The Phase Structure of Strong Interaction Matter from Lee-Yang Edge Singularities in Lattice QCD

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CRC–TR 211

Based on:

- P. Dimopoulos, L. Dini, F. Di Renzo, J. Goswami, G. Nicotra, CS, S. Singh, K. Zambello, F. Ziesché, PRD **105** (2022) 3, 034513, arXiv:2110.15933
- D. Bollweg, J. Goswami, O. Kaczmarek, F. Karsch, Swagato Mukherjee, P. Petreczky, CS, P. Scior arXiv:2202.09184

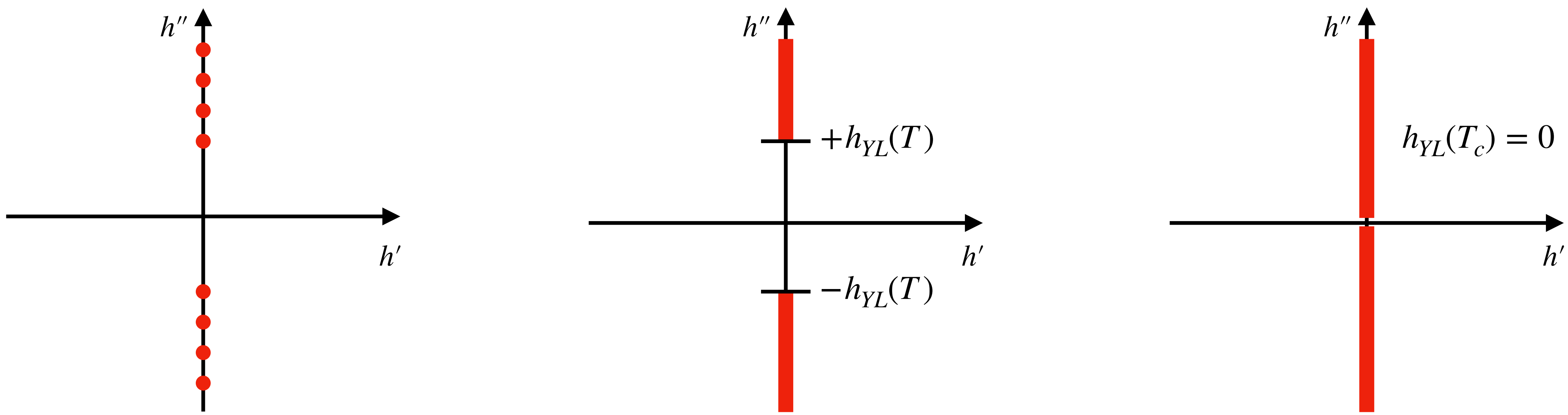
* Introduction and Motivation
* The multipoint Padé method
* Universal Scaling in the vicinity of the Roberge-Weiss transition
* Universal Scaling in the vicinity of the chiral transition
* The standard Padé resummation at $\mu_B = 0$ [talk by Frithjof]
* Universal Scaling in the vicinity of the QCD critical point

What is a Lee-Yang edge singularity?

Consider a generic ferromagnetic Ising or O(N) model:

- One finds zeros of the partition function only at imaginary values of the symmetry breaking field [Lee, Yang 1952]
- In the thermodynamic limit the zeros become dense on the line $h' = 0$

$$Z(V,T,h) \equiv 0, \quad h = h' + ih''$$



V finite, $T > T_c$ — $V \to \infty, T > T_c$ — $V \to \infty, T \to T_c$

- The density of Lee-Yang zeros $g(T,h'')$ behaves as $g(T,h'') \sim |h'' - h_{YL}(T)|^{\sigma_{LY}}$ for $h'' \to h_{LY}(T)$ from above [Kortman, Griffiths 1971; Fischer 1978].
- Fischer connected the edge-singularity with a phase transition in an φ^3-theory with imaginary coupling [Fischer 1978]
- 5-Loop calculation of this theory yields $\sigma_{LY} \sim 0.075$ (d=3) [Borinsky et al., Phys. Rev. D 103, 116024 (2021)]

Why should we care about Lee-Yang edge singularities?

- The approach $h_{LY} \to 0$ for $T \to T_c$ signals a ‘physical’ phase transition
  $\longrightarrow$ helps to determine a phase transition point. Search for QCD critical point?

- They limit the radius of convergence of any power series
  $\longrightarrow$ Taylor expansion method in QCD

- They provide important information on the singular part of the free energy, $f \sim |h'' - h_{YL}(T)|^{\sigma_{LY}+1}$ but also as the starting point of a branch cut
  $\longrightarrow$ improves analytic continuation, imaginary μ-method in QCD

- The position $h_{LY}(T)$ together with universal scaling provides us with another procedure to determine nonuniversal constants
  $\longrightarrow$ more precise determination of nonuniversal constants

What are the universal properties of Lee-Yang edge singularities?

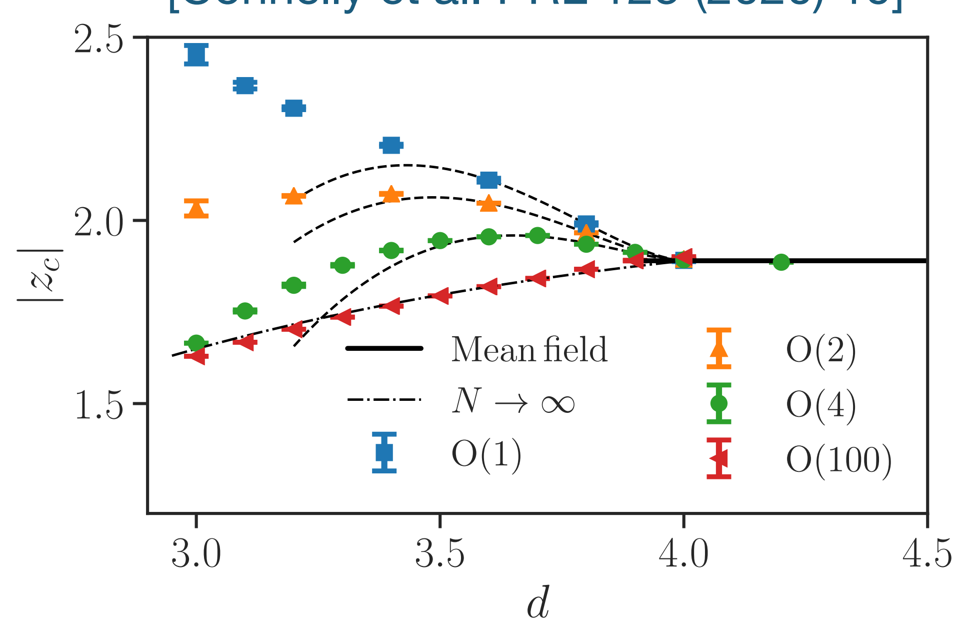
* Scaling relies on the assumption that the singular part of the free energy is a generalised homogeneous function $f(t,h) = b^{-d} f(b^{y_t} t, b^{y_h} h)$ with $t = T - T_c$. We can get rid of one argument by introducing a scaling variable, e.g., $z = t/h^{1/\beta\delta}$ which yields $f = h^{\frac{2-\alpha}{\beta\delta}} f_f(z)$.

* In terms of the scaling variable z, the position of the the Lee-Yang edge singularity is universal. We find $z_{LY} = |z_c| e^{i\frac{\pi}{2\beta\delta}}$. The modulus has been calculated recently by means of functional renormalization group methods

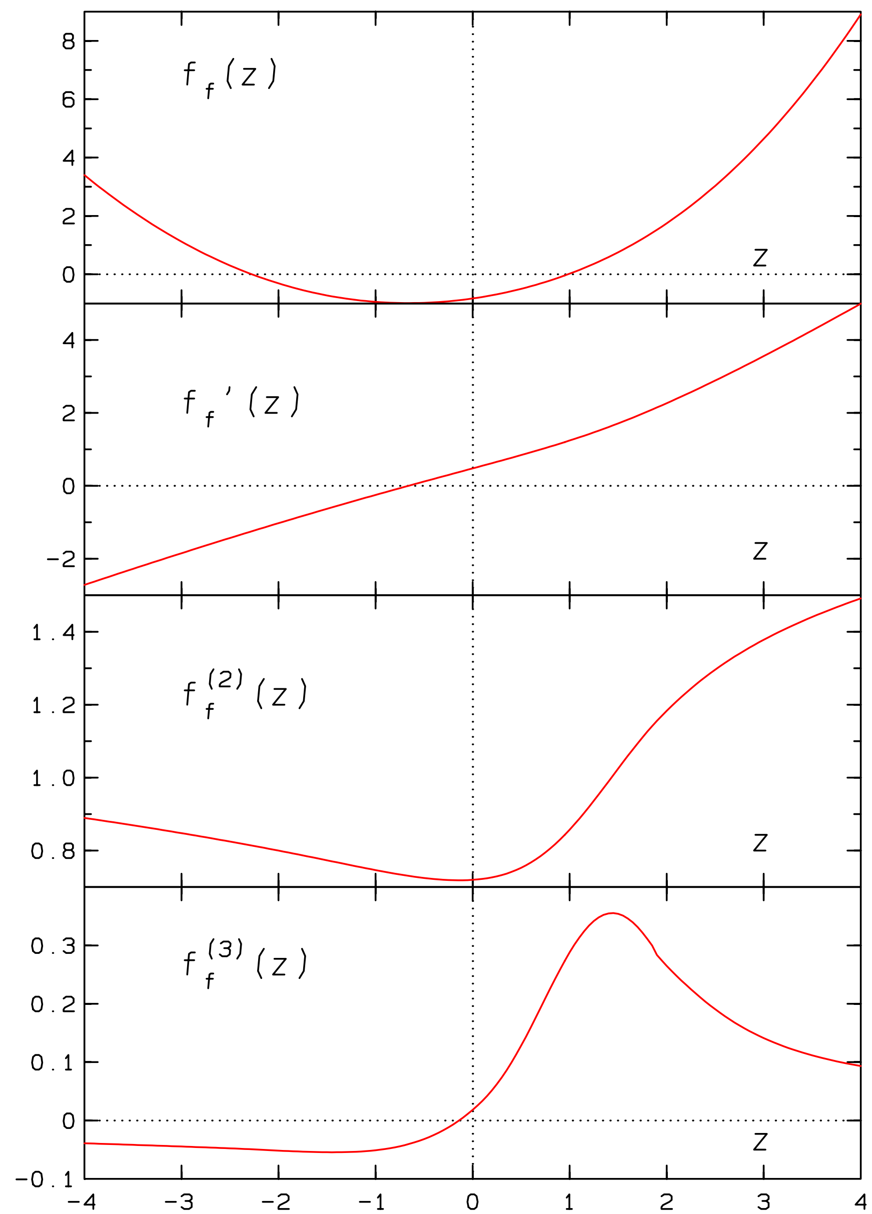
* The exponent σ_{LY} is also universal, and independent of the symmetry group (N)

* Eos: $M = h^{1/\delta} f_G(z)$;
  The universal scaling function $f_G(z)$ exhibits a branch cut starting at $z = z_{LY}$

[Connelly et al. PRL 125 (2020) 19]

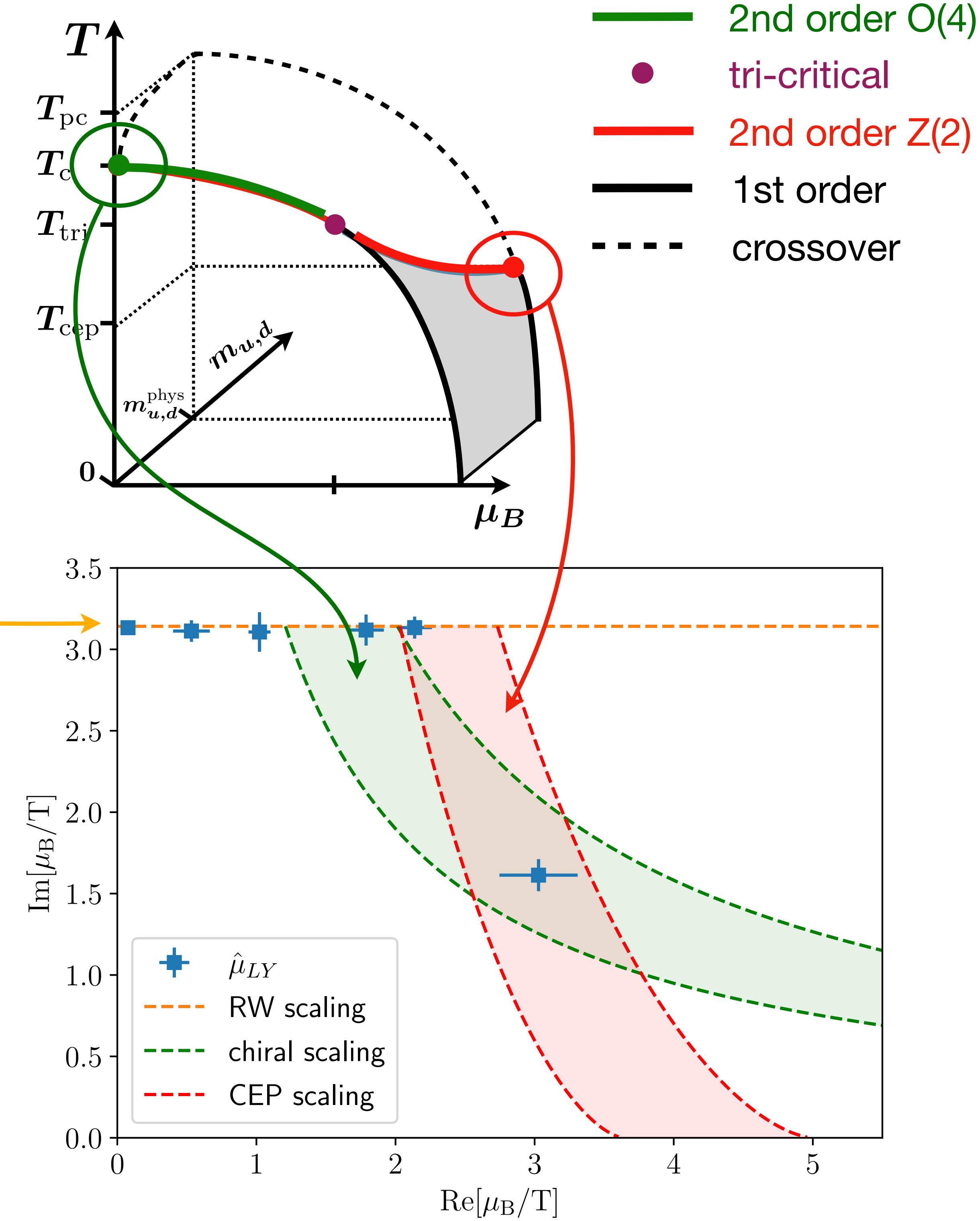


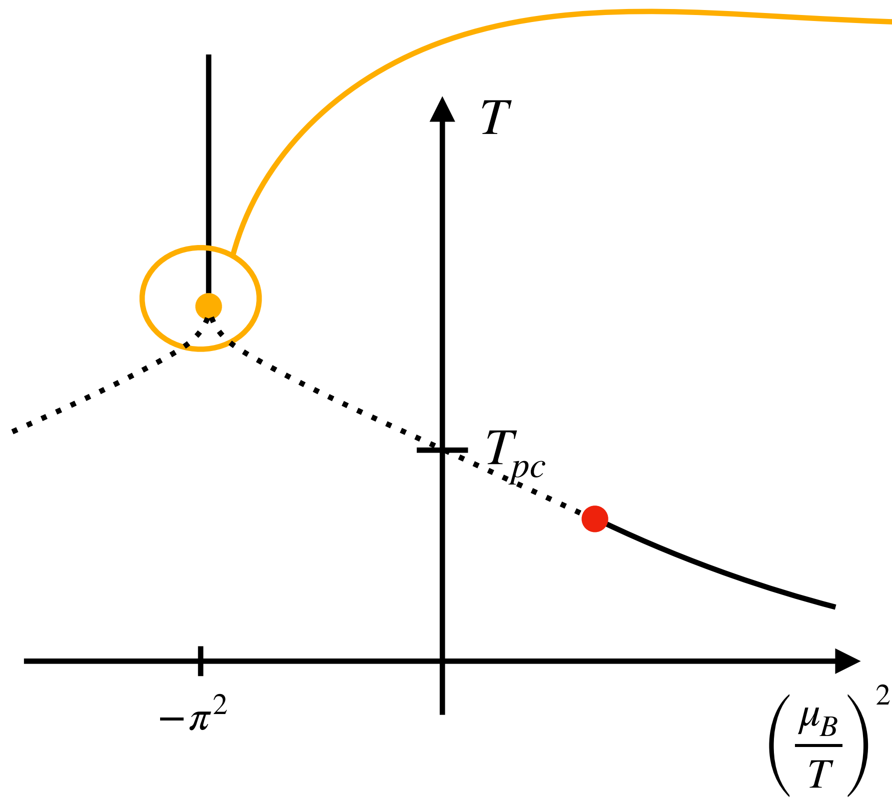
[Engels, Karsch, PRD 85 (2012) 094506]



Where can we apply our knowledge of Lee-Yang edge singularities in QCD?

- 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

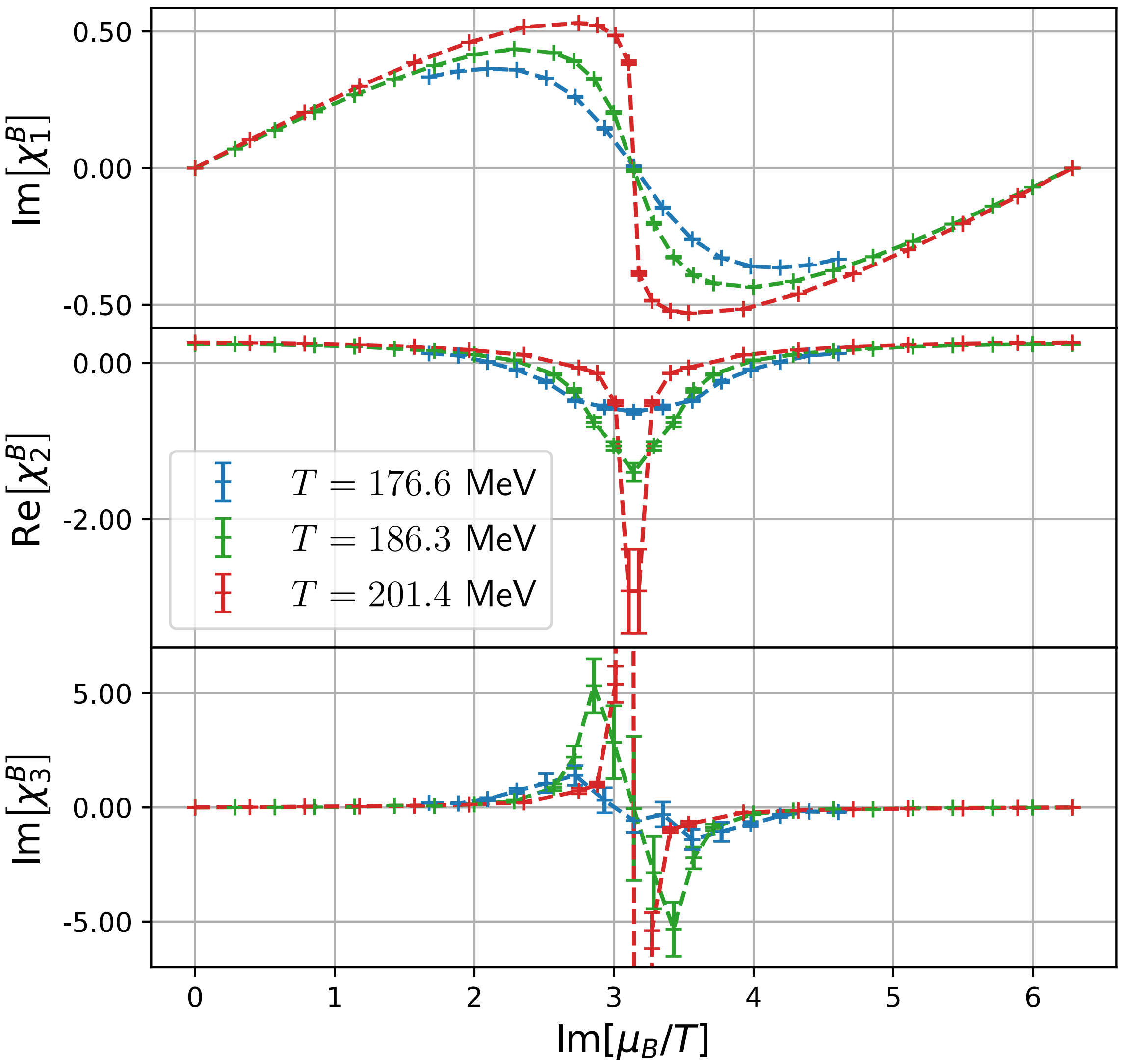




Input data from Lattice QCD:

- We use (2+1)-flavor of highly improved staggered quarks (HISQ)
- Simulations at $\mu_B > 0$ are not possible due to the infamous sign problem
- Instead we perform calculations at imaginary chemical potential $\mu_B = i\mu_B^I$ [De Frorcrand, Philipsen (2002); D'Elia, Lombardo (2003)]
- The temperature scale and line of constant physics is taken from previous HotQCD calculations [see e.g., Bollweg et al. PRD 104 (2021)]
- We measure cumulants of net baryon number in the interval $i\mu_B^I/T \in [0,\pi]$ [Allton et al. PRD 66 (2002)]
- The cumulants χ_n^B are odd and imaginary for n odd and even and and real for n even

Lattice size: $24^3 \times 4$



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

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

Standard Padé:

- Starting point is a power series

$$f(x) = \sum_{i=0}^{L} c_i\, x^i + \mathcal{O}(x^{L+1})\,.$$

- A Padé approximation is constructed such that the expansion of the Padé is identical to the Taylor series about $x = 0$

- We denote the [m/n]-Padé as

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

- One possibility to solve for the coefficients a_i, b_j, is by solving the tower of equations

$$P_m(0) - f(0)Q_n(0) = f(0)$$
$$P_m'(0) - f'(0)Q_n(0) - f(0)Q_n'(0) = f'(0)$$
$$\vdots$$

$\rightarrow$ Linear system of size $m + n + 1$, need $m + n$ derivatives of $f(x)$

Multipoint Padé:

- We have power series at several points x_k

- We demand that at all points x_k the expansion of the Padé is identical to the Taylor series about $x = x_k$

- One possibility (method I) to solve for the coefficients a_i, b_j, is by solving the tower of equations

$$P_m(x_0) - f(x_0)Q_n(x_0) = f(x_0)$$
$$P_m'(x_0) - f'(x_0)Q_n(x_0) - f(x_0)Q_n'(x_0) = f'(x_0)$$
$$\vdots$$
$$P_m(x_1) - f(x_1)Q_n(x_1) = f(x_1)$$
$$P_m'(x_1) - f'(x_1)Q_n(x_1) - f(x_1)Q_n'(x_1) = f'(x_1)$$
$$\vdots$$

$\rightarrow$ again a linear system of size $m + n + 1$, need much less derivatives, we have $m + n + 1 = \sum_k (L_k + 1)$

- Here we use $f = \chi_1^B$ and $x = \mu_B$
- Solving the linear system in the μ_B/T plane with two different *Ansatz* functions
- The most general form (*Ansatz* **NS**)

$$R_n^m(x) = \frac{\sum_{i=0}^{m} a_i\, x^i}{1 + \sum_{j=1}^{n} b_j\, x^j}$$

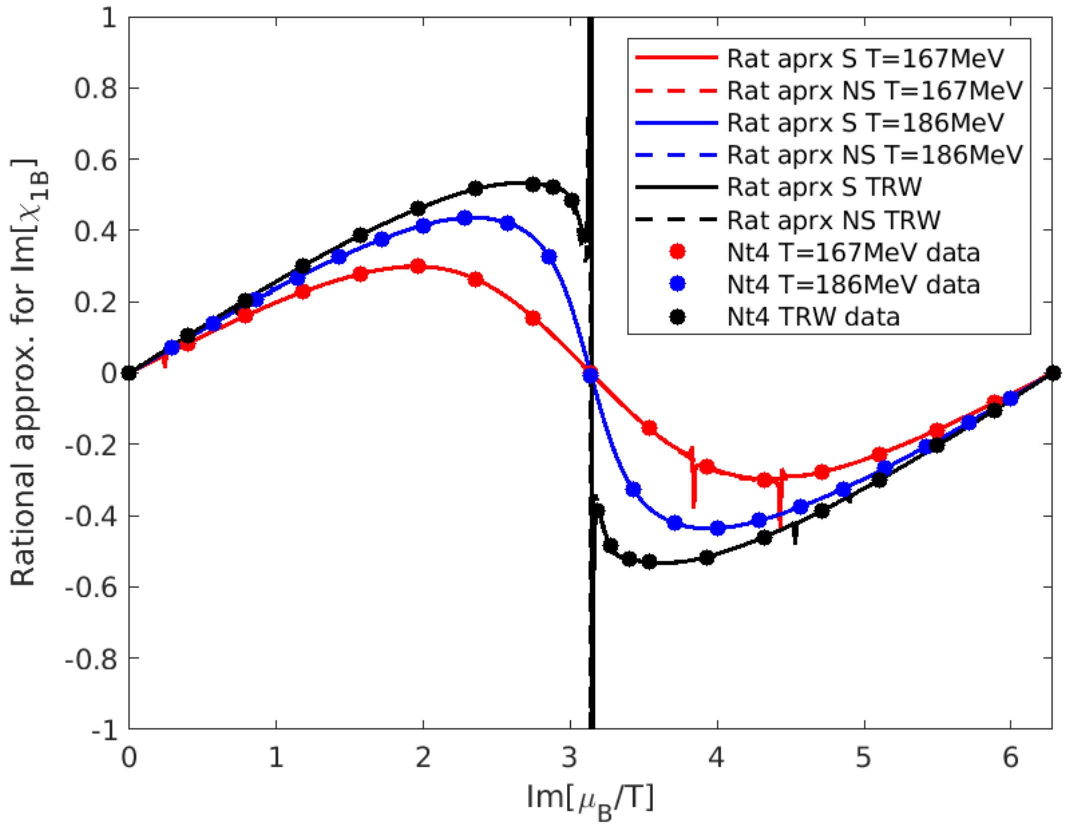
- Taking into account the expected parity of the net baryon number density (*Ansatz* **S**)

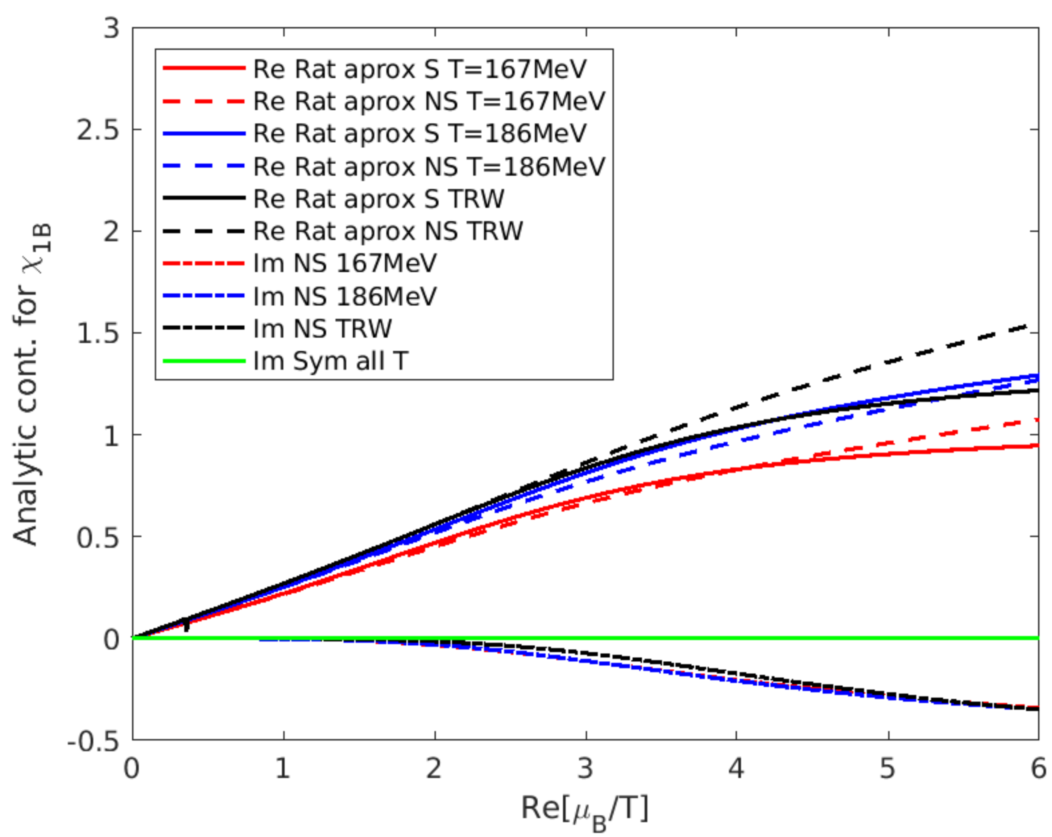
$$R_n^m(x) = \frac{\sum_{i=0}^{m'} a_{2i+1}\, x^{2i+1}}{1 + \sum_{j=1}^{n/2} b_{2j}\, x^{2j}} \qquad \text{with}$$

$$m = 2m' + 1; \;\; a_i, b_i \in \mathbb{R}; \;\; a_1 = \chi_2^B(T, V, 0)$$

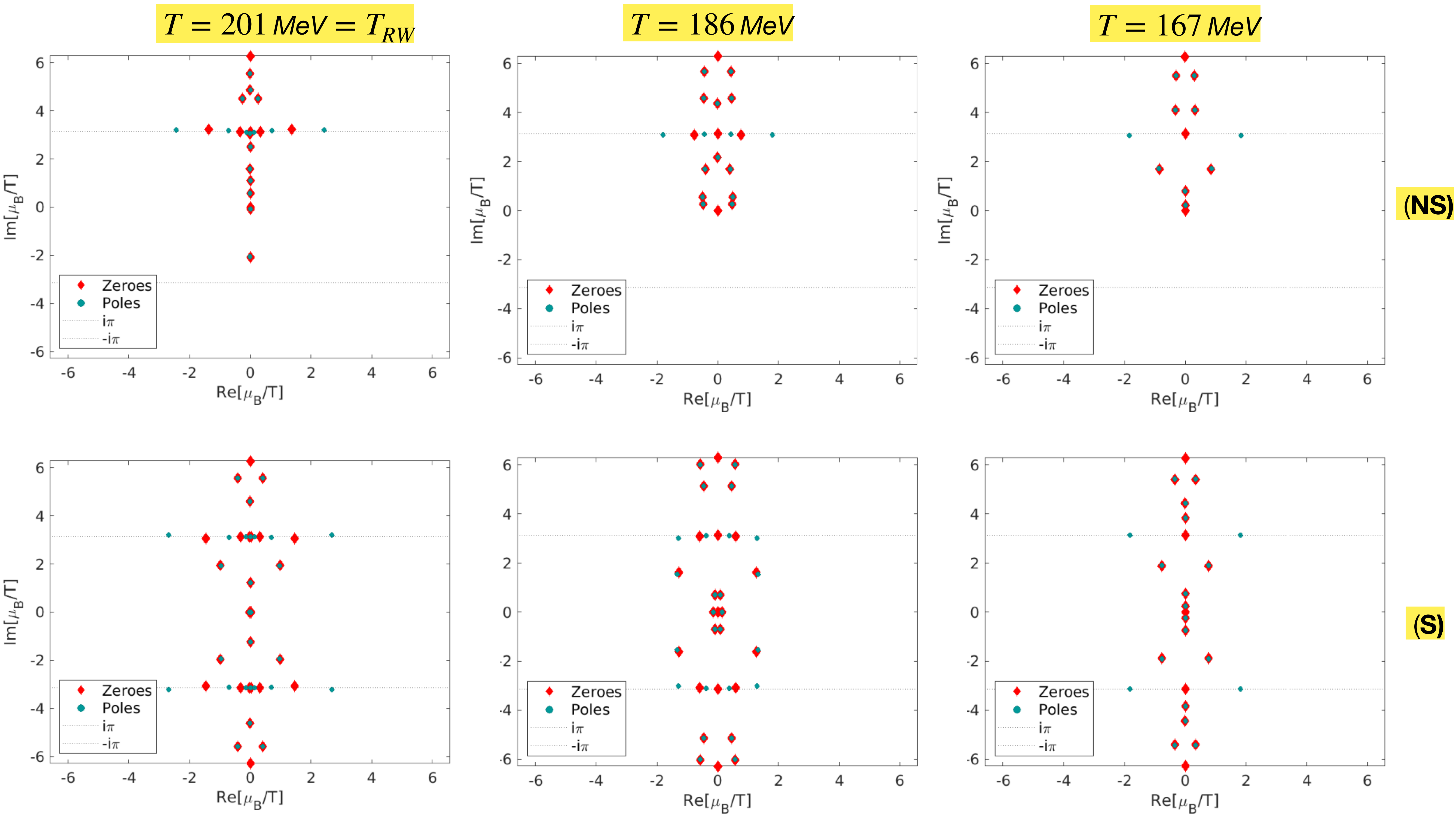
This ensures the correct parity for all χ_n^B, and a real valued analytic continuation.

→ find agreement in analytic continuation of both *for* $\mu_B/T \lesssim 2.5$





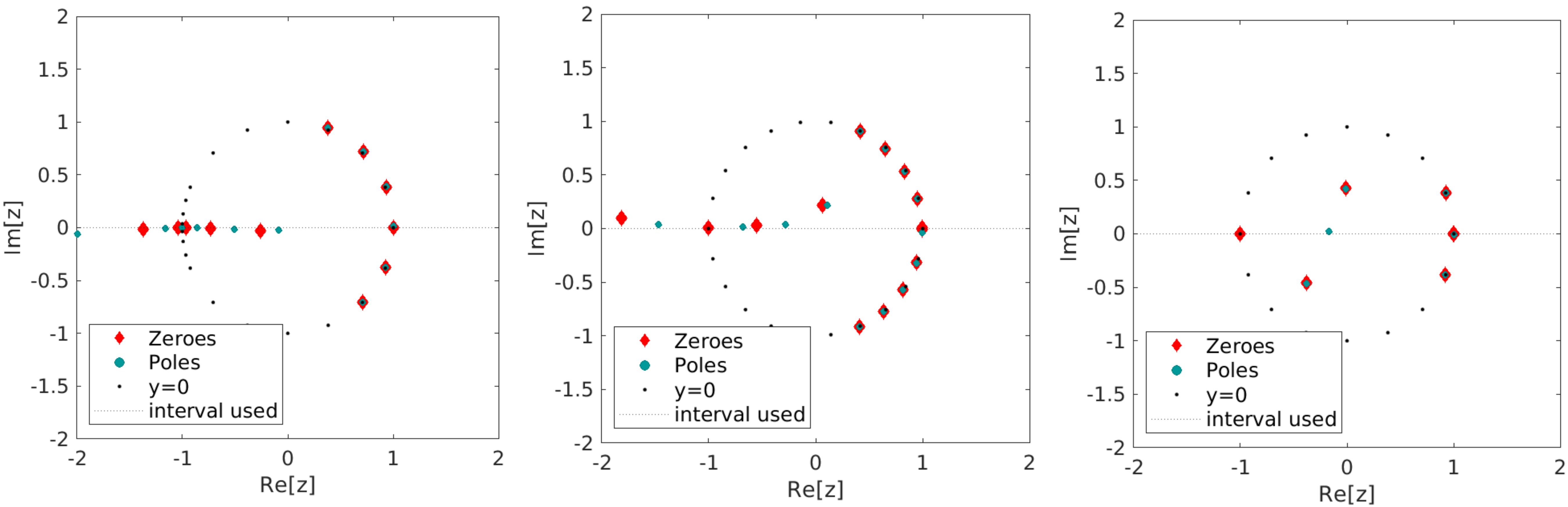
The multipoint Padé method - results singularity structure ($N_\tau = 4$)



→ find almost perfect cancelation of many zeros and poles

→ find signature for branch cut along $\mu_B/T = \mu_B^R \pm i\pi$ at $T = \{201{,}186\}$ MeV

The multipoint Padé method - results singularity structure ($N_\tau = 4$)



* We can solve the linear system in the fugacity plane

  → find signature for branch cut along $z = -z^R$ at $T = \{201{,}186\}$ MeV

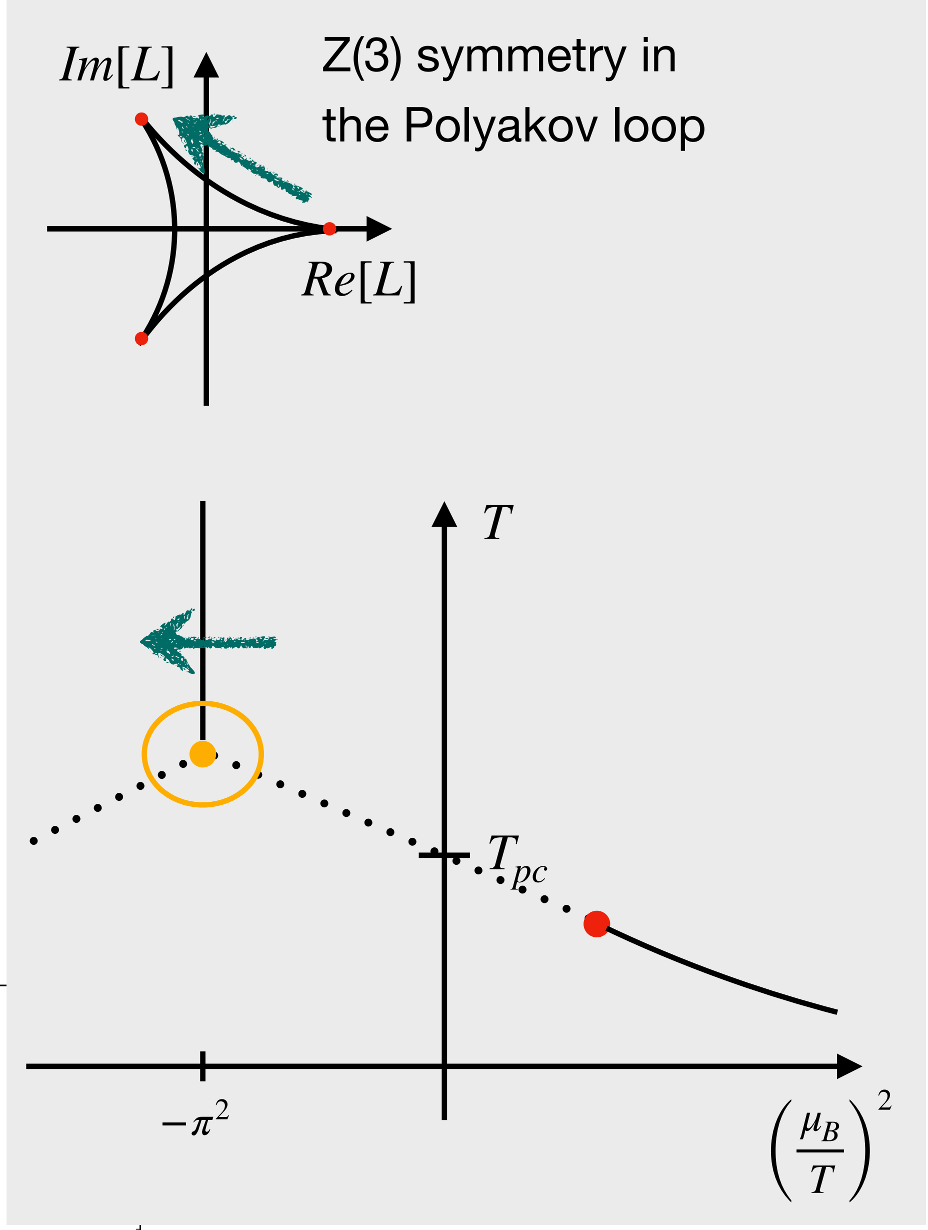
* First steps toward using more complicated conformal mappings [Skokov, Morita, Friman PRD 83 (2011); Basar Dunne 2112.14269]
* It has been argued that certain conformal mappings improve analytic continuation and sensitivity to the QCD critical point

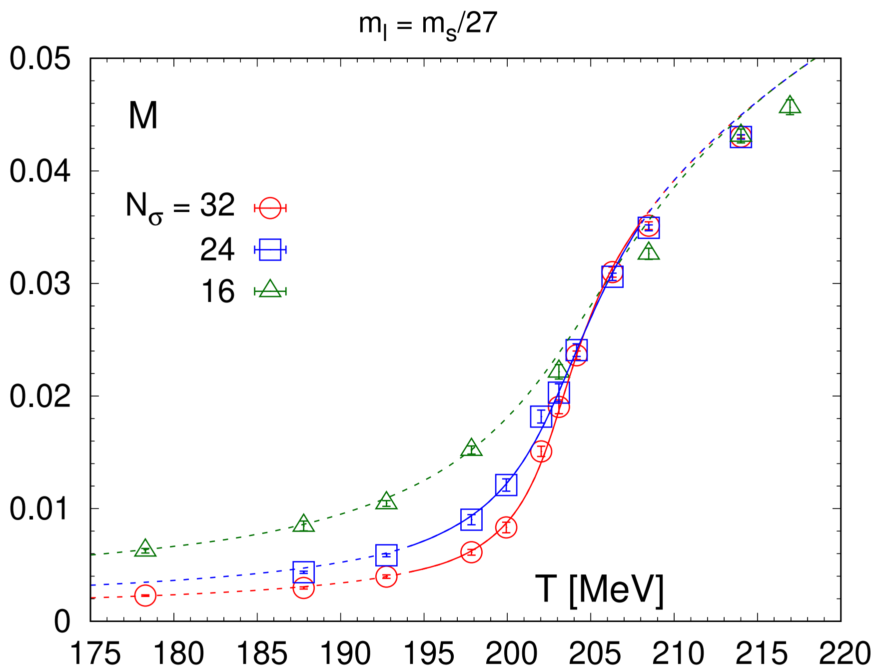
Can we interpret the closest singularity as Lee-Yang edge singularity?

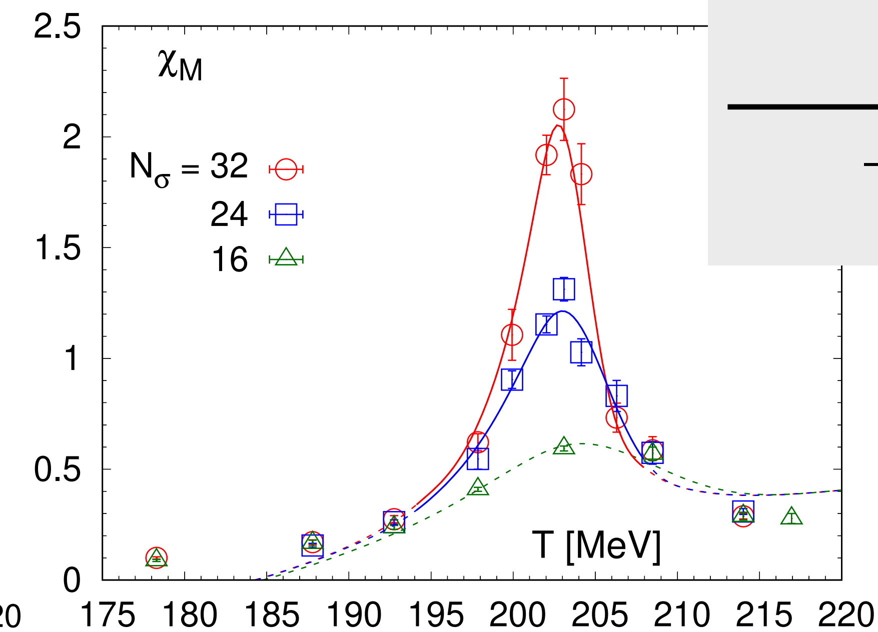
- At physical quark masses the Roberge-Weiss critical point is the Z(2) symmetric end point of a line of first order transitions.
- Need to map QCD parameter to the scaling fields t, h. For the Roberge-Weiss Transition we make the following Ansatz

$$t = t_0^{-1}\left(\frac{T_{RW} - T}{T_{RW}}\right) \quad \text{and} \quad h = h_0^{-1}\left(\frac{\hat{\mu}_B - i\pi}{i\pi}\right)$$

- For our lattice setup [(2+1)-flavor of HISQ, $N_\tau = 4$] we know the position of the critical point $(T_{RW}, \mu_{B_{RW}} = (201\text{ MeV}, i\pi))$







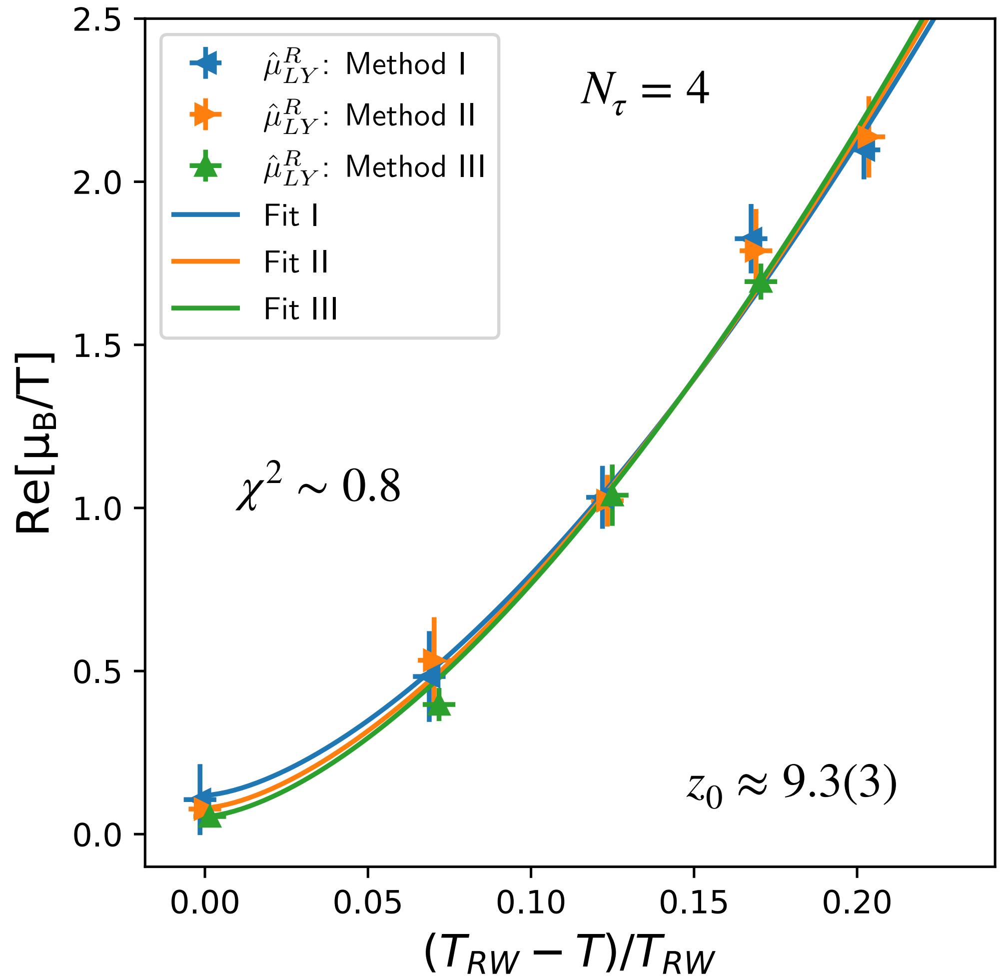
[J. Goswami, Lattice 2021]
[Bielefeld-Frankfurt, in preparation]

Can we interpret the closest singularity as Lee-Yang edge singularity?

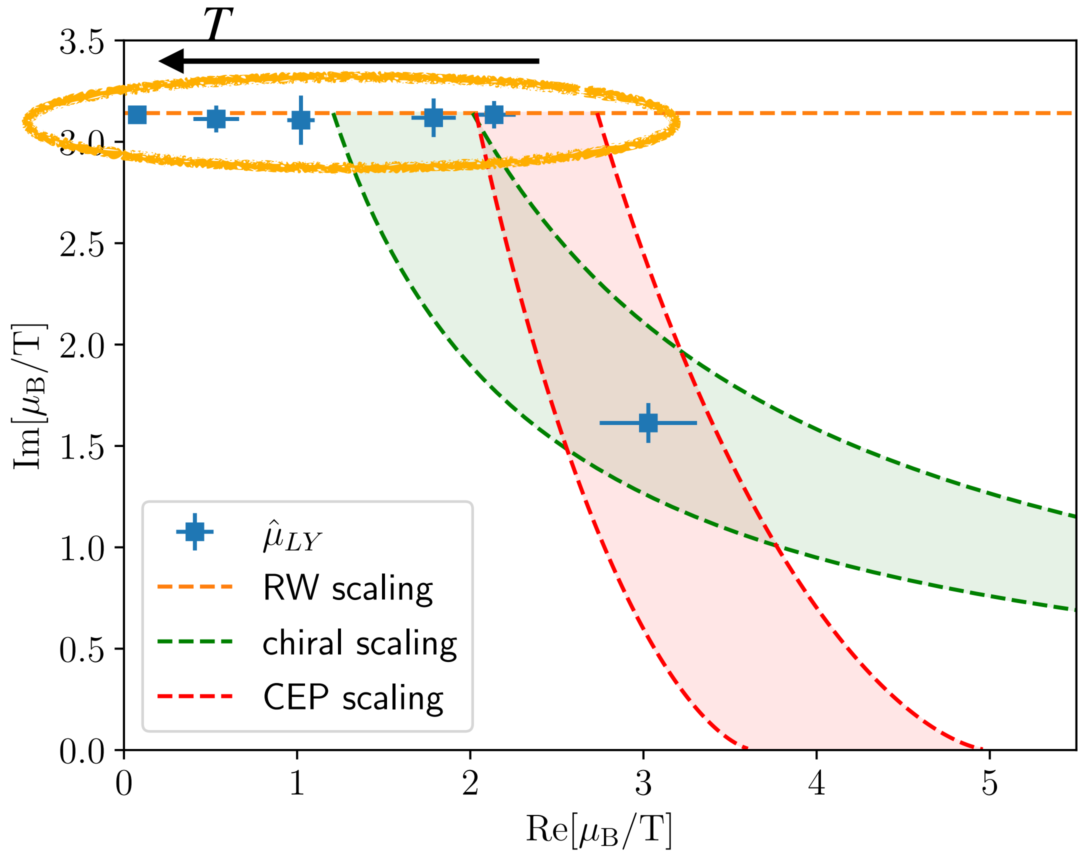
* We can look at the temperature dependence of our singularities. By solving $z = t/h^{1/\beta\delta} \equiv z_c$ we find

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

with $z_0 = h_0^{1/\beta\delta}/t_0$ and $\hat{\mu} = \mu/T$.



→find good agreement with RW-scaling



Method I: solving the linear system in the $\hat{\mu}_B$ plane

Method II: minimize a generalised $\tilde{\chi}^2$, (combined fit to all data)

$$\tilde{\chi}^2 = \sum_{j,k} \frac{\left|\frac{\partial^j R^m_n}{\partial \hat{\mu}^j_B}(\hat{\mu}_{B,k}) - \chi^B_{j+1}(\mu_{B,k})\right|^2}{|\Delta\chi^B_{j+1}(\hat{\mu}_{B,k})|^2}$$

Method III: solving the linear system in the z plane, and mapping the result back to $\hat{\mu}_B$

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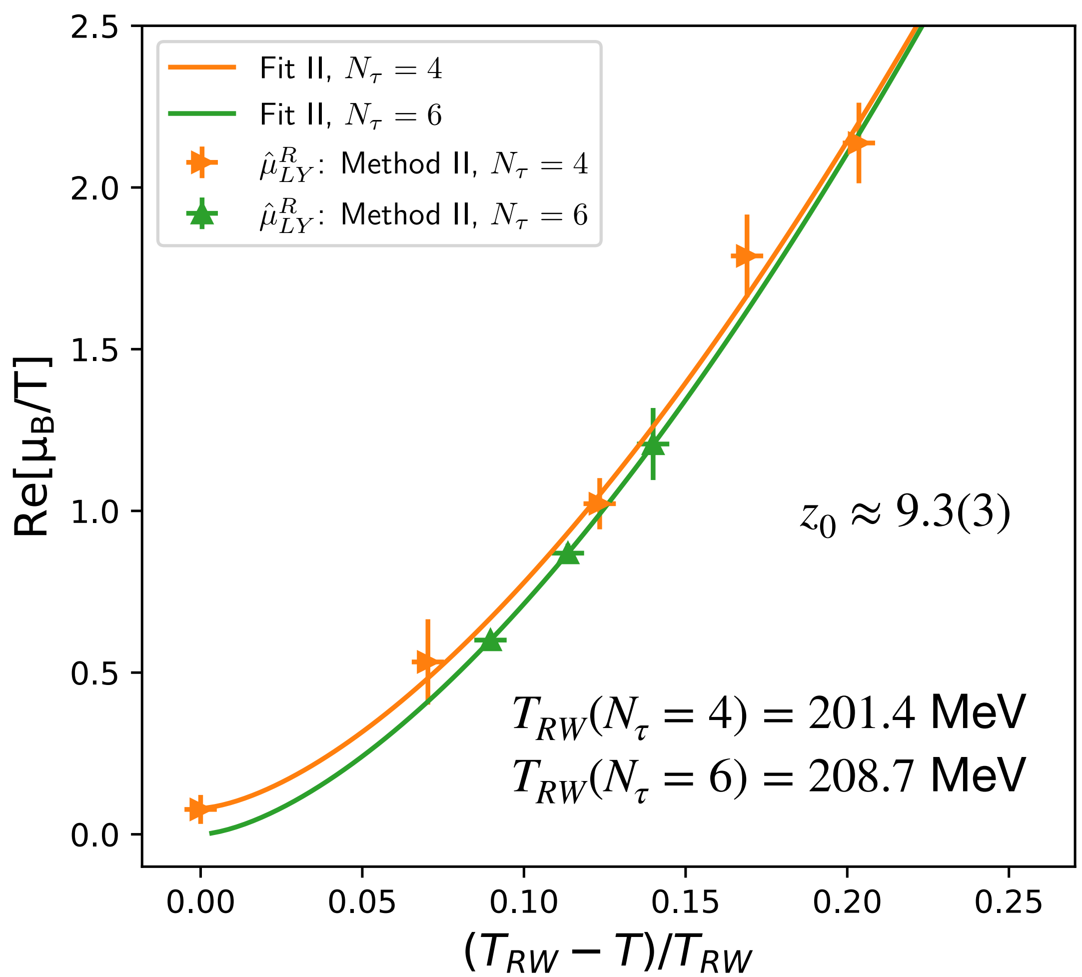

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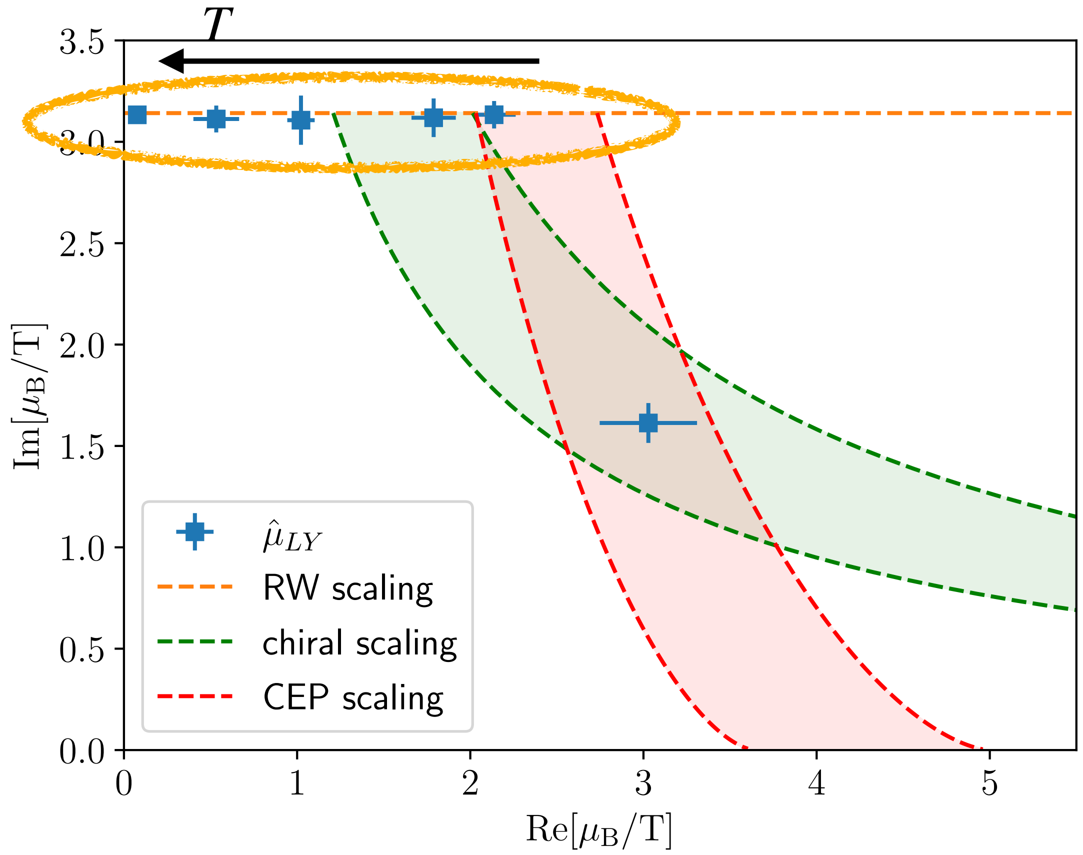

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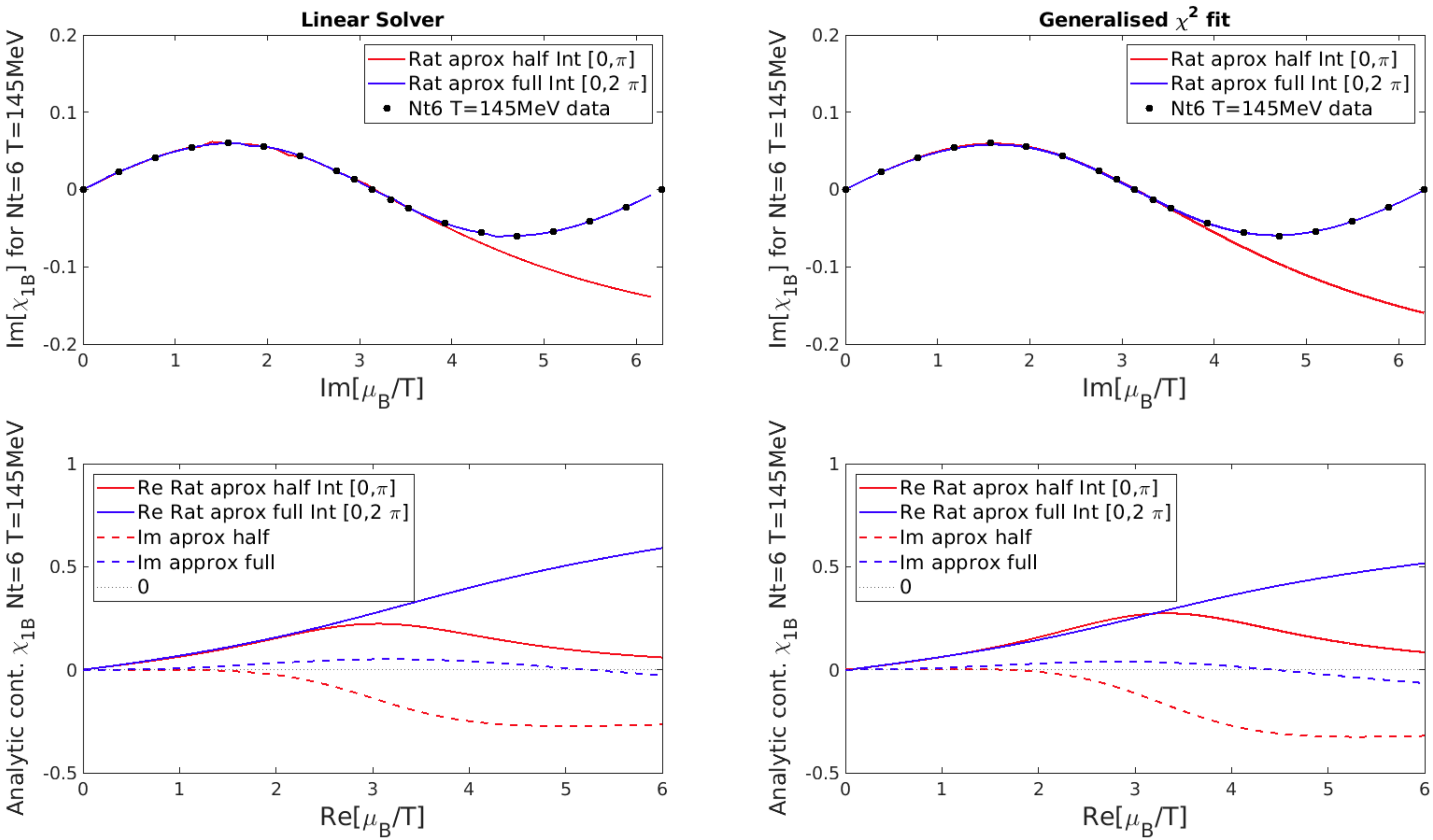
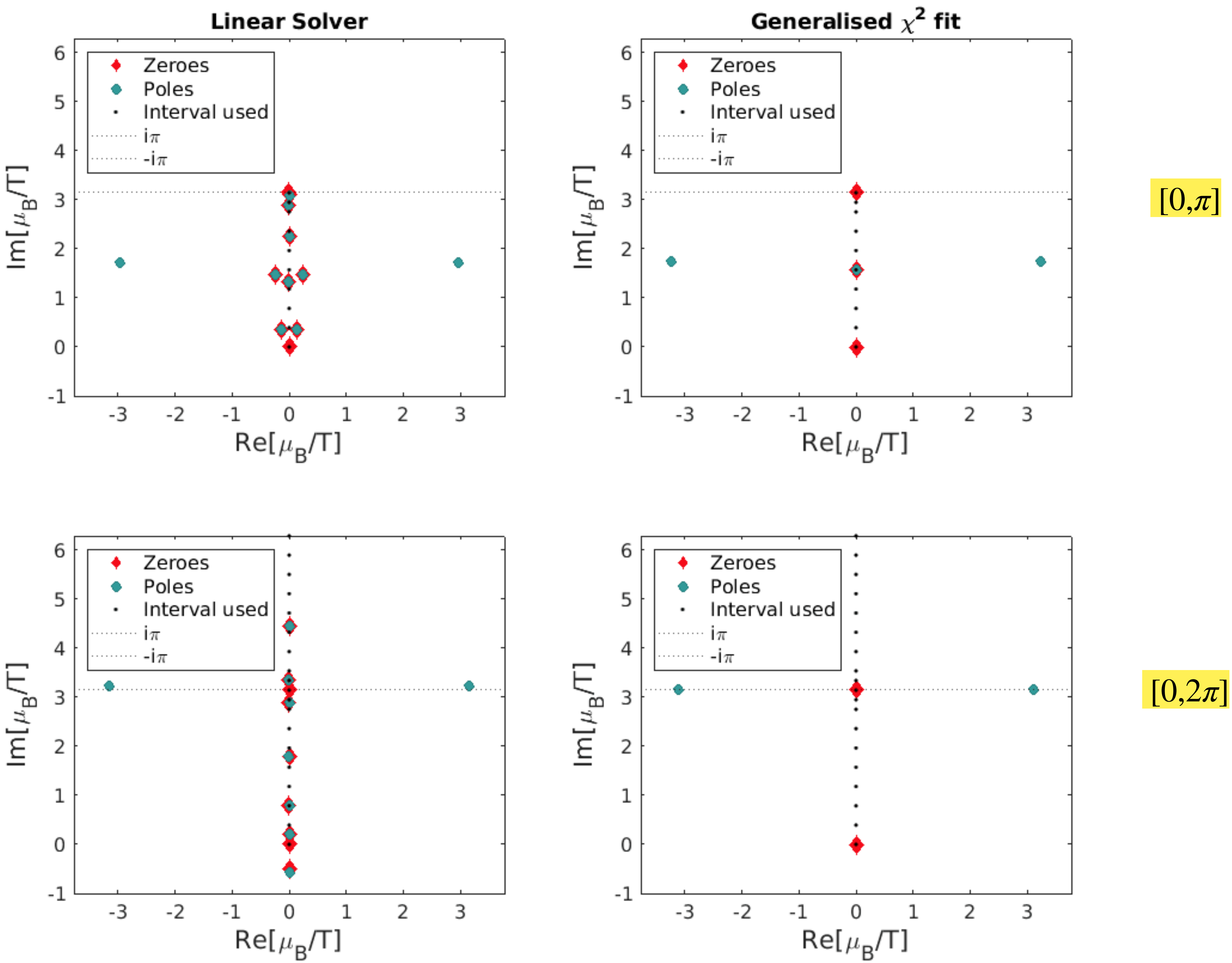
* Calculations at $T = 145$ MeV on $36^3 \times 6$ lattices



→find dependence on the probed interval, but not on the method



→find dependence on the probed interval, but not on the method

* The chiral transition is very well studied by the HotQCD collaboration. Important nonuniversal constants are known.

* Ansatz for the scaling fields is give by

$$t = \frac{1}{t_0}\left[\frac{T-T_c}{T_c} + \kappa_2^B\left(\frac{\mu_B}{T}\right)^2\right]$$

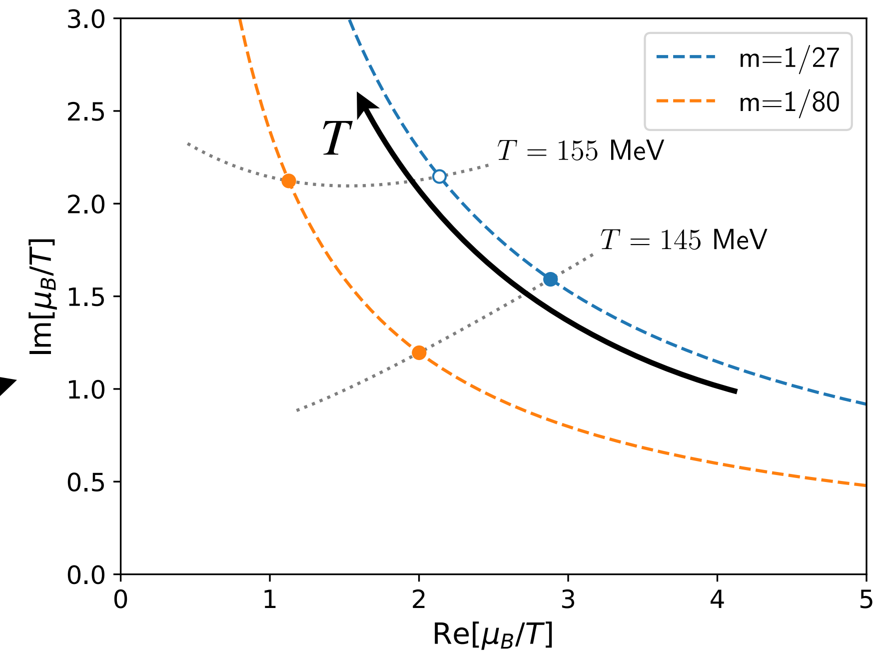
$$h = \frac{1}{h_0}\frac{m_l}{m_s^{\text{phys}}}$$

* We solve again for $\hat{\mu}_{LY}$ by setting $z = z_c$ and obtain

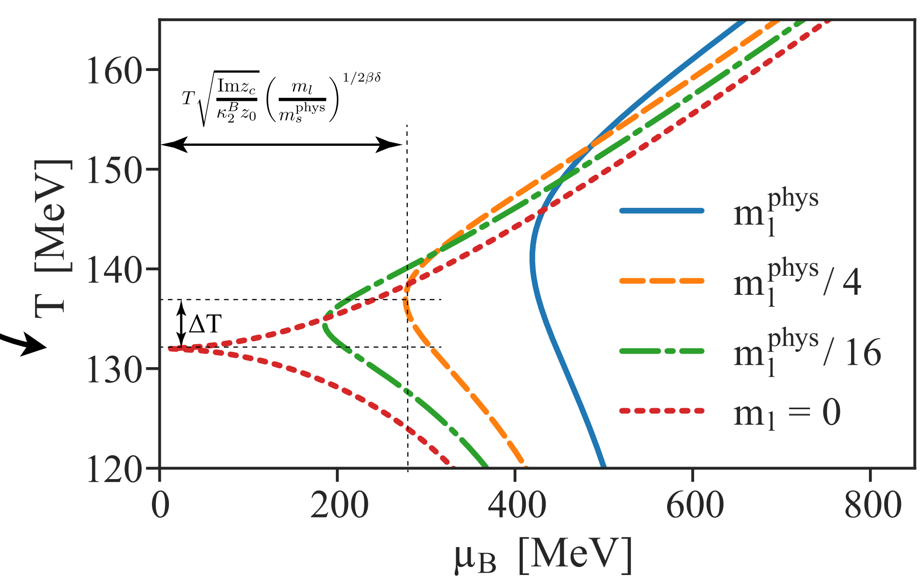
$$\hat{\mu}_{LY} = \left[\frac{1}{\kappa_2^B}\left(\frac{z_c}{z_0}\left(\frac{m_l}{m_s^{\text{phys}}}\right)^{1/\beta\delta} - \frac{T-T_c}{T_c}\right)\right]^{1/2}$$

Required input: T_c, κ_2^B, z_0, z_c

Position of the LYE

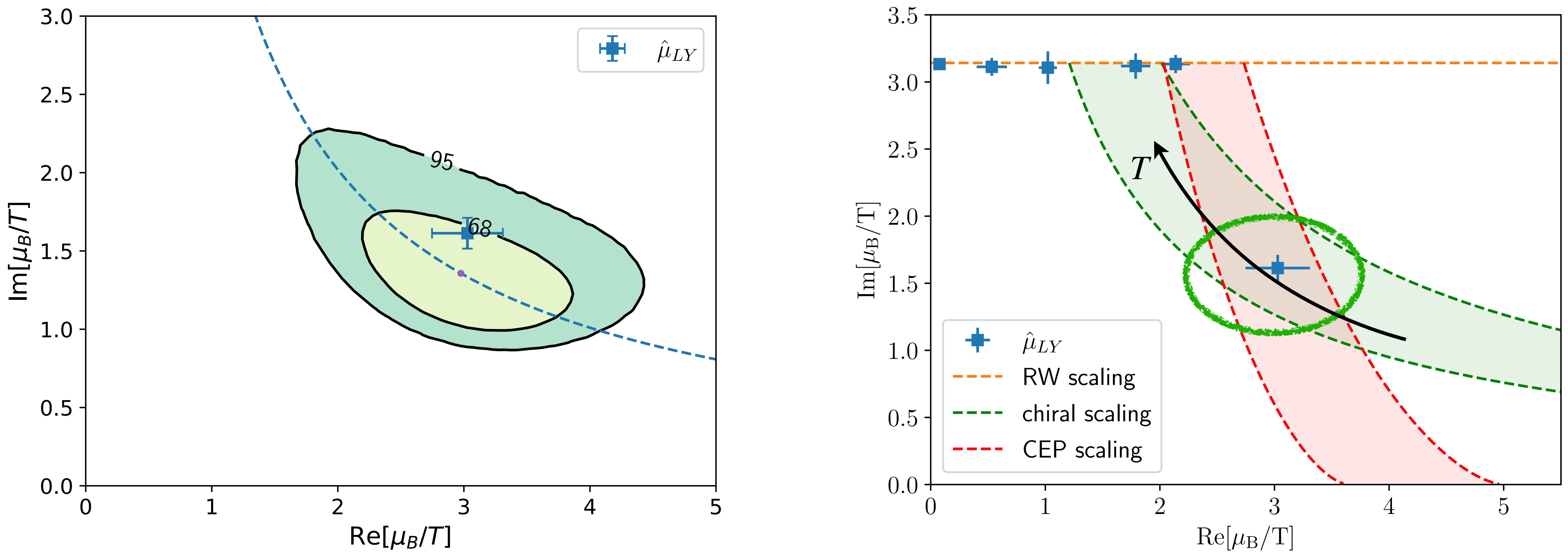


The radius of convergence



[Mukherjee, Skokov, PRD 103 (2021) 071501]

* Comparison of the prediction with the actually found singularity of the multipoint Padé



* 68% and 95% confidence regions of the prediction are generated with the following $N_\tau = 6$ specific values for the nonuniversal constants

$$\left.\begin{aligned} T_c &= (147 \pm 6)\ \text{MeV}, \\ z_0 &= 2.35 \pm 0.2, \\ \kappa_2^B &= 0.012 \pm 0.002, \end{aligned}\right\}$$ [HotQCD], Gaussian error distribution assumed

$|z_c| = 2.032$ (O(2)) value [Connelly et al. PRL 125 (2020) 19]

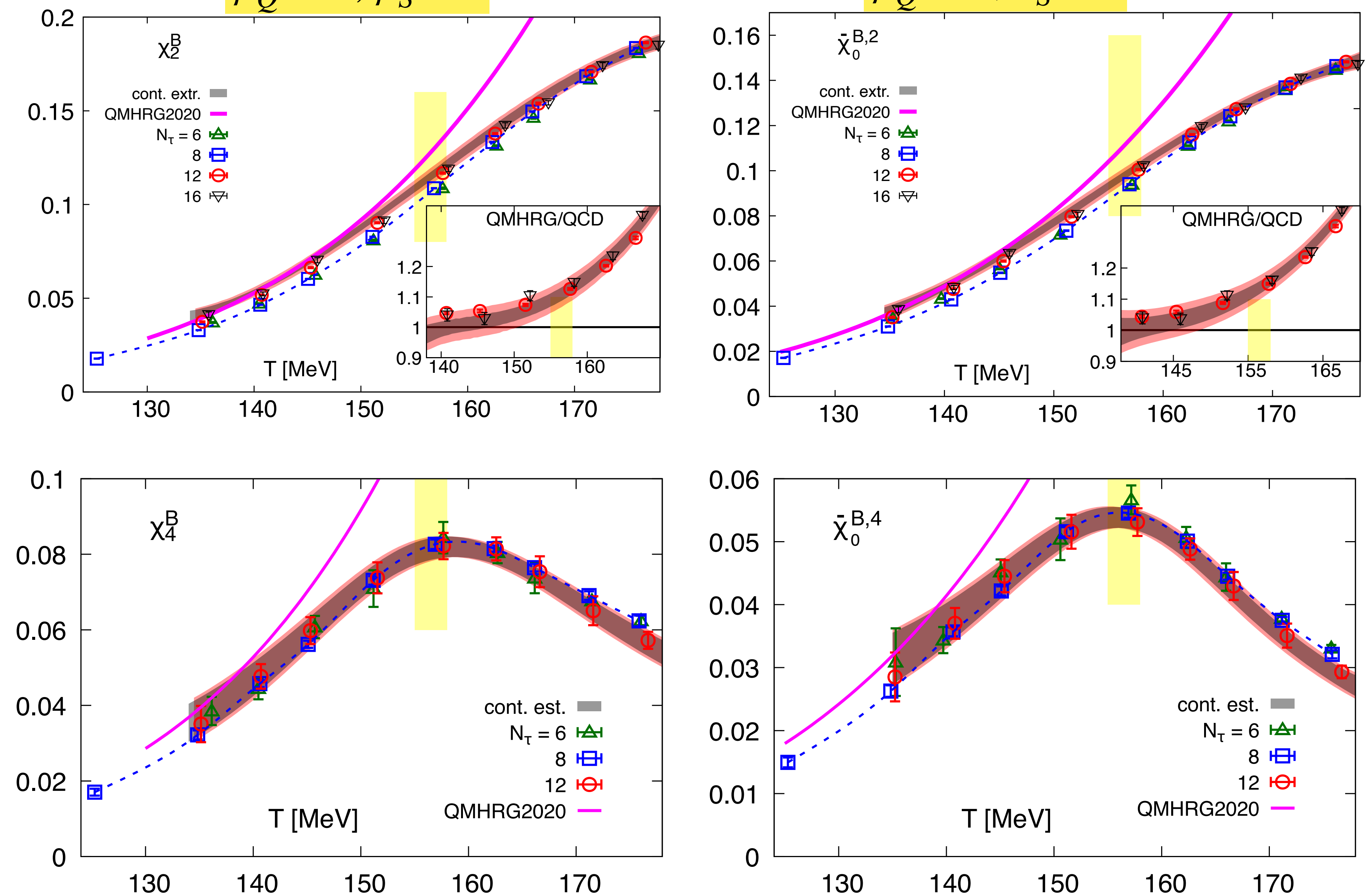
→find good agreement. Coincidence? Need more data.

- We will now consider the pressure series

$$\frac{P}{T^4} = \frac{1}{VT^3} \ln \mathcal{Z}(T, V, \vec{\mu}) = \sum_{i,j,k=0}^{\infty} \frac{\chi_{ijk}^{BQS}}{i!\,j!\,k!} \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k \quad \rightarrow \quad f(x) = \sum_n^{\infty} c_n x^n$$

- Very high statistics, over 1M configurations per temperature ($N_\tau = 8$), generated by HotQCD over the past decade
- Consider two cases of a series in one variable:
- Fist two orders are strictly positive

$\mu_Q = 0,\ \mu_S = 0$ | $\mu_Q = 0,\ n_S = 0$



[Bollweg et al. [HotQCD] arXiv:2202.09184]

Padé resummation of the Taylor series about $\mu_B = 0$ $(N_\tau = 8)$

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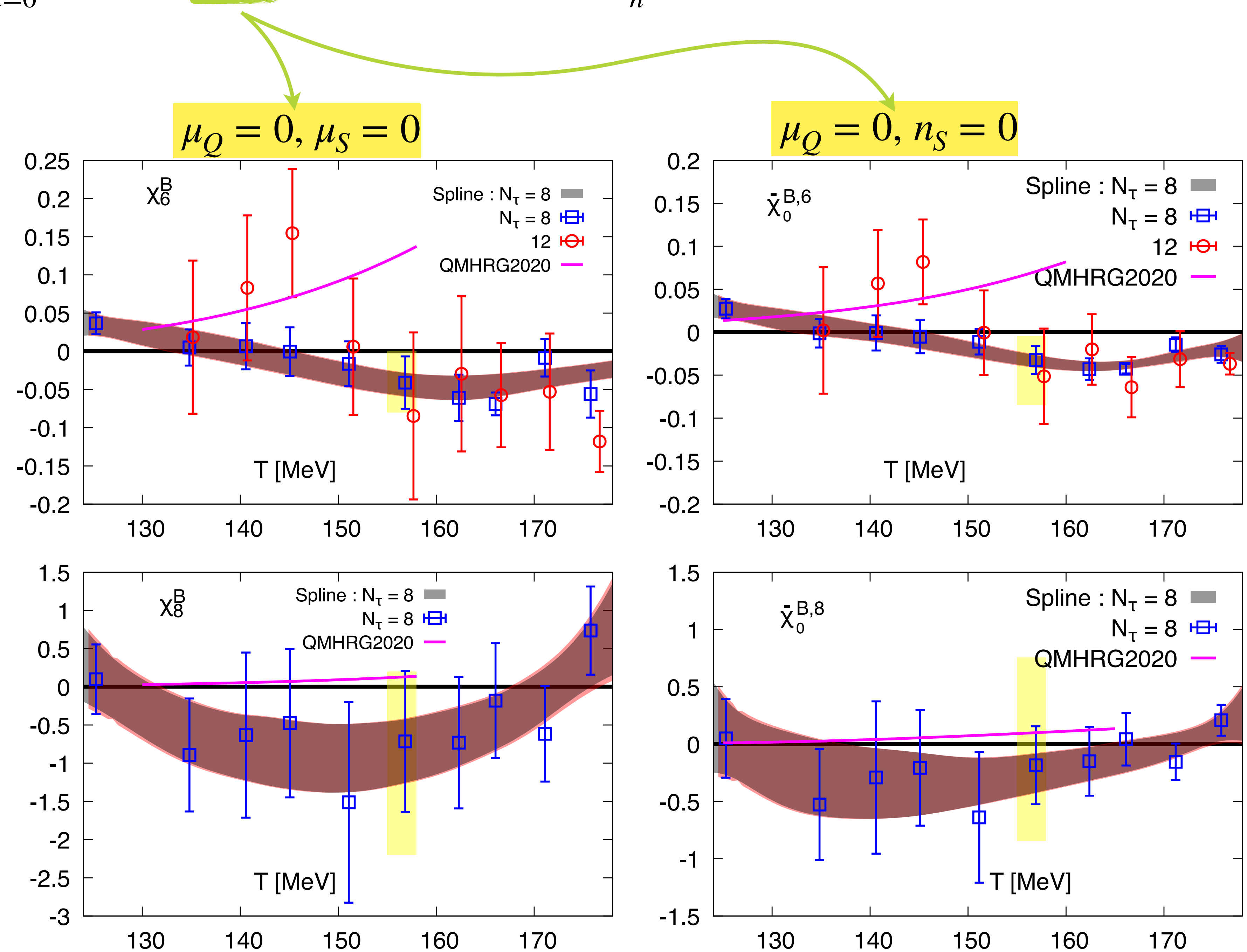


[Bollweg et al. [HotQCD] arXiv:2202.09184]

* We can estimate the radius of convergence $r_c = \lim_{n\to\infty} r_{c,n}$ by ratios of expansion coefficients

Simple ratio estimator: $r_{c,n} = \sqrt{|A_n|}$ $\quad A_n = \frac{c_n}{c_{n+2}}$, n even

Mercer-Roberts estimator: $r^{MR}_{c,n} = |A^{MR}_n|^{1/4}$ $\quad A^{MR}_n = \frac{c_{n+2}\,c_{n-2} - c_n^2}{c_{n+4}\,c_n - c_{n+2}^2}$, n even

* The Estimators A_n and A_n^{MR} are related to the poles of the [n,2] and [n,4] Padé, respectively.

* For the analysis of the Padé, we take advantage of the positivity of $\chi_2^B\,(\bar\chi_2^B)$ and $\chi_4^B\,(\bar\chi_4^B)$ and rescale the pressure series by a factor P_4/P_2^2 and redefine the expansion parameter to $\bar{x} = \sqrt{P_4/P_2}\ \hat\mu_B \equiv \sqrt{\bar\chi_4^B/(12\bar\chi_2^B)}\ \hat\mu_B$.

$$\frac{(\Delta P(T,\mu_B)/T^4)P_4}{P_2^2} = \sum_{k=1}^{\infty} c_{2k,2}\bar{x}^{2k} = \bar{x}^2 + \bar{x}^4 + c_{6,2}\bar{x}^6 + c_{8,2}\bar{x}^8 + \ldots$$

with $c_{6,2} = \frac{P_6 P_2}{P_4^2} = \frac{2}{5}\frac{\bar\chi_6^B\bar\chi_2^B}{(\bar\chi_4^B)^2}$ and $c_{8,2} = \frac{P_8 P_2^2}{P_4^3} = \frac{3}{35}\frac{\bar\chi_8^B(\bar\chi_2^B)^2}{(\bar\chi_4^B)^3}$

→The singular structure of the 8th order expansion depends only on two coefficients

Padé resummation of the Taylor series about $\mu_B = 0$ $(N_\tau = 8)$

* In term of the expansion parameter $\bar{x}$, the Padé is given as

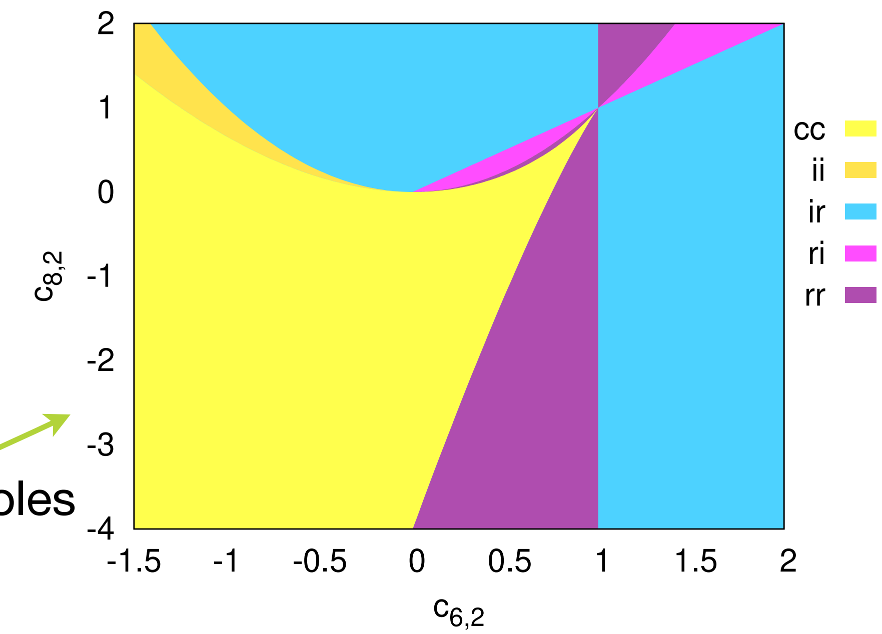
$$P[2,2] = \frac{\bar{x}^2}{1-\bar{x}^2}$$

Poles on the real axis at

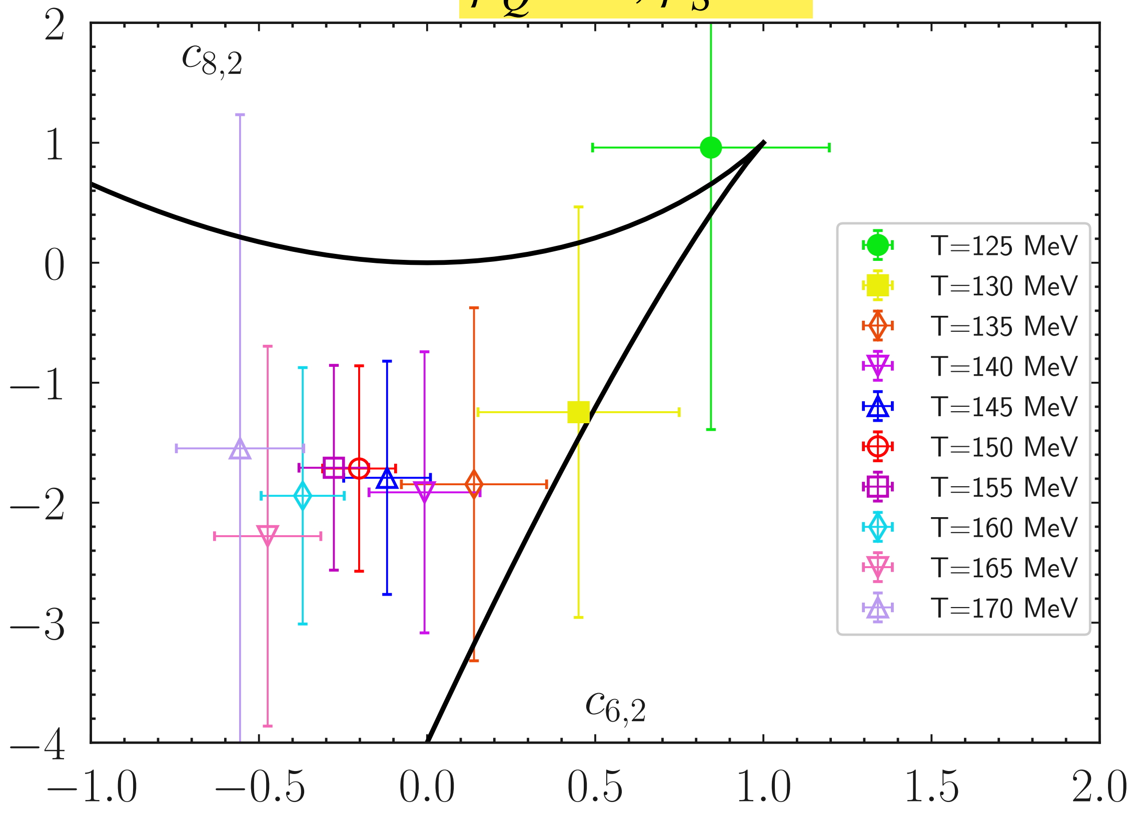
$$\bar{x}^2 = 1 \quad \Leftrightarrow \quad \hat{\mu}_{B,c} = \sqrt{12\bar{\chi}^B_2/\bar{\chi}^B_4}$$

$$P[4,4] = \frac{(1-c_{6,2})\bar{x}^2 + \left(1-2c_{6,2}+c_{8,2}\right)\bar{x}^4}{(1-c_{6,2}) + (c_{8,2}-c_{6,2})\bar{x}^2 + (c_{6,2}^2-c_{8,2})\bar{x}^4}$$

4 poles (two pairs)



$\mu_Q = 0,\ \mu_S = 0$



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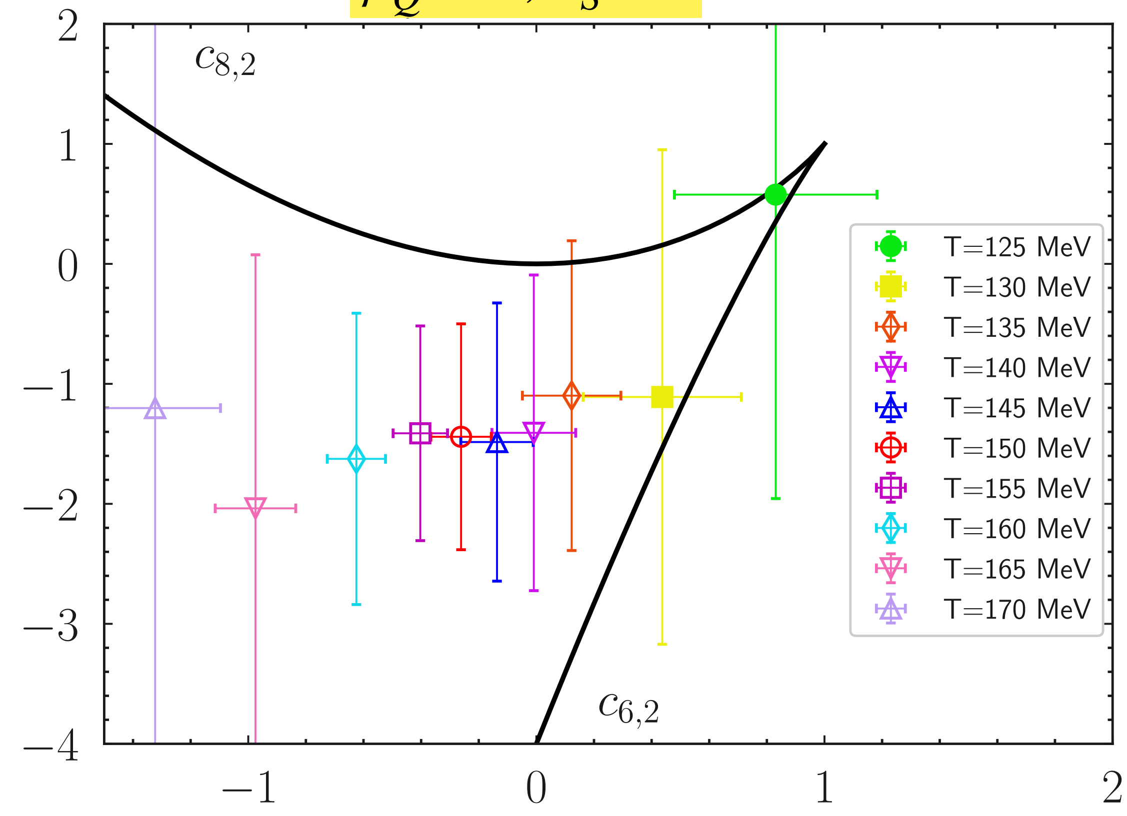
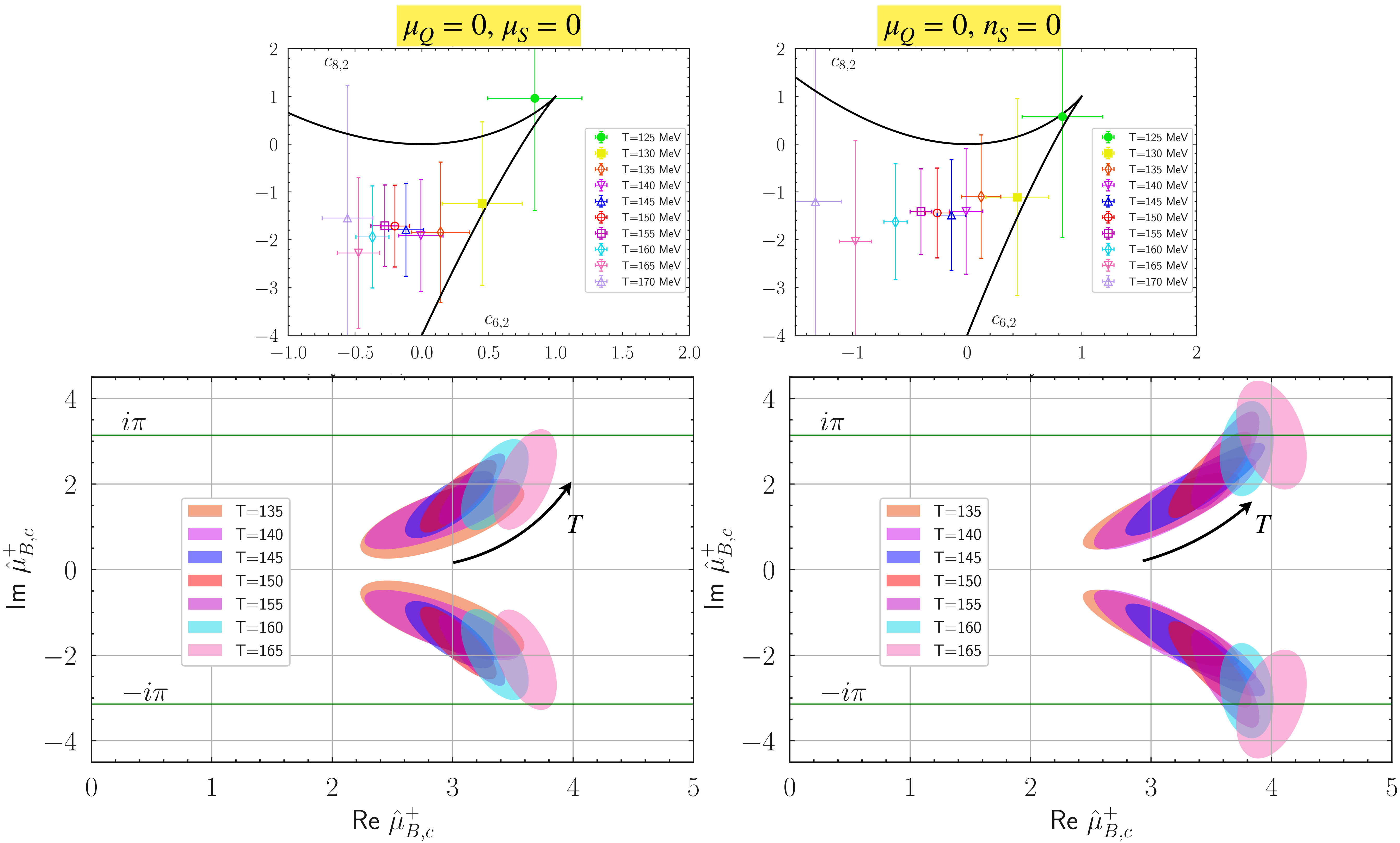


→ For $T > 135$ MeV we find only complex poles

Padé resummation of the Taylor series about $\mu_B = 0$ $(N_\tau = 8)$

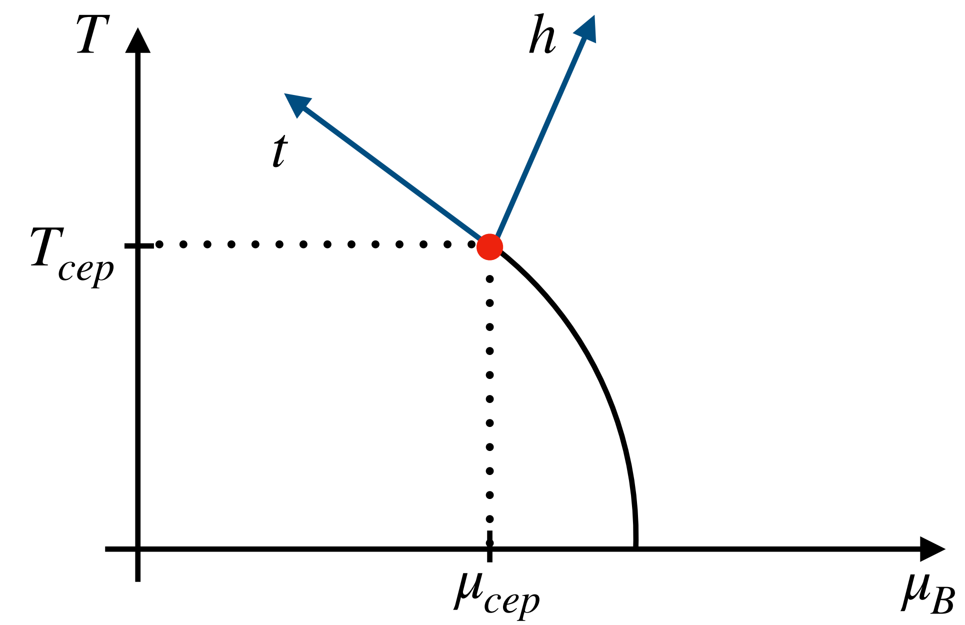


→ Poles approach the real axis with decreasing temperature

→Temperature dependence is currently not in consistence with expected universal scaling

- Scaling fields are unknown, a frequently used *ansatz* is given by a linear mapping

$$t = \alpha_t(T - T_{cep}) + \beta_t(\mu_B - \mu_{cep})$$
$$h = \alpha_h(T - T_{cep}) + \beta_h(\mu_B - \mu_{cep})$$



- For the Lee-Yang edge singularity we obtain

$$\mu_{LY} = \mu_{cep} - c_1(T - T_{cep}) + ic_2|z_c|^{-\beta\delta}(T - T_{cep})^{\beta\delta},$$

Real part: linear in T

Imaginary part: power law

The coefficient only depends on the slope of the crossover line

$$c_1 = \beta_T/\beta_\mu$$

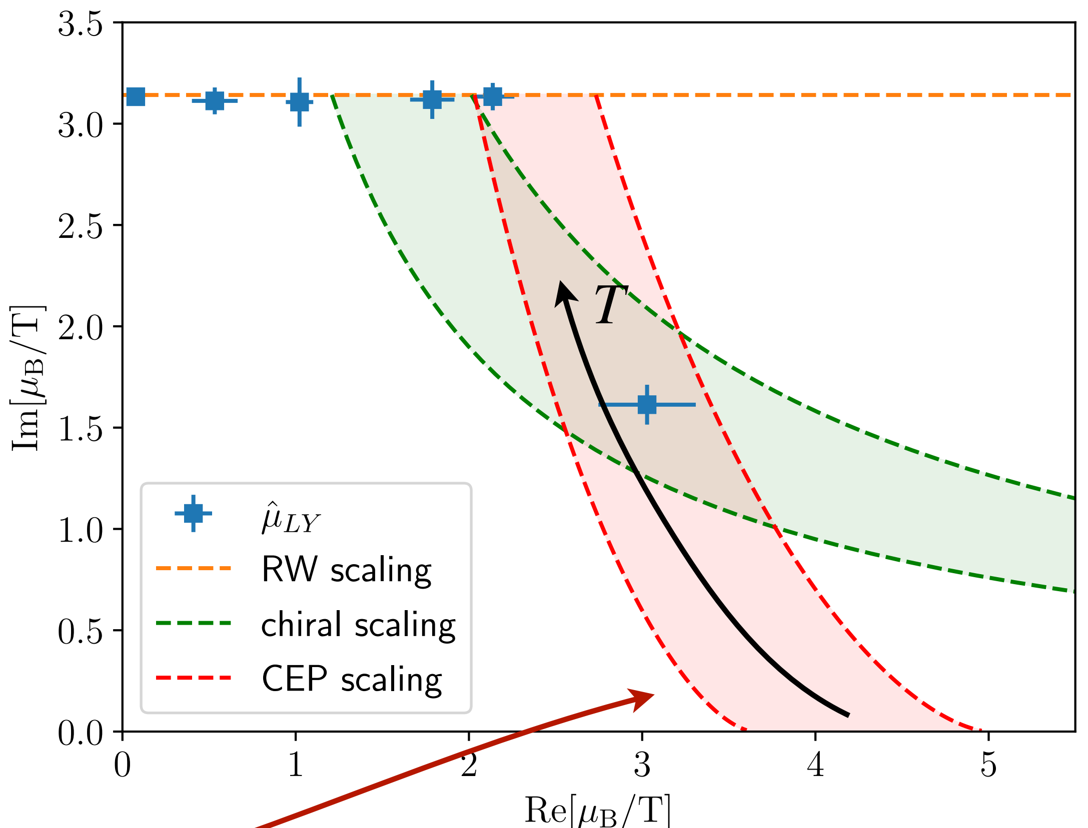
- To visualise the scaling we use some ad-hoc values

$\mu_{cep} = 500 - 630$ MeV

$T_{cep} = T_{pc}(1 - \kappa_2^B \hat{\mu}_B^2)$

$\kappa_2^B = 0.012$ $\quad c_1 = 0.024$

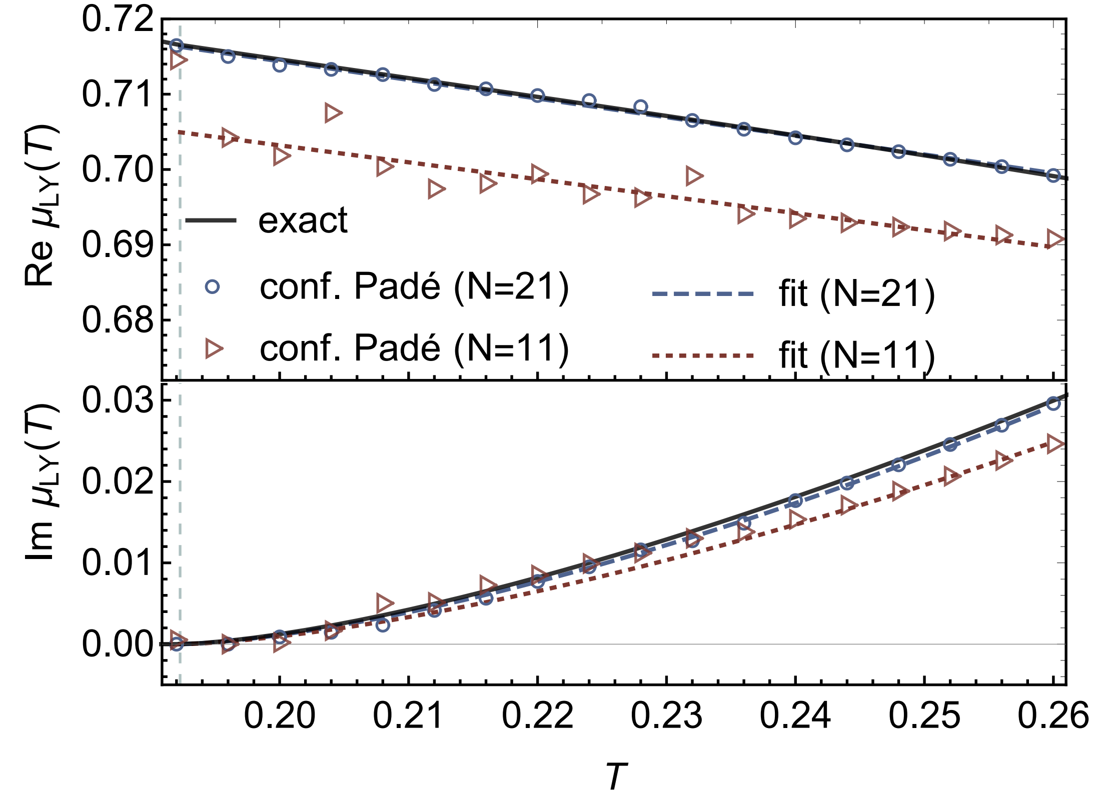
$T_{pc} = 156.5$ MeV $\quad c_2 = 0.5$



* In the Gross-Neveu model, it has been demonstrated that a scaling analysis of the Lee-Yang edge singularities can be used to determine the critical point

* However, 8th order is not sufficient to extract the correct results.

→ Need more precise data from lattice QCD



[Basar, PRL 127 (2021) 171603]

New Method

- We [Bielefeld-Parma] have developed a multipoint Padé method to extract singularities of the net baryon number density in the $\hat{\mu}_B$ plane

Close to the RW transition

- Find evidence for a brunch cut along $\hat{\mu}_B = \hat{\mu}_B^R \pm i\pi$
- Find Z(2) scaling of closest singularities
- Hence, our singularities can be identified with the Lee-Yang edge singularities

Close to the chiral transition

- Multipoint Padé: find one singularity which is in good agreement with expectation, need to verify the scaling in T and m_l

Close to the critical end-point

- Padé with high statistics $N_\tau = 8$ data [HotQCD]: singularities also in the correct bulk part, they approach the real μ_B axis, but not in consistency with universal scaling
- Bound on the critical point: $\hat{\mu}_{cep} > 2.5$ and $T_{cep} < 135$ MeV