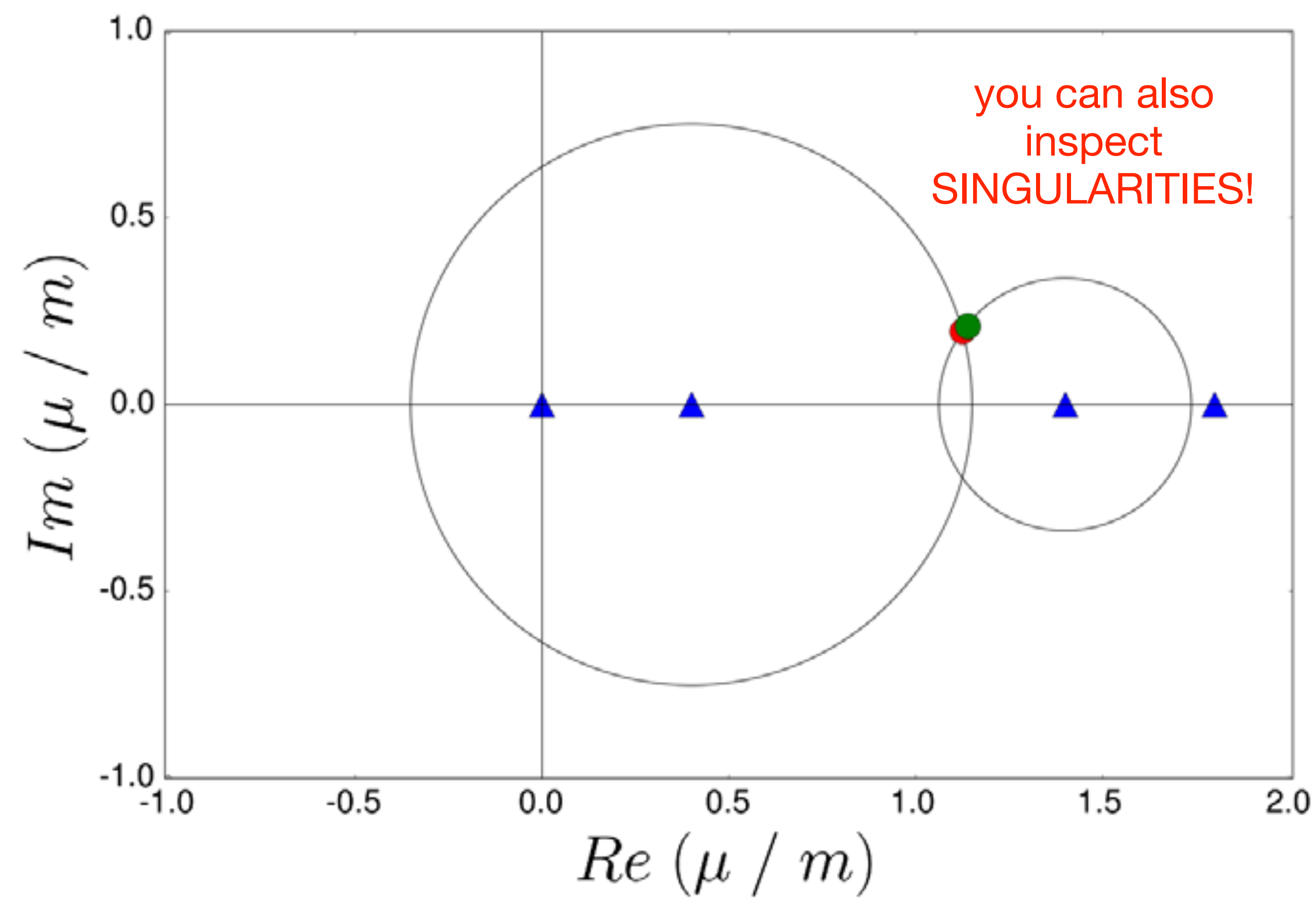
Di Renzo, Singh, Zambello (2021)

THIMBLE DECOMPOSITION is DISCONTINUOUS across STOKES points, but PHYSICAL OBSERVABLES are NOT!

First idea: compute TAYLOR EXPANSIONS in regions where single decomposition holds and BRIDGE!

Second (better) idea: once you have TAYLOR EXPANSIONS compute PADÈ APPROXIMANTS and BRIDGE!





In the following

- A recap of our approach: (multi-point) Padé approximants for cumulants of the net baryon density and information on singularities in the complex chemical potential plane

- Test of the method on a prototype computation: the critical point of 2D Ising model

- Preliminary steps for a Temperature Padé and the quest for singularities in the complex temperature plane

PADÈ approximants for dense QCD

Bielefeld Parma (2021)

What can we compute in dense lattice QCD, given the sign problem?

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Taylor expansions at ZERO μ_B

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Observables at IMAGINARY values of μ_B

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Let's merge the two and then go for a (multi-point) PADÈ !

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$$\chi_n^B(T,V,\mu_B) = \left(\frac{\partial}{\partial\hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$
$$= \left(\frac{1}{3}\frac{\partial}{\partial\hat{\mu}_l} + \frac{1}{3}\frac{\partial}{\partial\hat{\mu}_s}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

cumulants of the net baryon density are computed at a number of imaginary values of $\hat{\mu}_B \equiv \mu/T$ (including zero…)

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cumulants of the net baryon density are computed at a number of imaginary values of $\hat{\mu}_B \equiv \mu/T$ (including zero...)

and approximated by rational functions (x is $\frac{\mu_B}{T}$)

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

A bit more on multi-point PADÈ

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which we want to account (at many points) for a function $f(x)$
and its derivatives

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which we want to account (at many points) for a function $f(x)$
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Solve a linear system …

$$P_m(x_1) - f(x_1)Q_n(x_1) = f(x_1),$$
$$P'_m(x_1) - f'(x_1)Q_n(x_1) - f(x_1)Q'_n(x_1) = f'(x_1),$$
$$\cdots,$$
$$P_m(x_2) - f(x_2)Q_n(x_2) = f(x_2),$$
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$$\cdots,$$
$$P_m(x_N) - f(x_N)Q_n(x_N) = f(x_N),$$
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A bit more on <u>multi-point</u> PADÈ

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A few alternatives…

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A few alternatives…

- $$R_n^m(x) = \frac{\sum_{i=0}^{m'} a_{2i+1} x^{2i+1}}{1+\sum_{j=1}^{n/2} b_{2j} x^{2j}},$$

odd function…

$$(m = 2m'+1, a_1 = \chi_2^B(T,V,0))$$

A bit more on <u>multi-point</u> PADÈ

$$\chi_n^B(T,V,\mu_B) = \left(\frac{\partial}{\partial\hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$
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* $$R_n^m(x) = \frac{P_m(x)}{\tilde{Q}_n(x)} = \frac{P_m(x)}{1+Q_n(x)} = \frac{\sum_{i=0}^m a_i x^i}{1+\sum_{j=1}^n b_j x^j}$$

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$$(m = 2m'+1,\, a_1 = \chi_2^B(T,V,0))$$

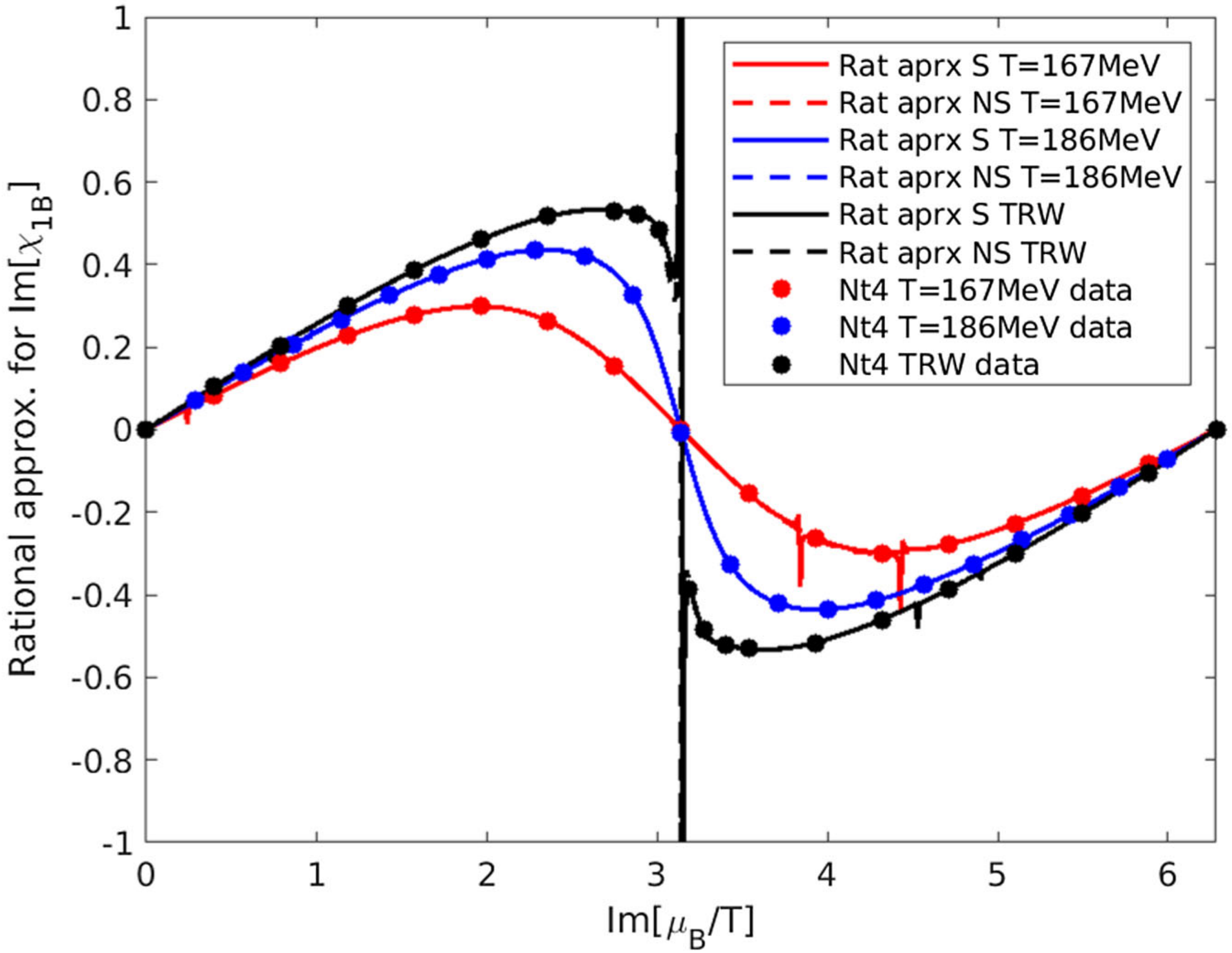
odd function…

$$c_j^{(k)} \equiv \frac{\partial^j f}{\partial x^j}(x_k) \simeq \frac{\partial^j R_n^m}{\partial x^j}(x_k)$$

* minimise $$\tilde{\chi}^2 = \sum_{j,k} \frac{\left|\frac{\partial^j R_n^m}{\partial x^j}(x_k) - c_j^{(k)}\right|^2}{|\Delta c_j^{(k)}|^2}$$

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4, physical masses

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



PRETTY GOOD DESCRIPTION OF DATA, BUT THERE ARE (ALSO) SPIKES …

as you should expect…

$$R_n^m(x) = \frac{P_m(x)}{\tilde{Q}_n(x)}$$

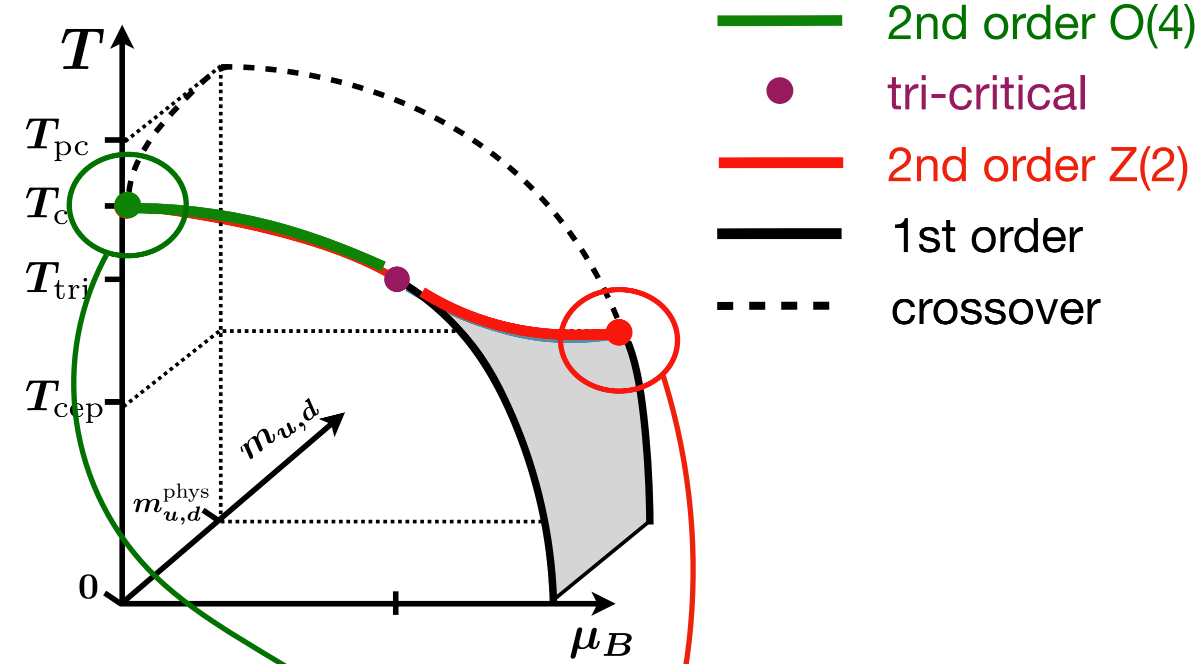
Let's now look for the SINGULARITY STRUCTURE

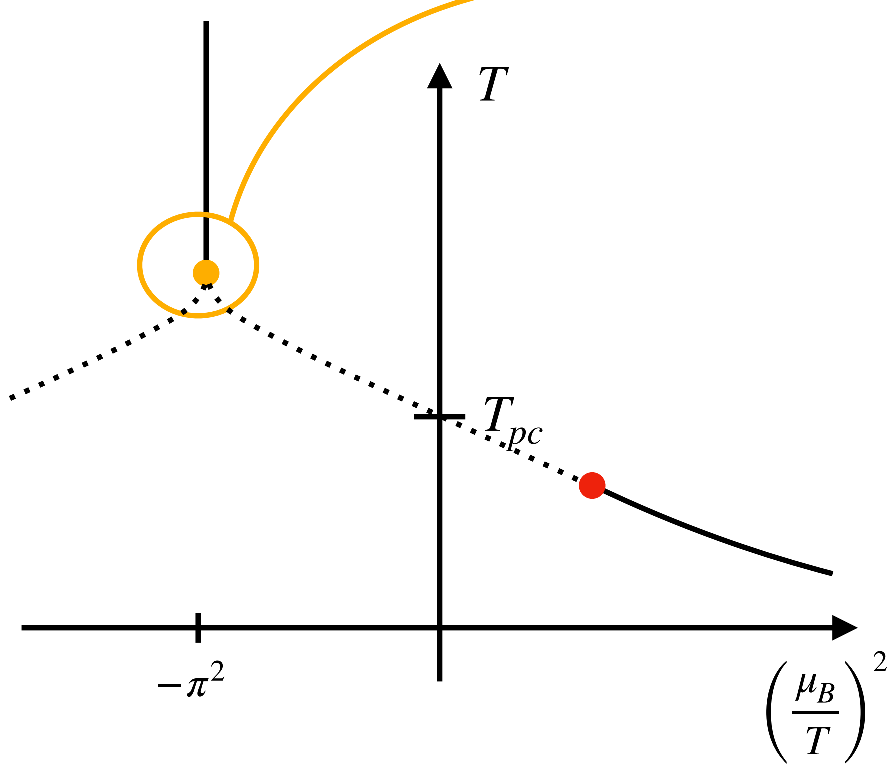
(we hunt for LEE YANG ZEROS, i.e. zeros of the partition function)

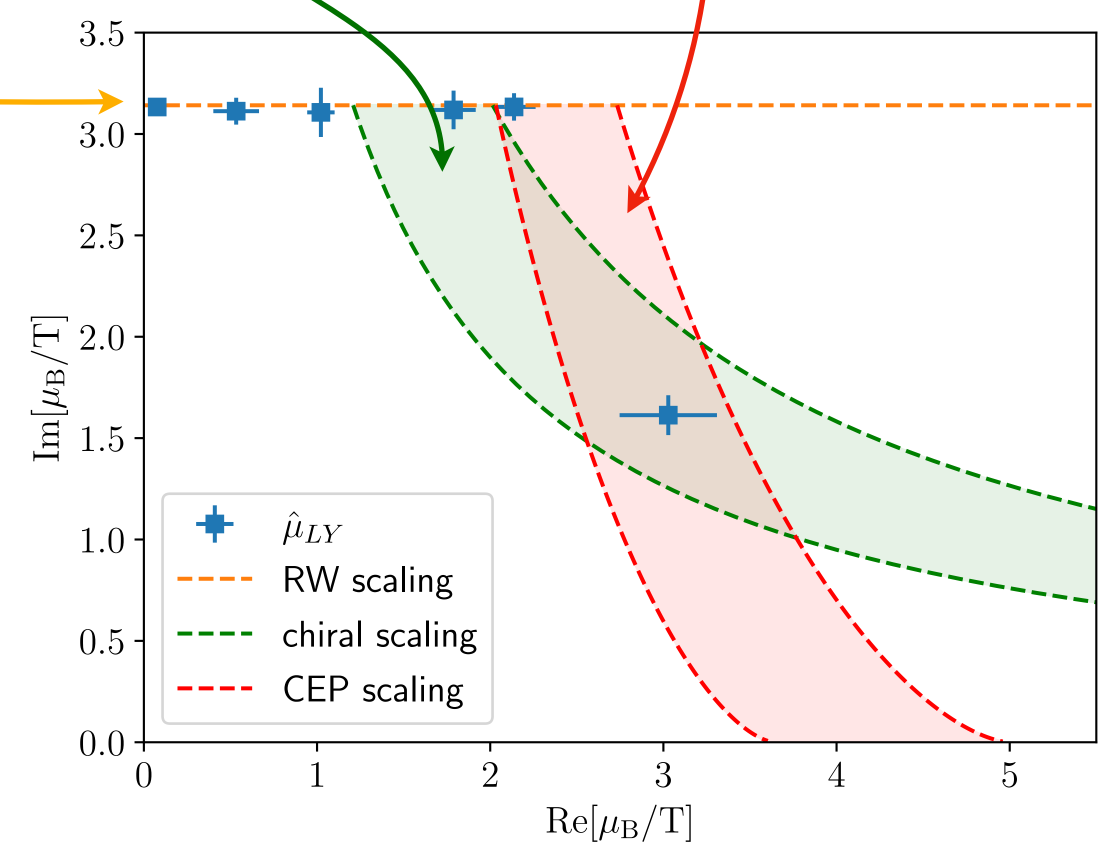
The big picture of Lee Yang edge singularities in QCD

Slide produced by Christian Schmidt

- The ultimate goal is the location of the QCD critical point
- We can think of three distinct critical points/ scaling regions: Roberge Weiss transition, chiral transition, QCD critical point







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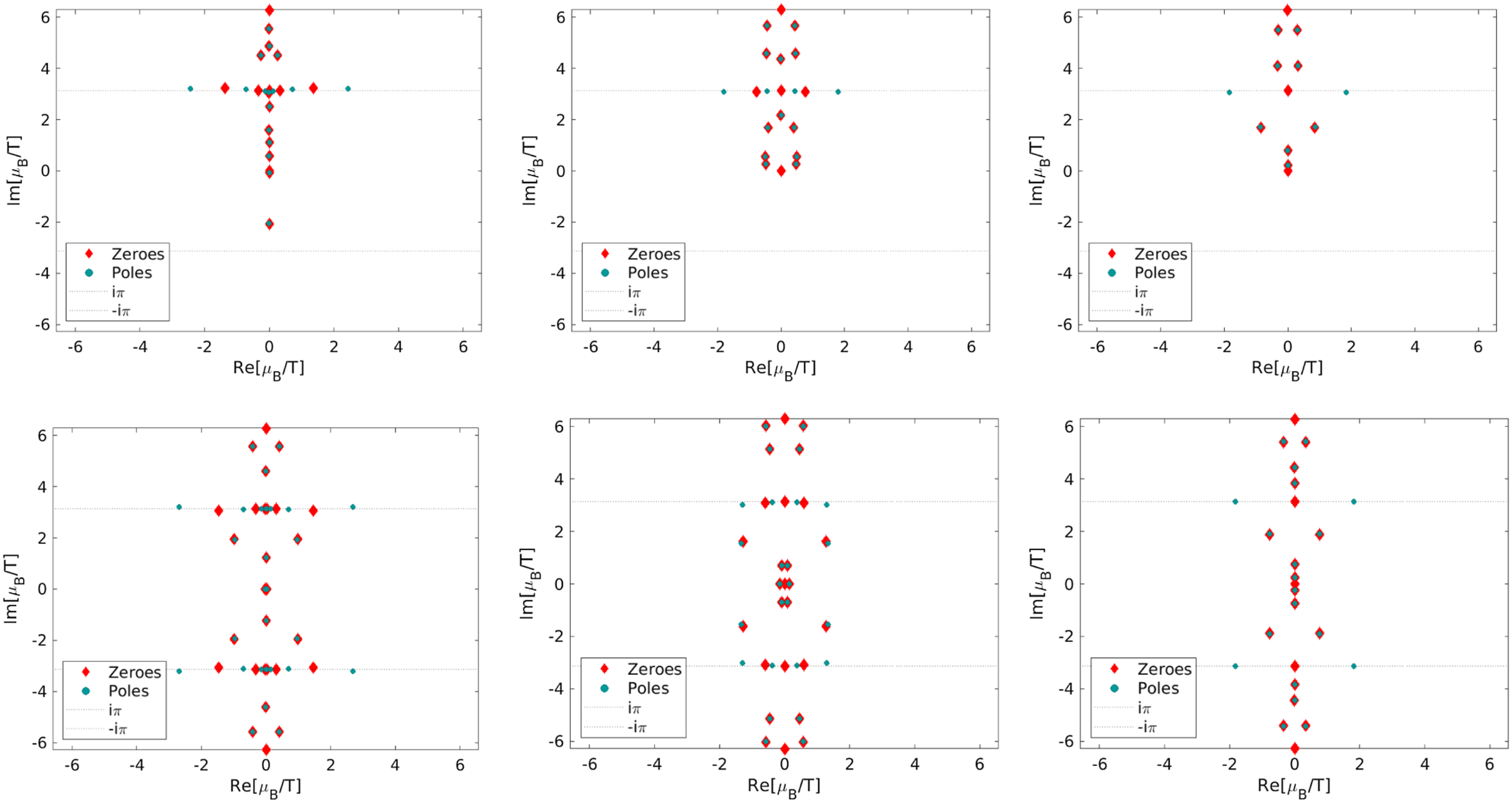
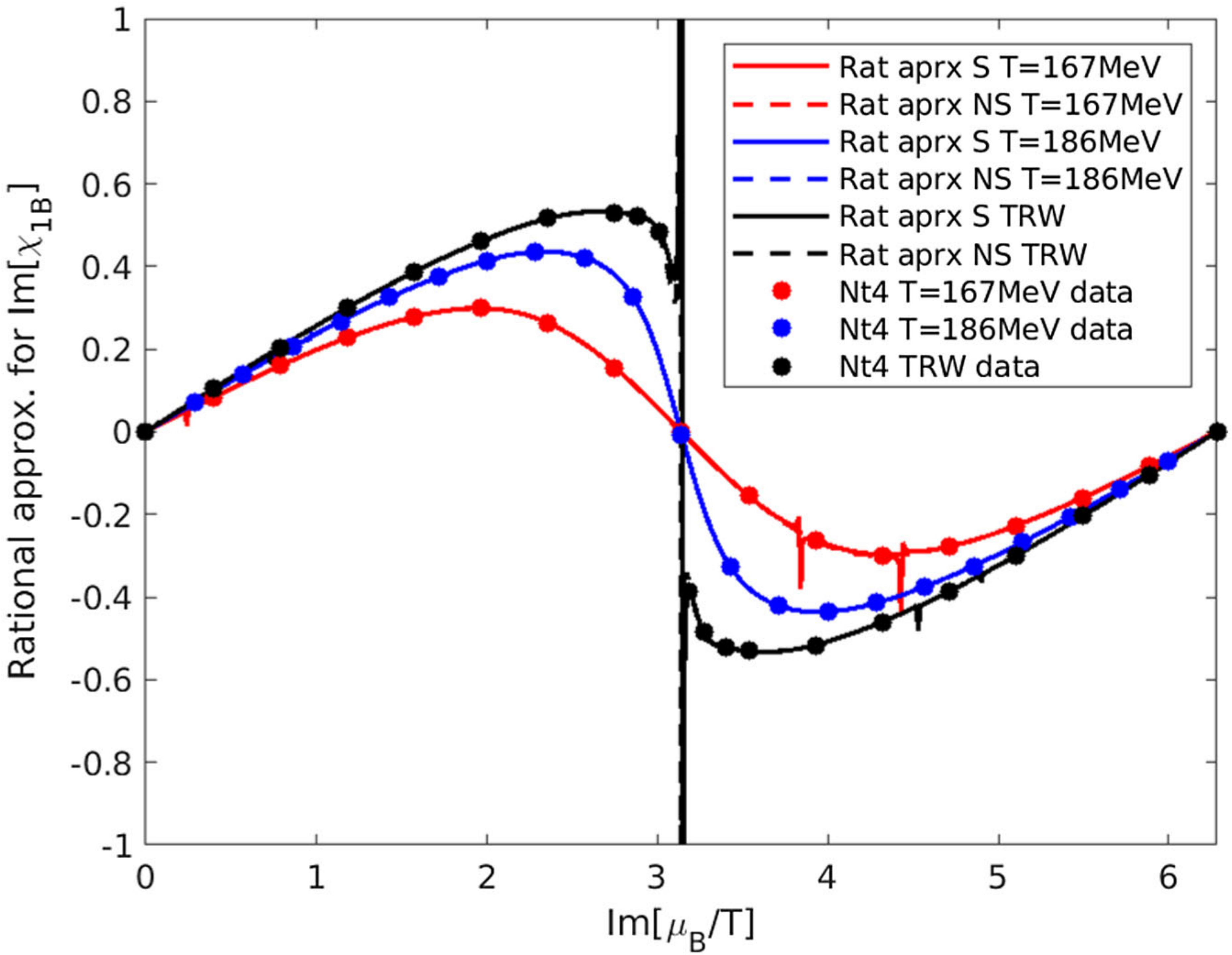


zeros and poles* show up where they are expected || large number of cancelations || relevant vs NON relevant pieces of informations

* zeros of numerator and denominator, actually…

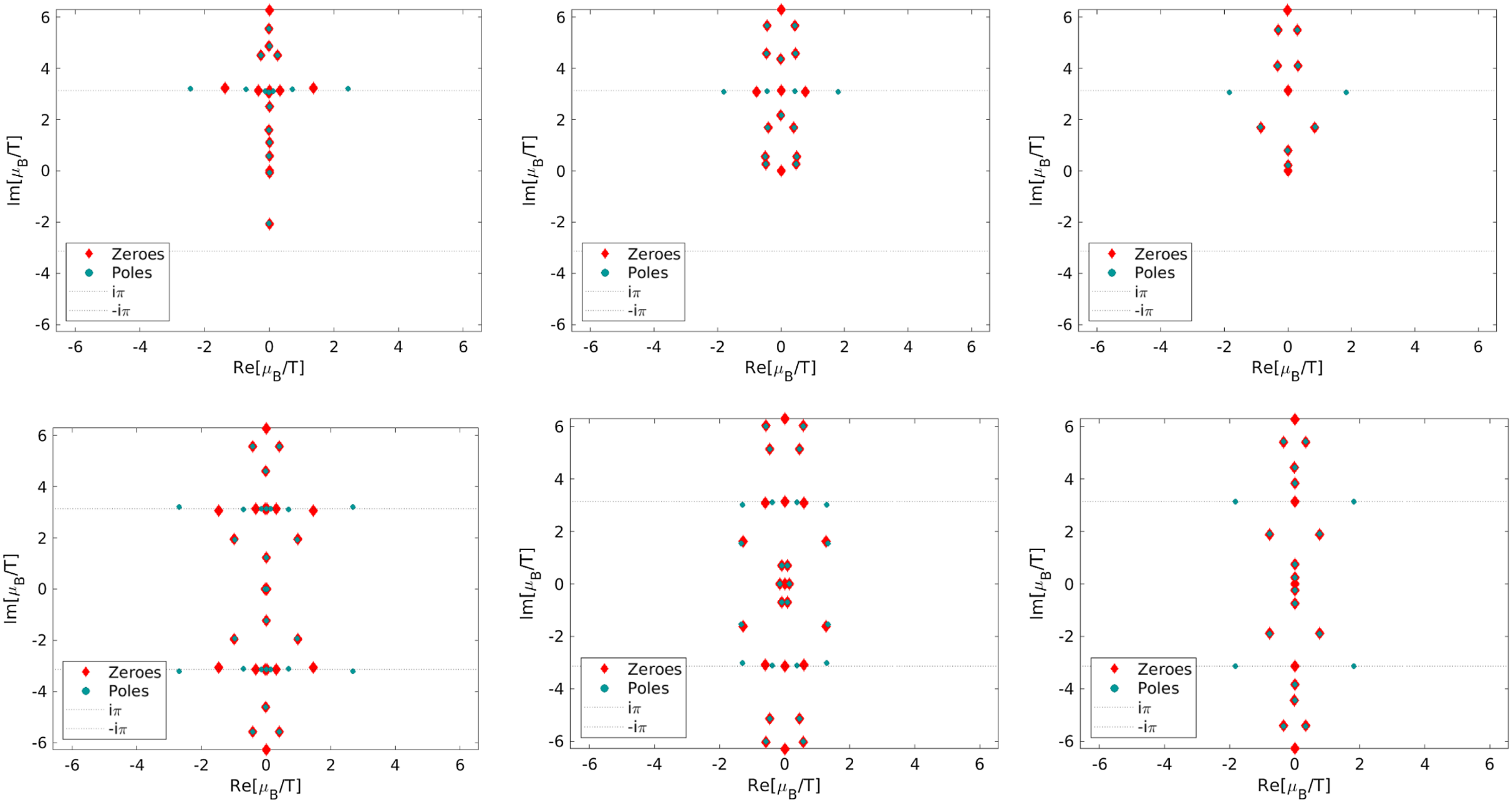


… so we can account for SPIKES … remember …

$$R_n^m(x) = \frac{P_m(x)}{\tilde{Q}_n(x)}$$

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4, physical masses

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



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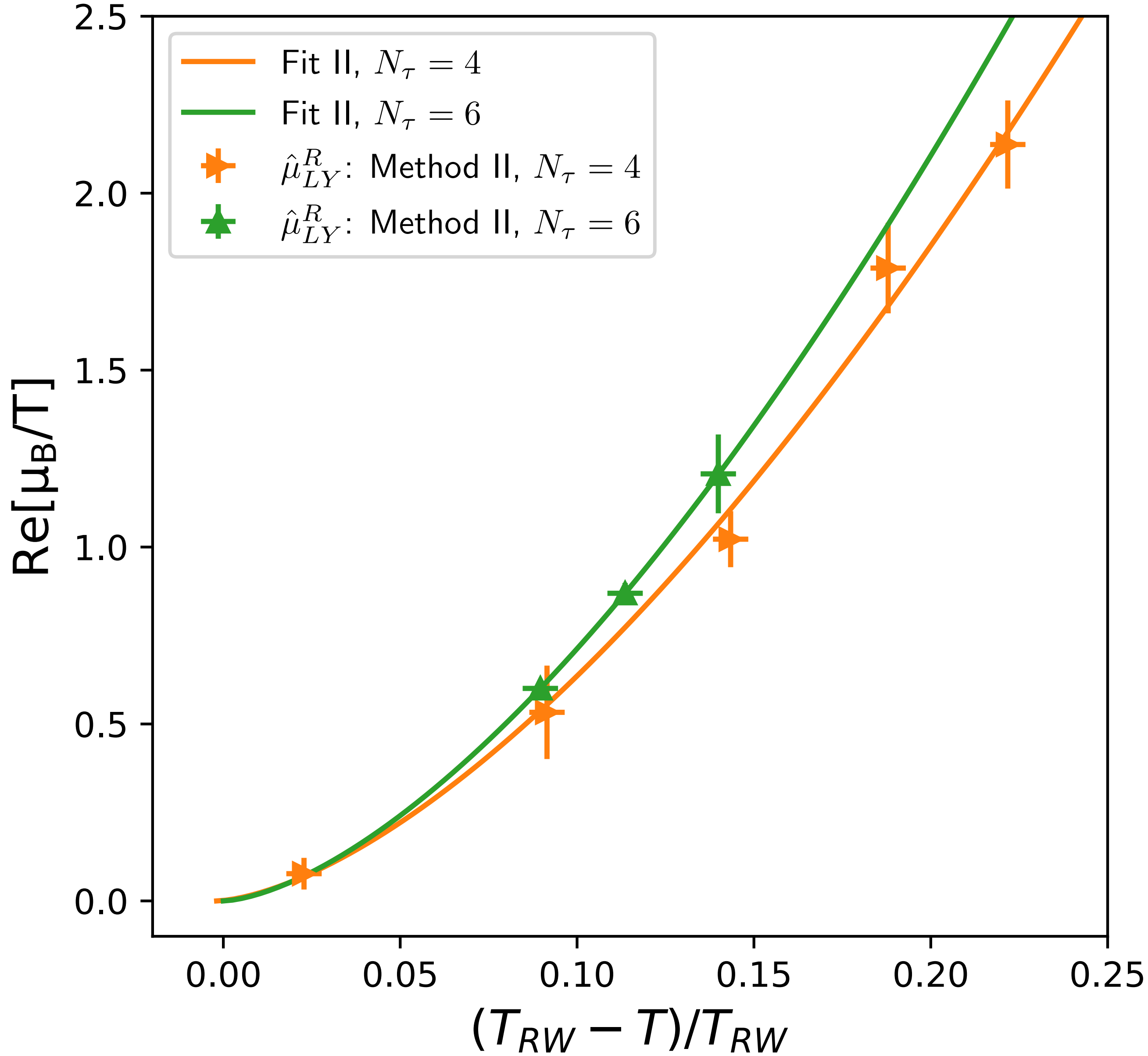


Order parameter near a 2nd order phase transition

$$M = h^{1/\delta} f_G(z) + M_{\text{reg}} \qquad z \equiv t/|h|^{1/\beta\delta}$$

$$t = t_0^{-1}\left(\frac{T_{\text{RW}} - T}{T_{\text{RW}}}\right)$$

scaling fields

$$h = h_0^{-1}\left(\frac{\hat{\mu}_B - i\pi}{i\pi}\right) \qquad \hat{\mu}_B = \mu_B/T$$

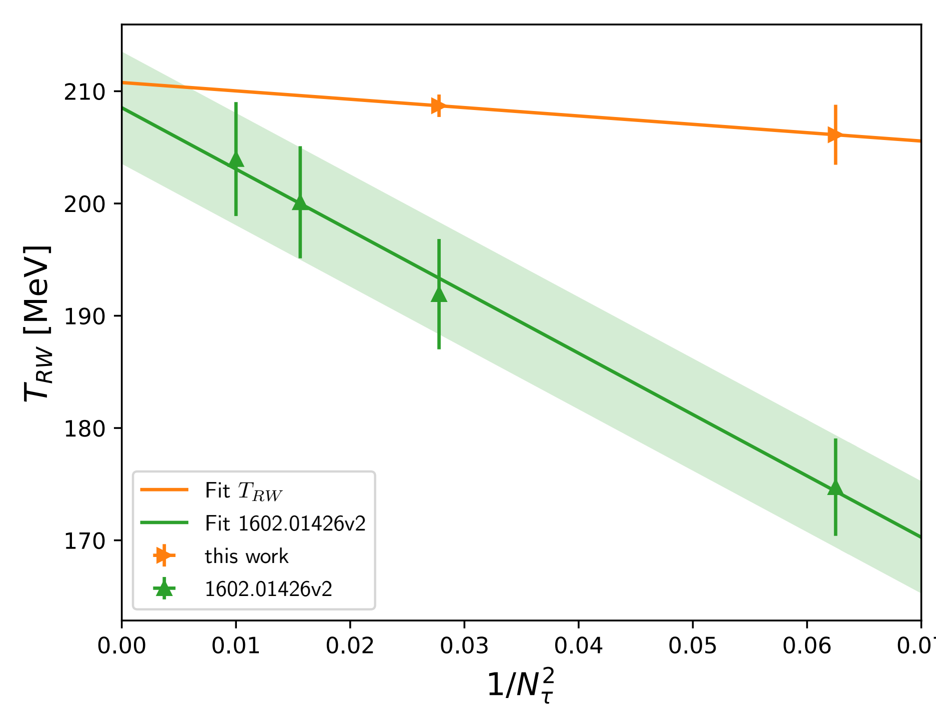
$$\hat{\mu}^R_{\text{LY}} = \pm\pi\left(\frac{z_0}{|z_c|}\right)^{\beta\delta}\left(\frac{T_{\text{RW}} - T}{T_{\text{RW}}}\right)^{\beta\delta}$$

$$\hat{\mu}^I_{\text{LY}} = \pm\pi,$$

From the fit we get

T_{RW} = 206.7(2.6) MeV

T_{RW} = 208.705(0.002) MeV



2+1 HISQ, at a lower (145 MeV) temperature, N_t=6

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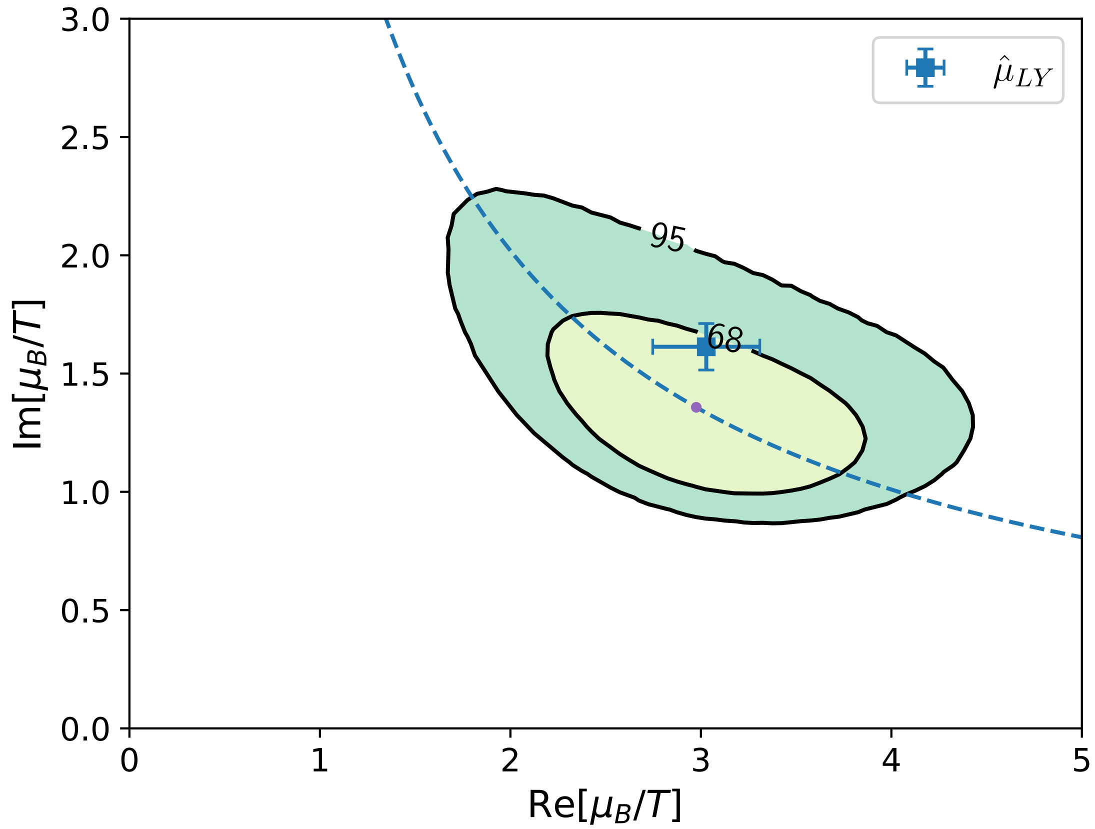

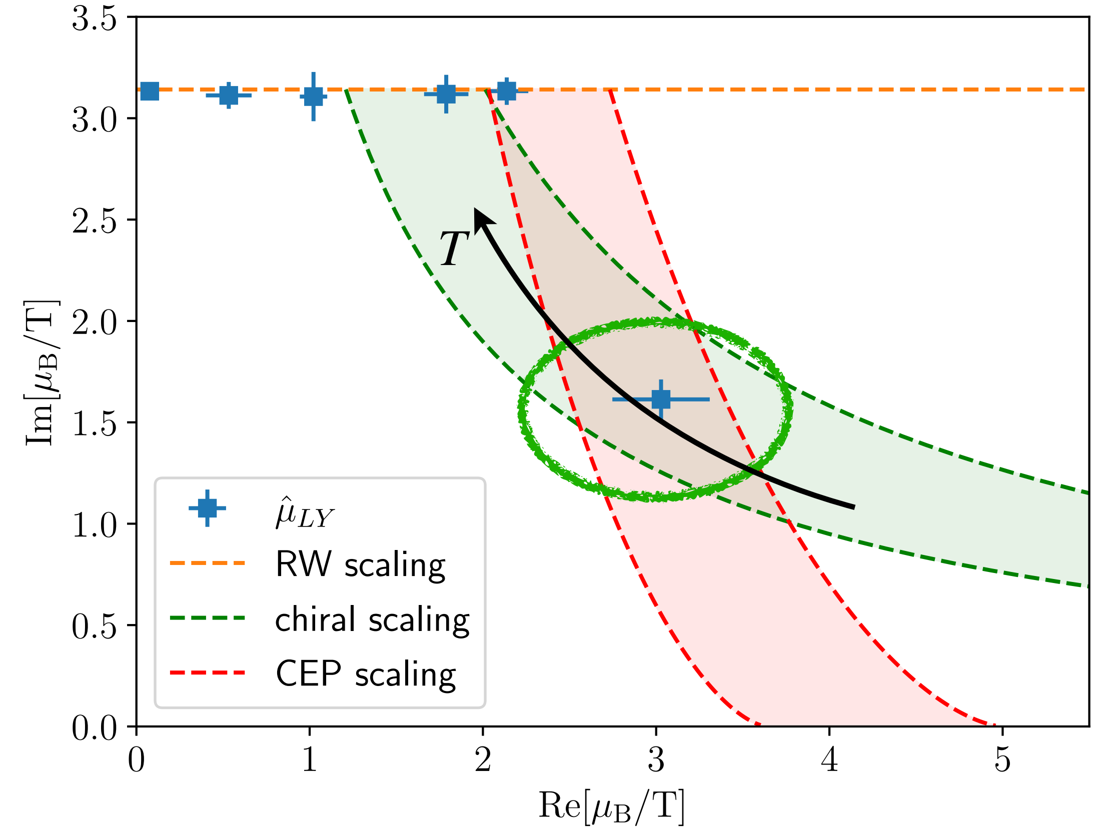

Care needed! … but intriguing … what we found is compared with 68% and 95% confidence regions of a theoretical prediction (no fit!)
Our first, preliminary indication of a chiral singularity…

MORE ON THIS IN K. ZAMBELLO'S TALK!

Can we trust all this ?!?

Let's test 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.

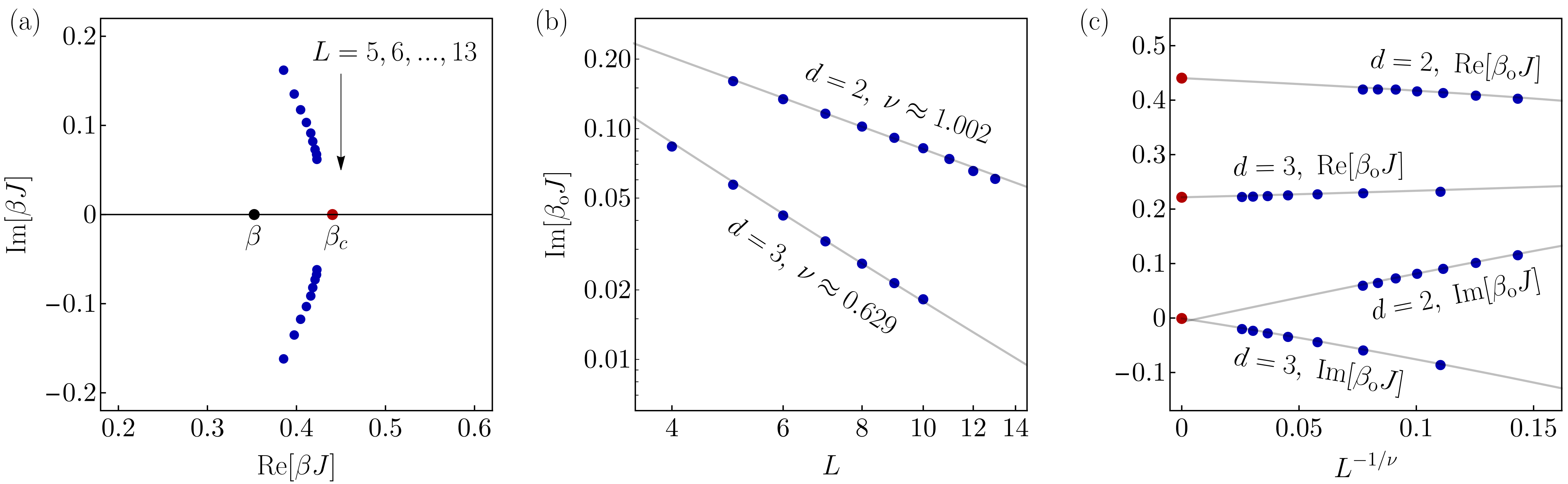

FIG. 2. Fisher zeros and critical exponents. (a) The leading Fisher zeros (blue circles) for the Ising model with $d = 2$ are extracted from the energy cumulants of order $n = 6, 7, 8, 9$. With increasing system size, the Fisher zeros approach the critical inverse temperature $\beta_c J \simeq 0.4404$

PHYSICAL REVIEW RESEARCH 1, 023004 (2019)

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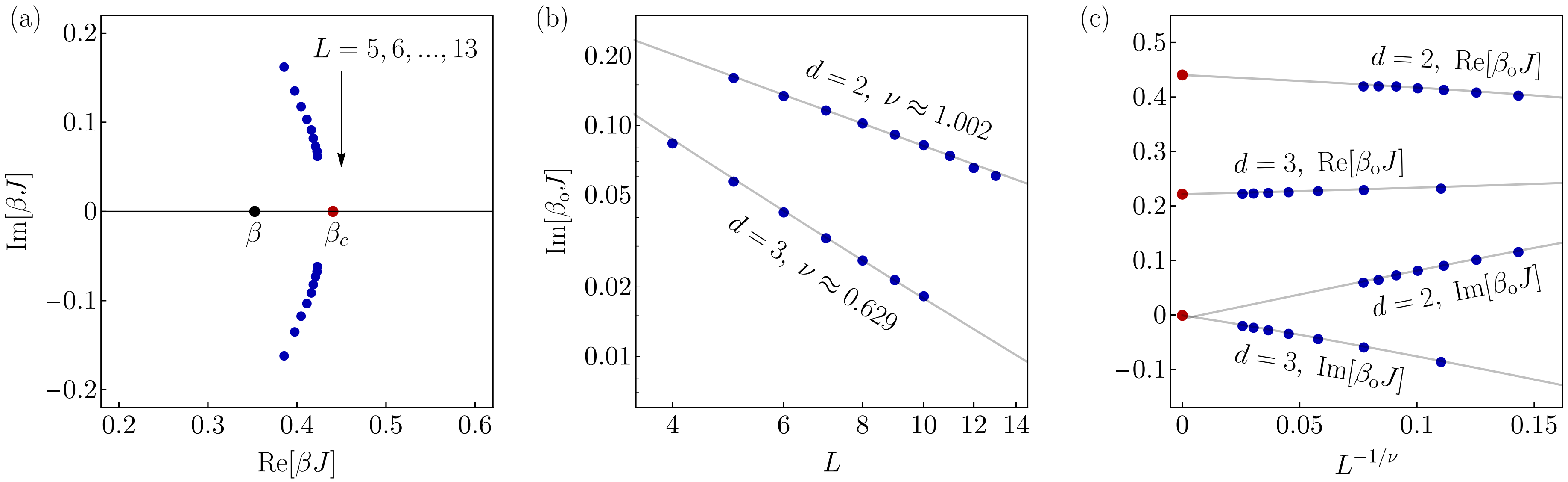
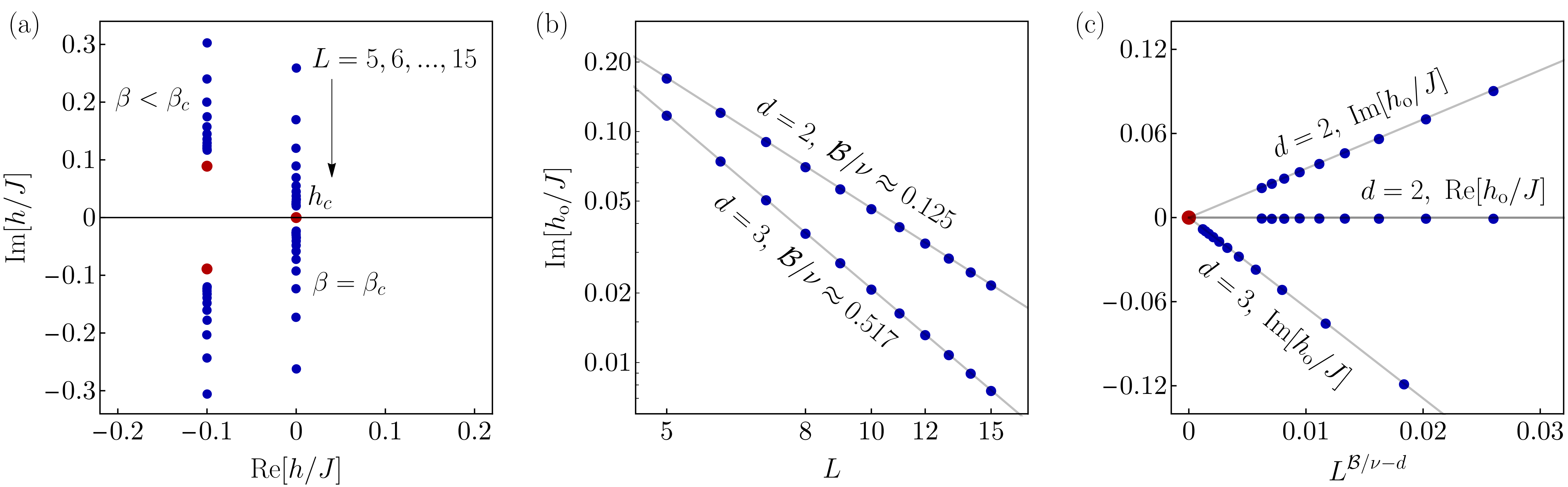
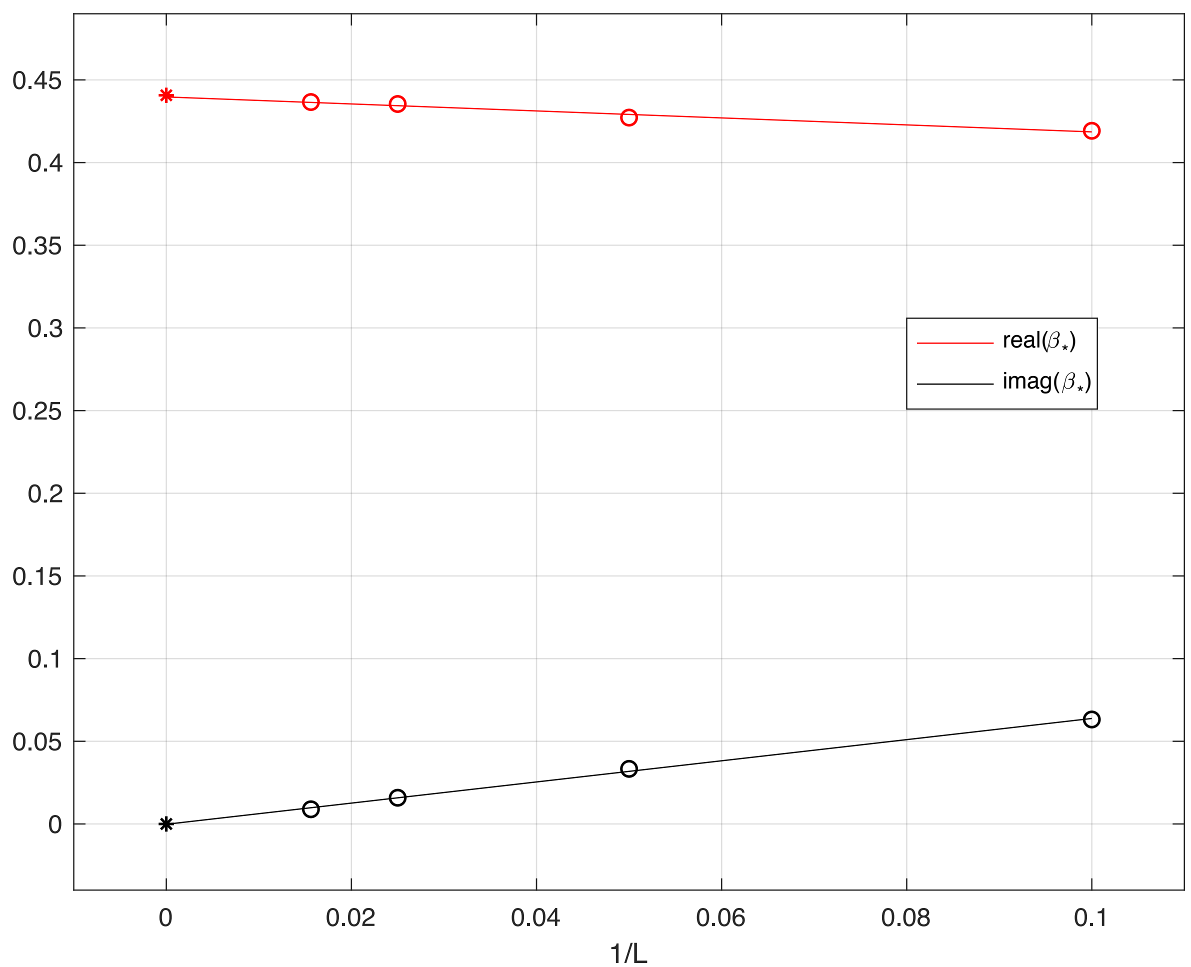


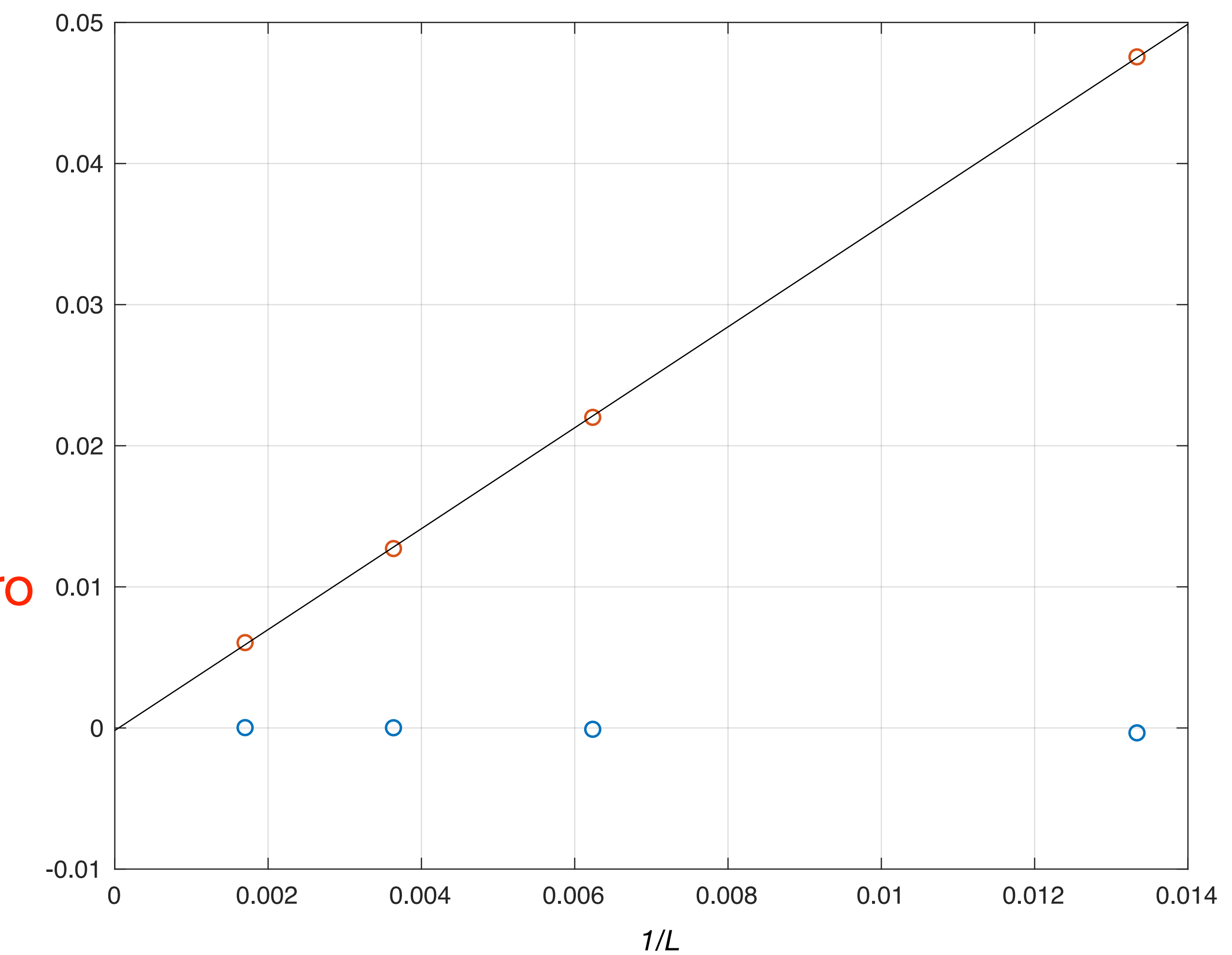
Dealing now with leading zeros from magnetisation cumulants (now derive with respect to magnetic field)



… and this is what we can get with our multi-point PADÈ method!

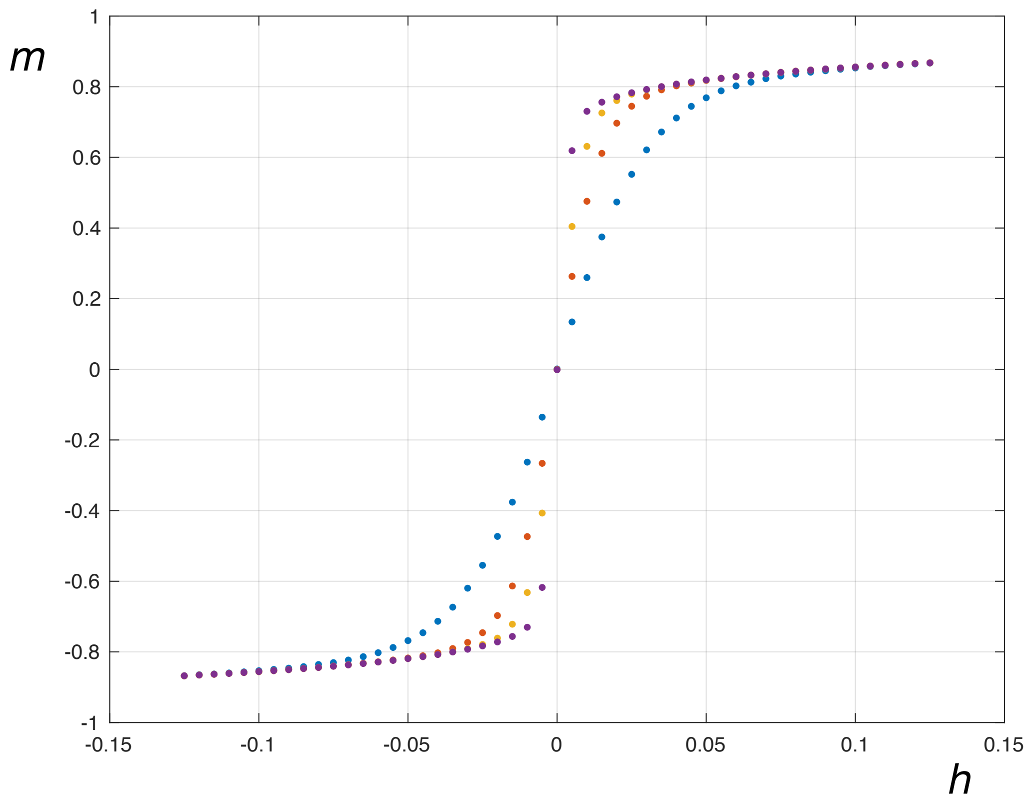


Real and imaginary parts of the leading (Fisher) zero as a function of (inverse) lattice size (from the computation of specific heat at different temperatures and lattice sizes)



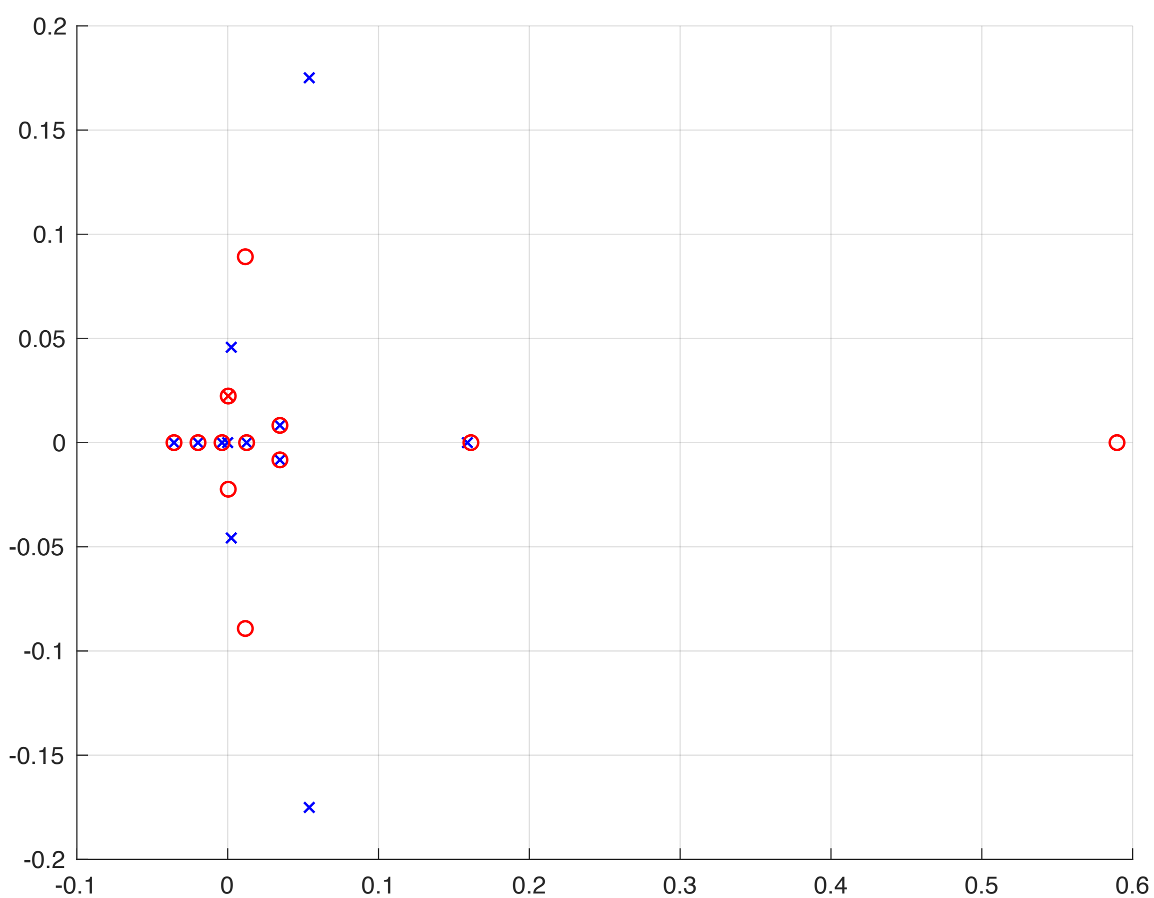
Real and imaginary parts of the leading (Lee Yang) zero as a function of (inverse) lattice size (from the computation of magnetisation at different magnetic fields and lattice sizes)

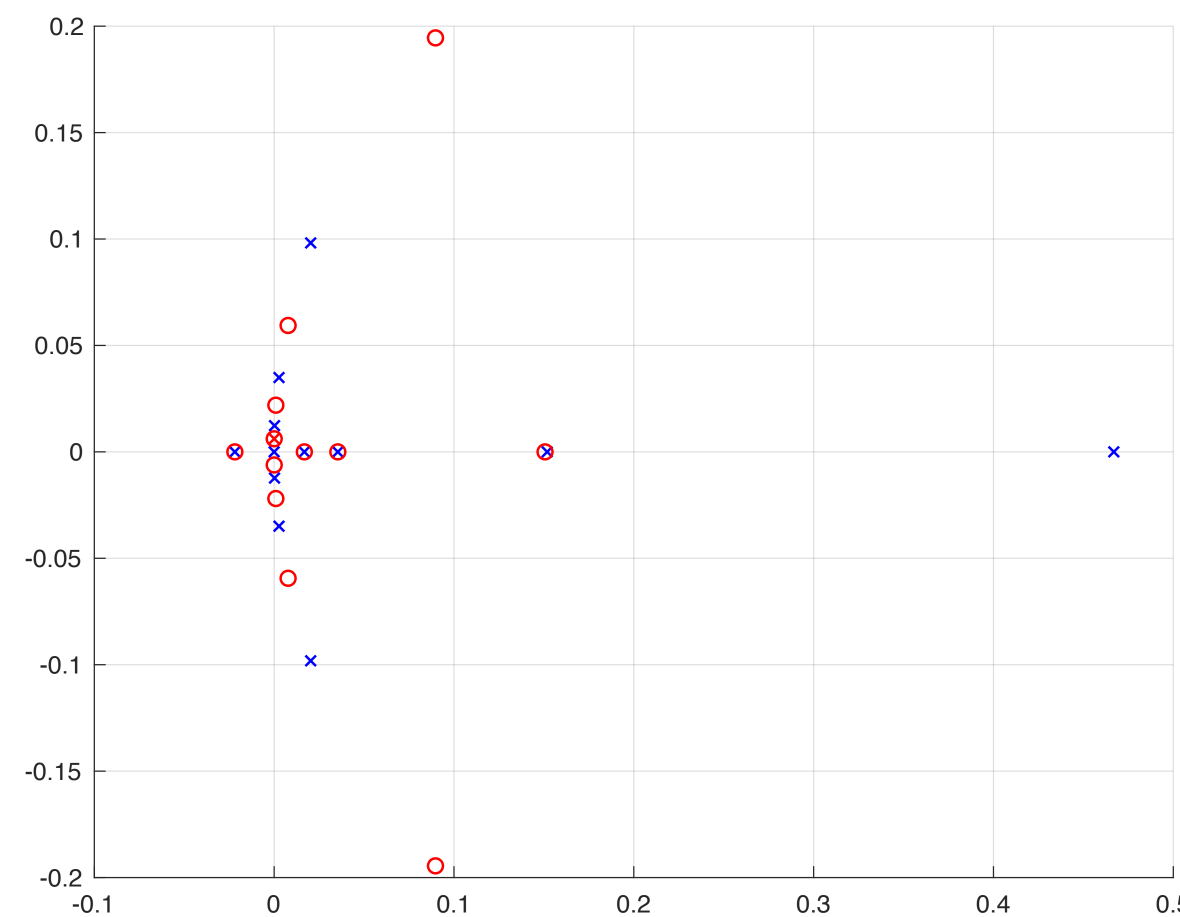
Remember what it means … (we take the case of m vs h)



- computation of magnetisation at different magnetic fields and lattice size
- determination of the leading pole (red symbols) from the Padè approximants
- scaling of the leading zero

(figures are in complex h plane)





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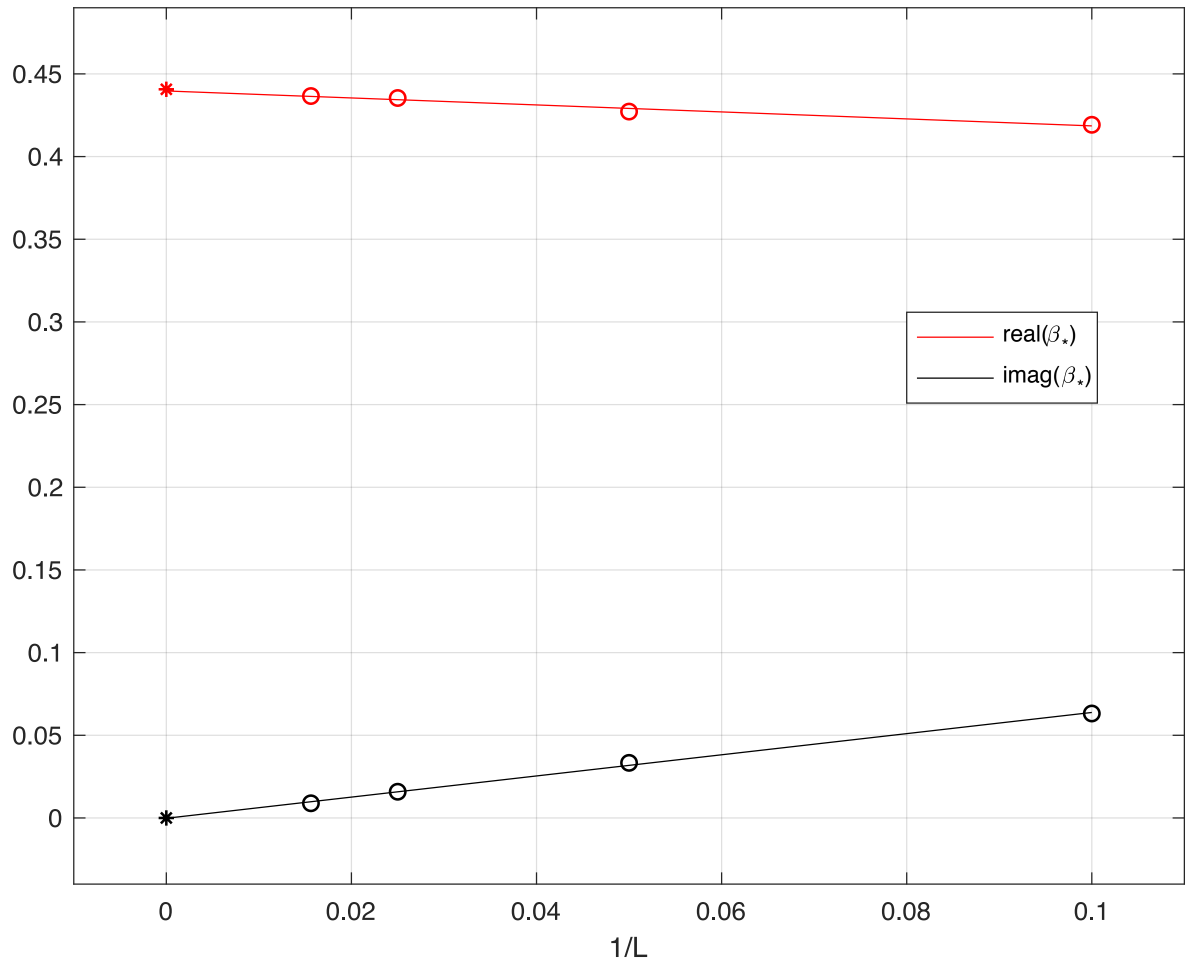
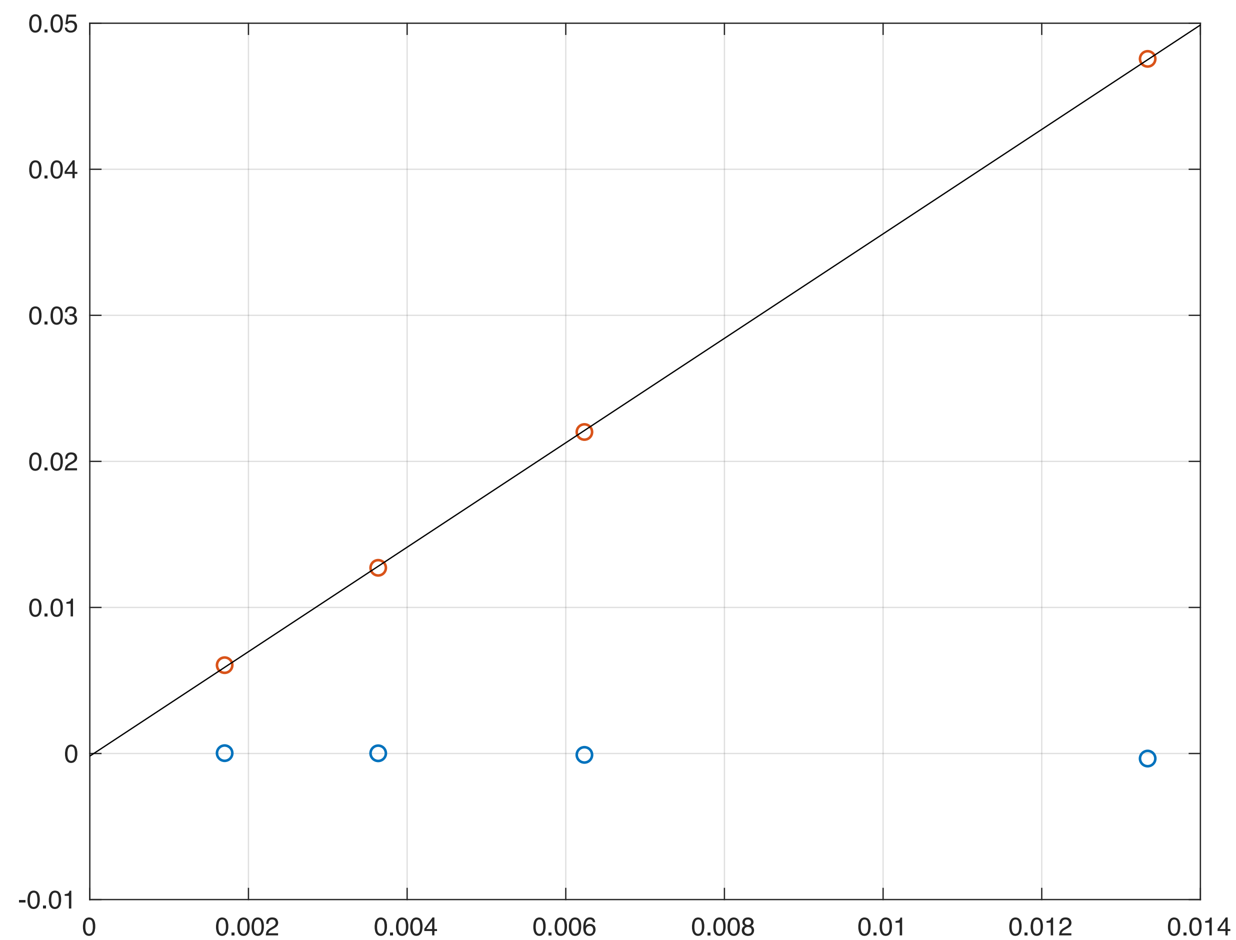


(Errors are smaller than symbols sizes)

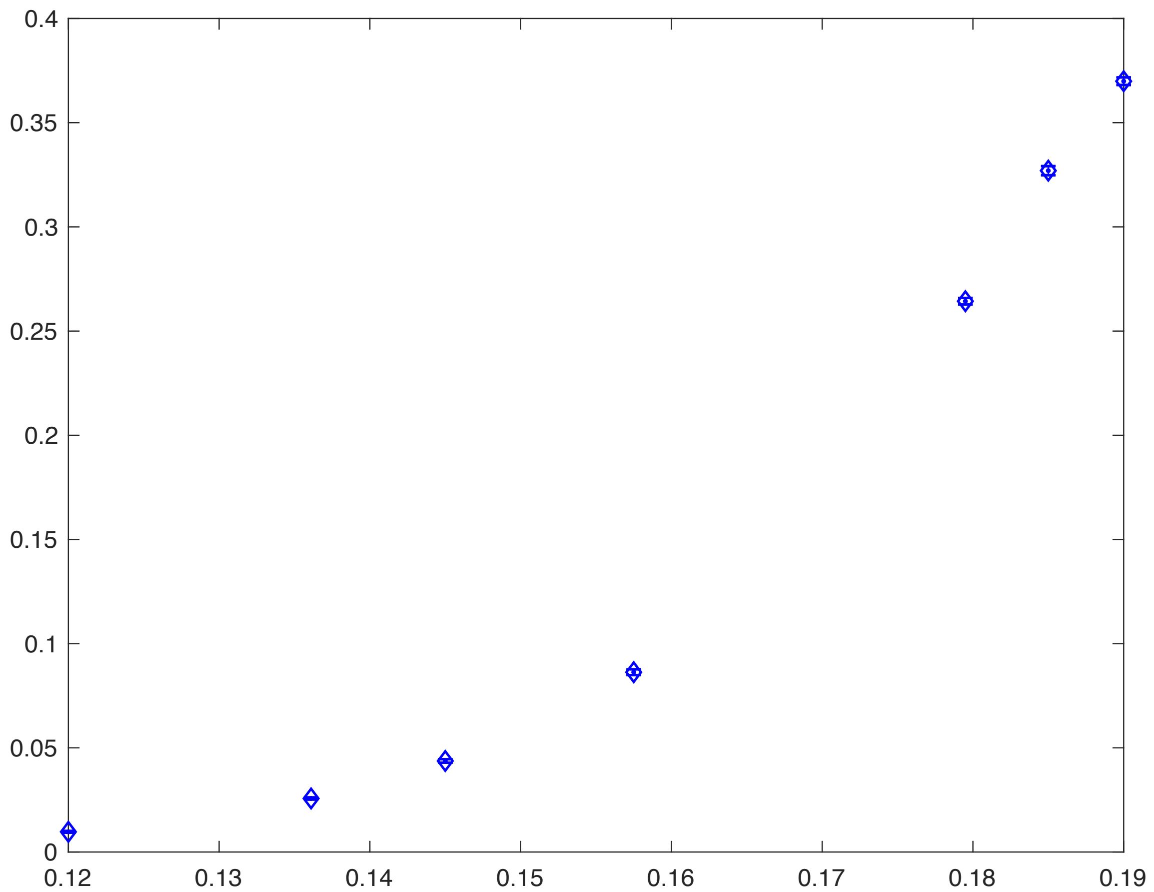
Critical exponents got at a few per mille level



Something new:

Temperature Padé approximants

Play again the Padé game, this time in T!



We computed the baryon density at different values of (imaginary) baryonic chemical potential and temperatures.

(Here we plot at a given value of chemical potential for different temperatures)

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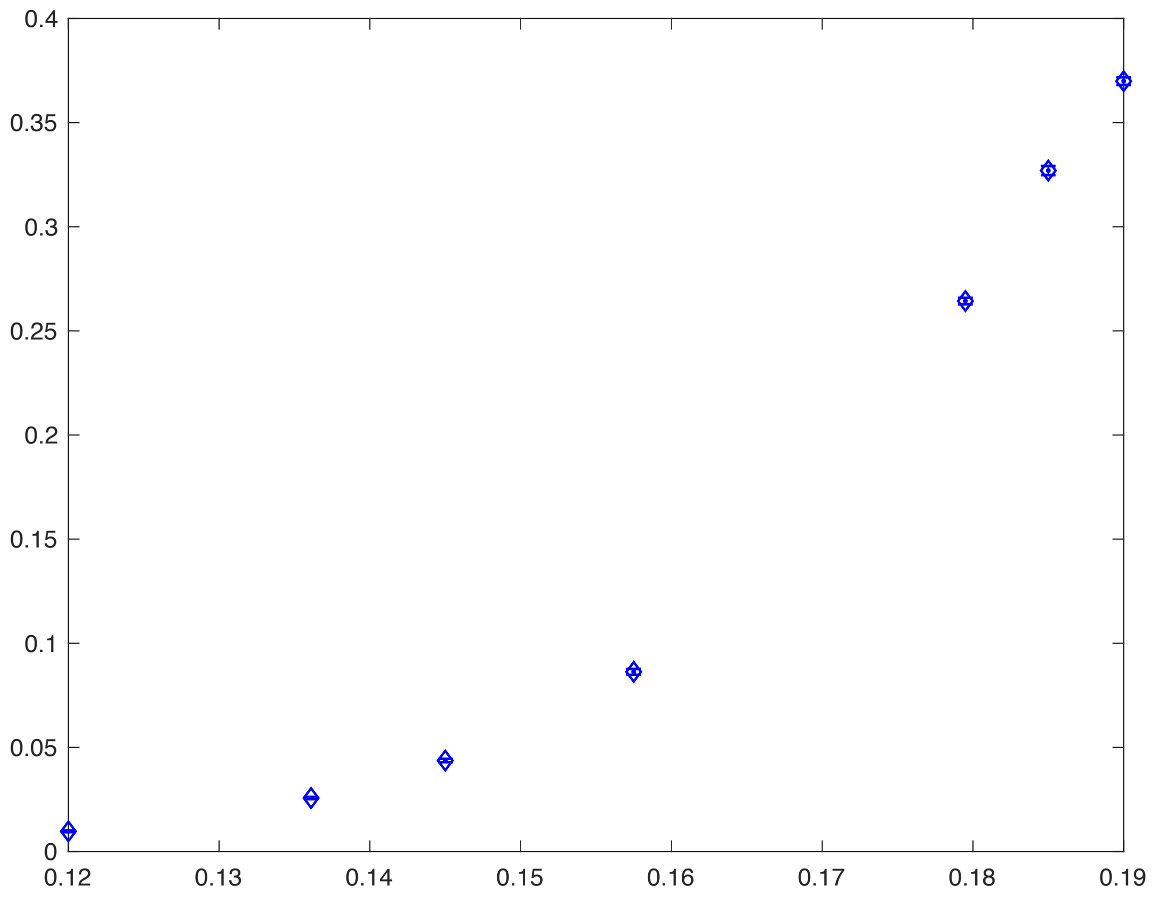
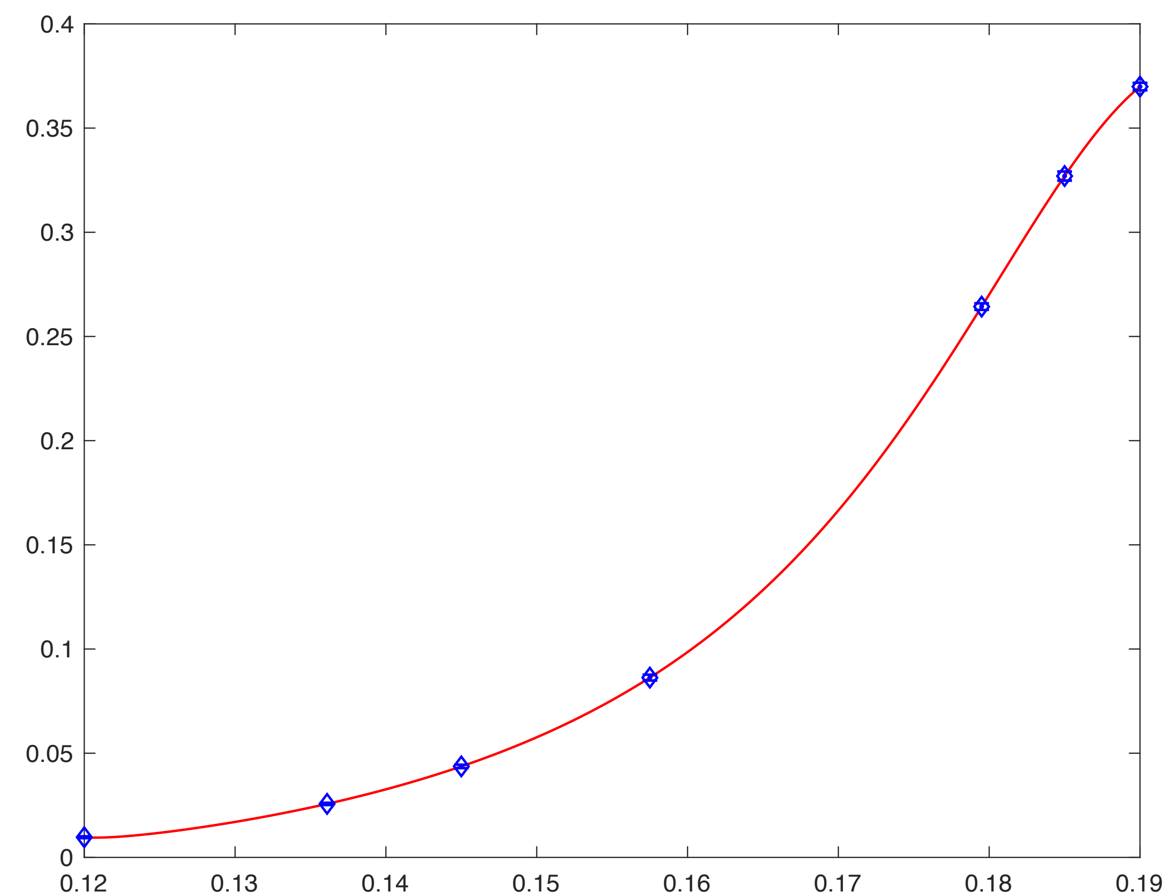


We computed the baryon density at <u>different values</u> of (imaginary) baryonic chemical potential and temperatures.

(Here we plot at a given value of chemical potential for different temperatures)

We now compute Padé approximants which are ratios of polynomials in the temperature…

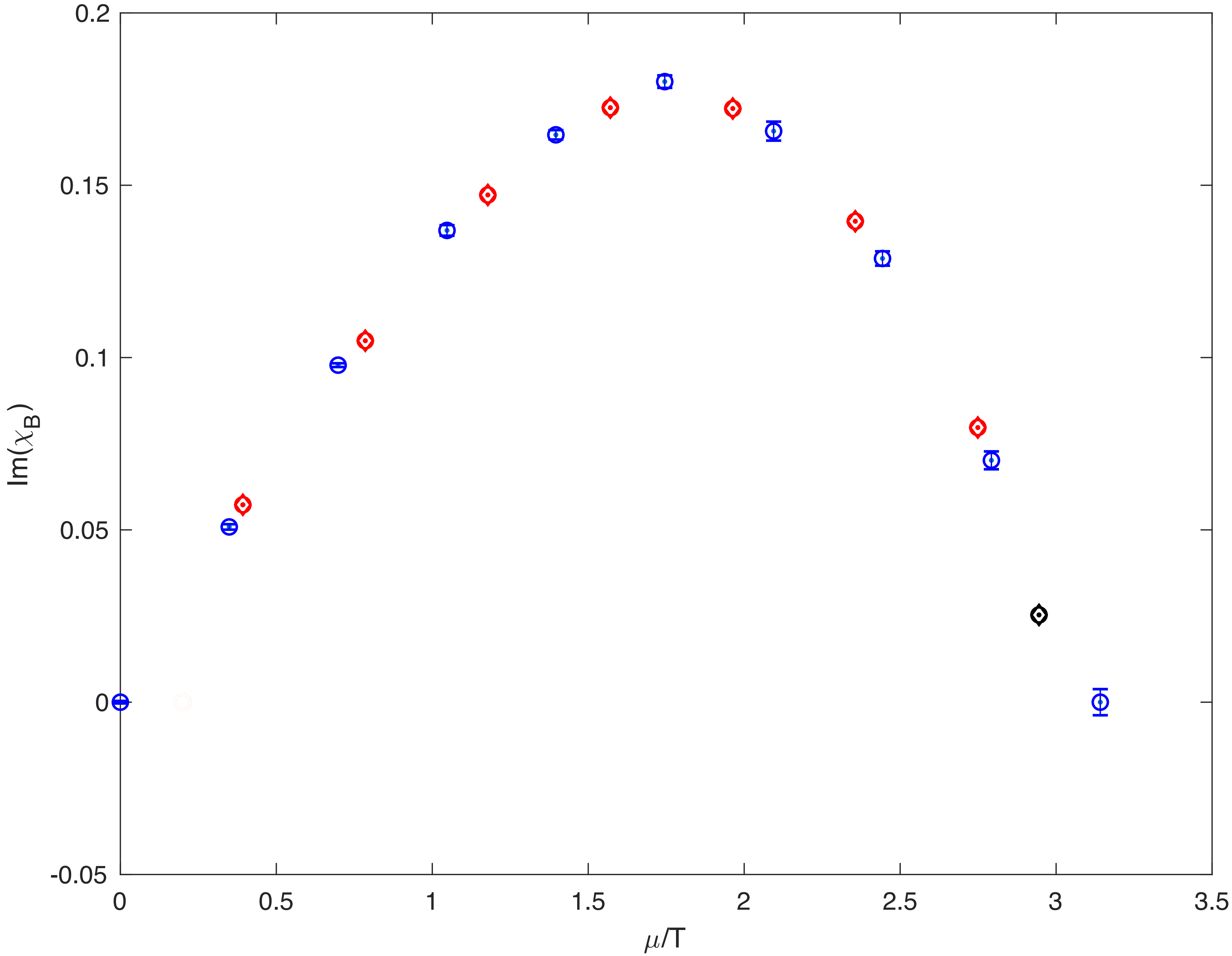
…looking pretty good in interpolating…



Indeed we are doing pretty well!

We now reconstruct the $\frac{\mu}{T}$ dependence at a given temperature!

(actual measurements and values dictated by Padé plotted together)

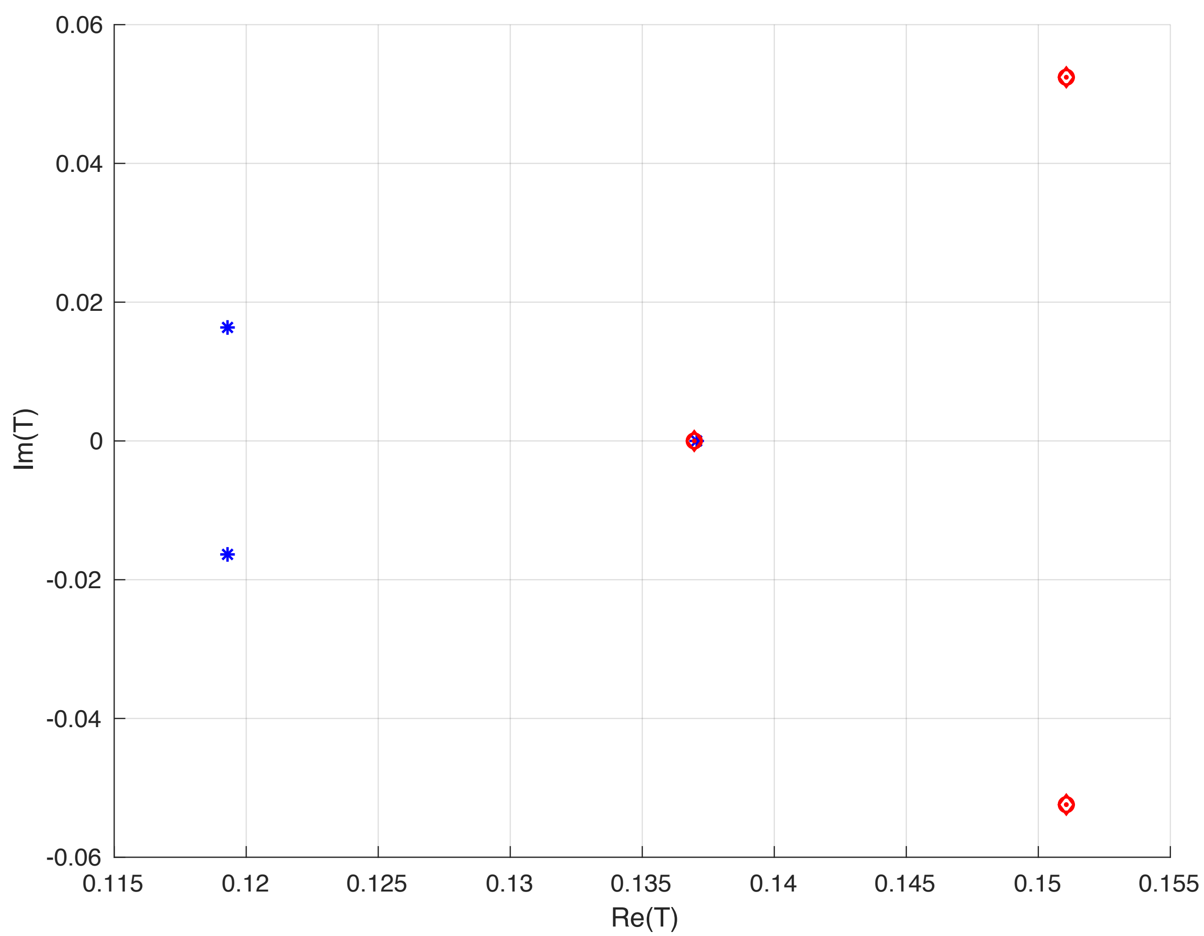


What about the (would-be) POLES in complex T plane?

(look at RED symbols)

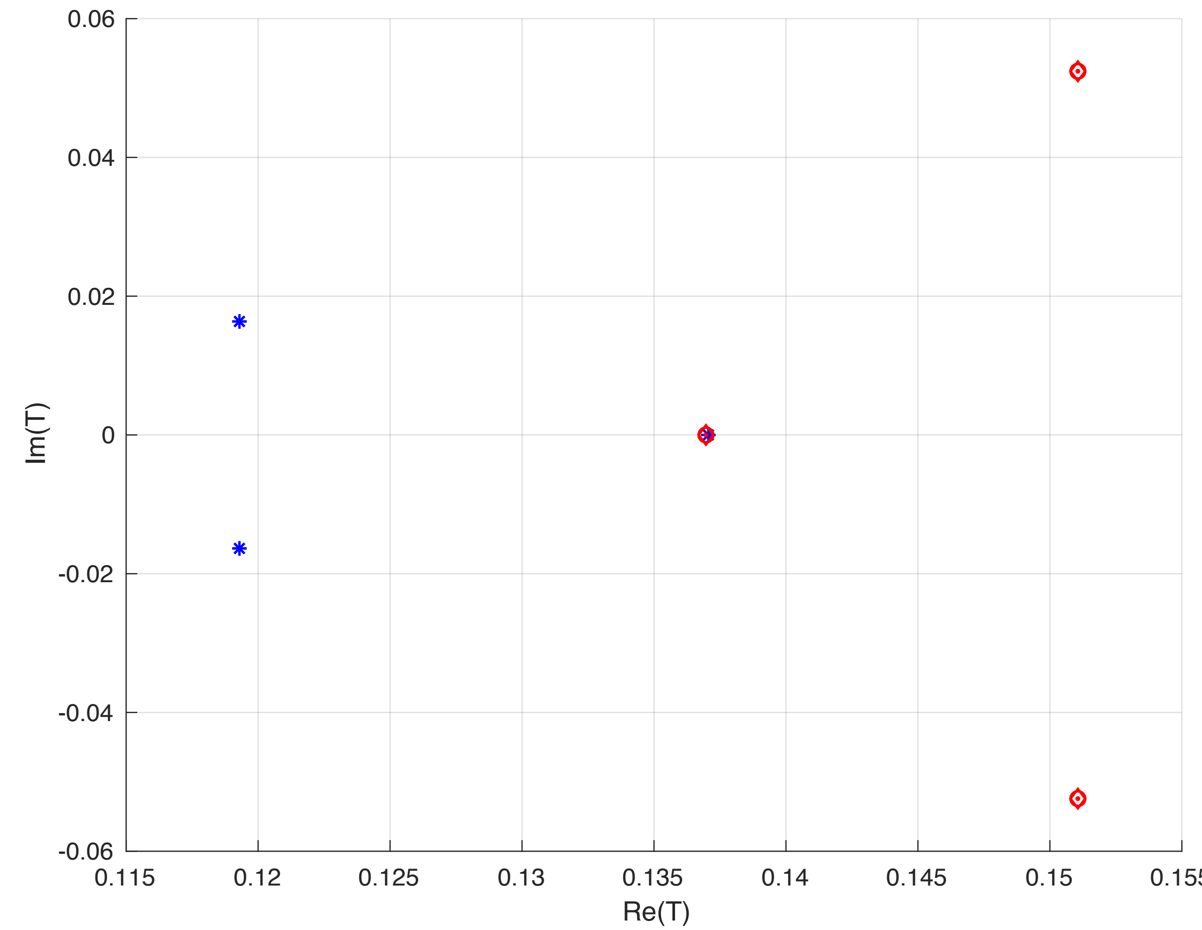
Here we are close to zero (imaginary) baryonic chemical potential…

… in the end, it makes sense …



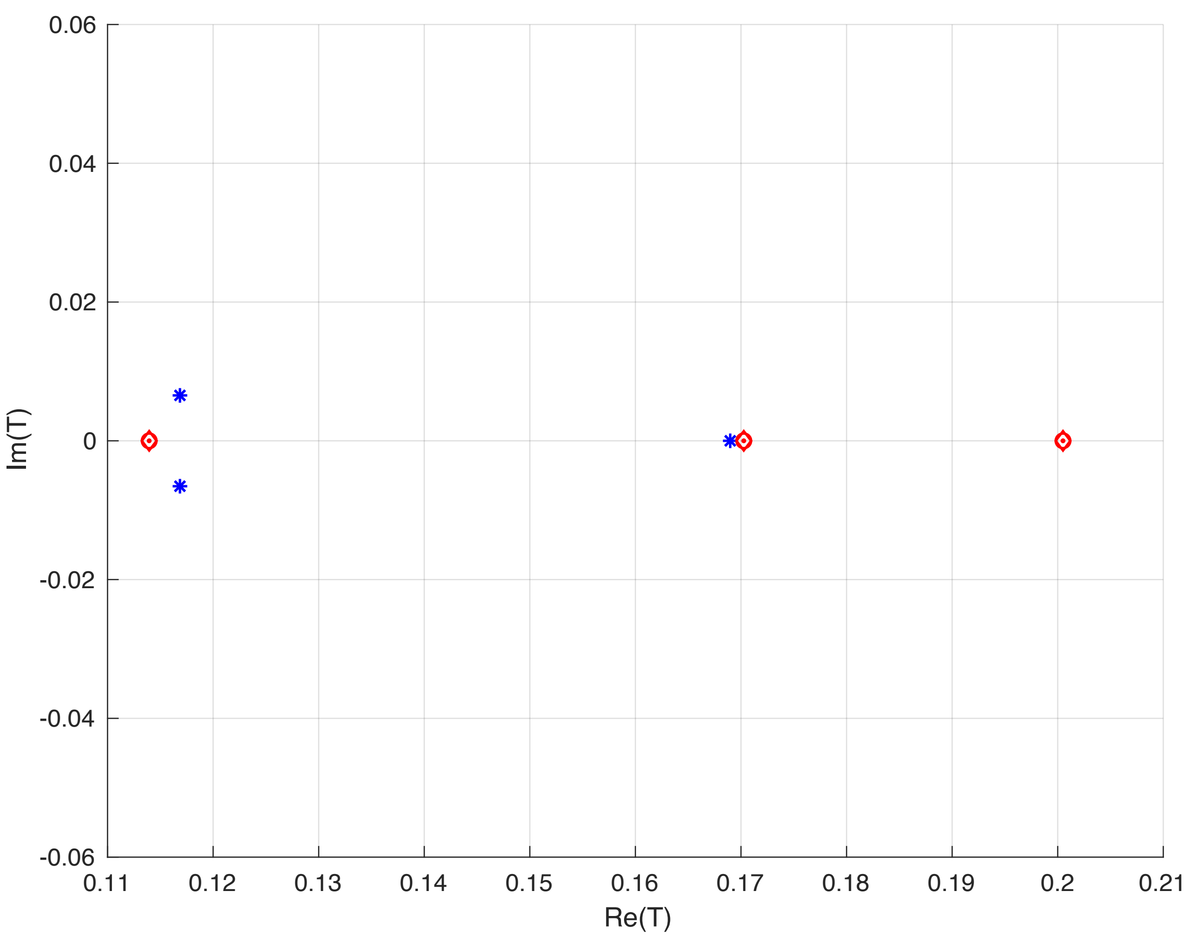
What about the (would-be) POLES in complex T plane?

(look at RED symbols)



Here we are close to zero (imaginary) baryonic chemical potential…

… in the end, it makes sense …



Here we are at high (imaginary) baryonic chemical potential…

… and in the end, again it makes 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, we are trying to better understand chiral transition. The Holy Grail (needless to say) is the critical point… **MORE ON THIS IN THE NEXT TALK!**

2. We are gaining more and more confidence in the method itself (works very well for Ising 2d)

3. We presented preliminary steps for Padé analysis in the complex temperature plane. Results started making sense…