The QCD phase diagram and Lee-Yang zeros

Christian Schmidt

UNIVERSITÄT BIELEFELD
Faculty of Physics

CRC-TR 211

PUNCH 4NFDI

HotQCD Collaboration:
Dennis Bollweg, David Clarke, Jishnu Goswami, Olaf Kaczmarek, Frithjof Karsch, Swagato Mukherjee, Peter Petreczky, CS, Sipaz Sharma

[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]
[PRD 105 (2022) 7, 074511, arXiv: 2202.09184]

Bielefeld Parma Collaboration:
David Clarke, Petros Dimopoulos, Francesco Di Renzo, Jishnu Goswami, Guido Nicotra, CS, Simran Singh, Kevin Zambello

[arXiv: 2405.10196]
[PRD 105 (2022) 3, 034513, arXiv: 2110.15933]

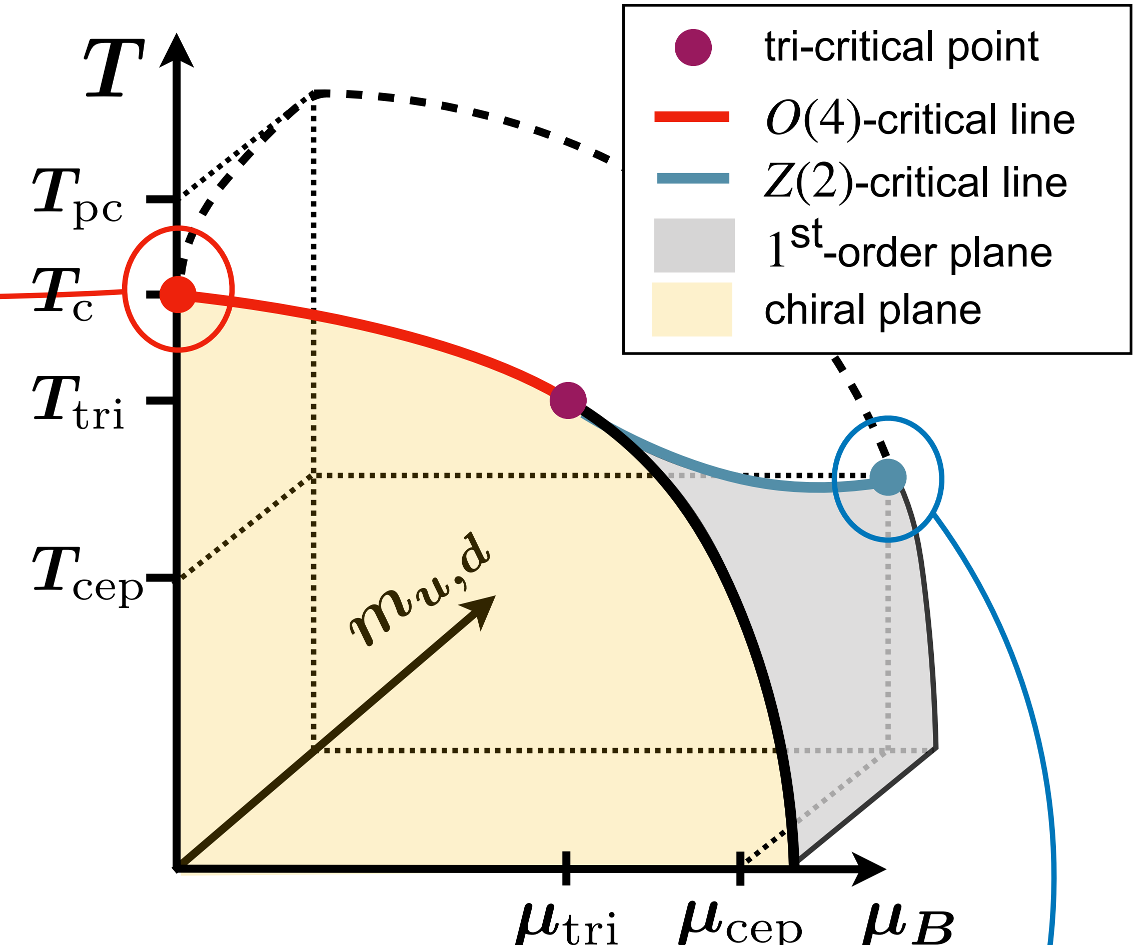
Wrocław, July 2-4, 2024

Spontaneous chiral symmetry breaking

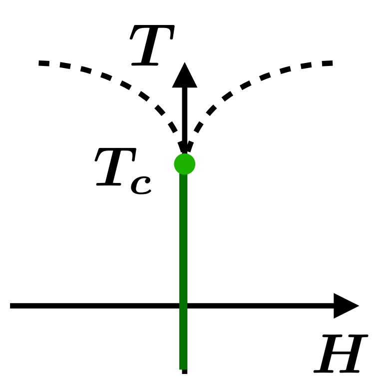
$$\mathrm{U}(1)_V \times \cancel{\mathrm{U}(1)}_A \times \mathrm{SU}(N_f)_L \times \mathrm{SU}(N_f)_R$$

$$\rightarrow \mathrm{U}(1)_V \times \cancel{\mathrm{U}(1)}_A \times \mathrm{SU}(N_f)_V \times \cancel{\mathrm{SU}(N_f)}_A$$

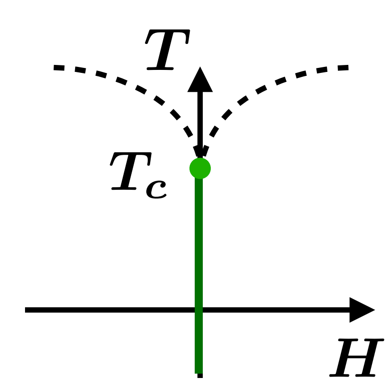
The QCD phase diagram



O(4)-symmetric model



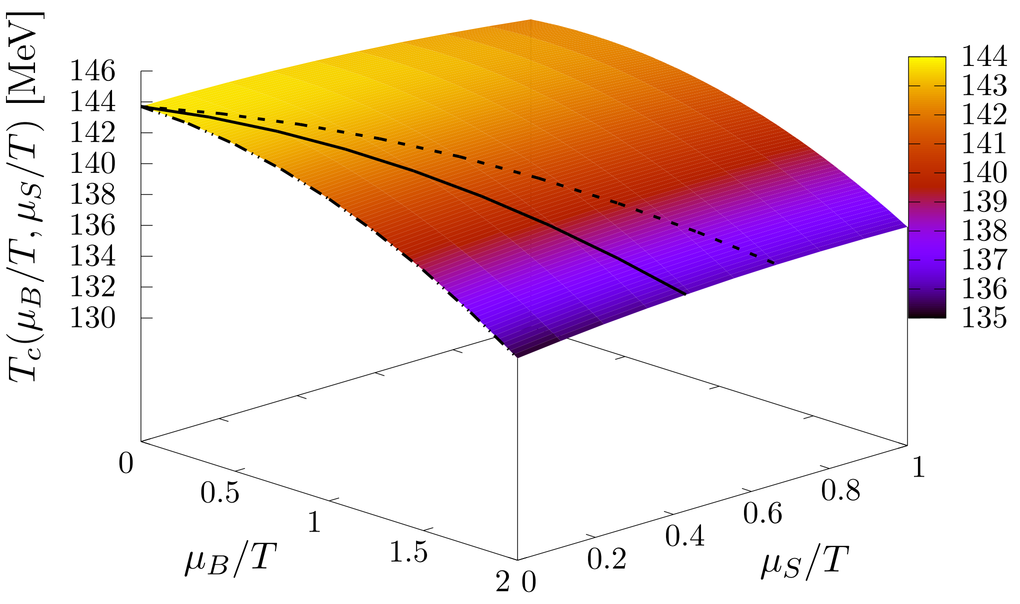
Z(2)-symmetric model



- Map is defined by the scaling directions and few non-universal constants T_c, t_0, h_0, … → need to be determined
- Critical exponents, critical amplitudes and scaling functions are universal and well known and can be used
- Verifying universality classes is more difficult

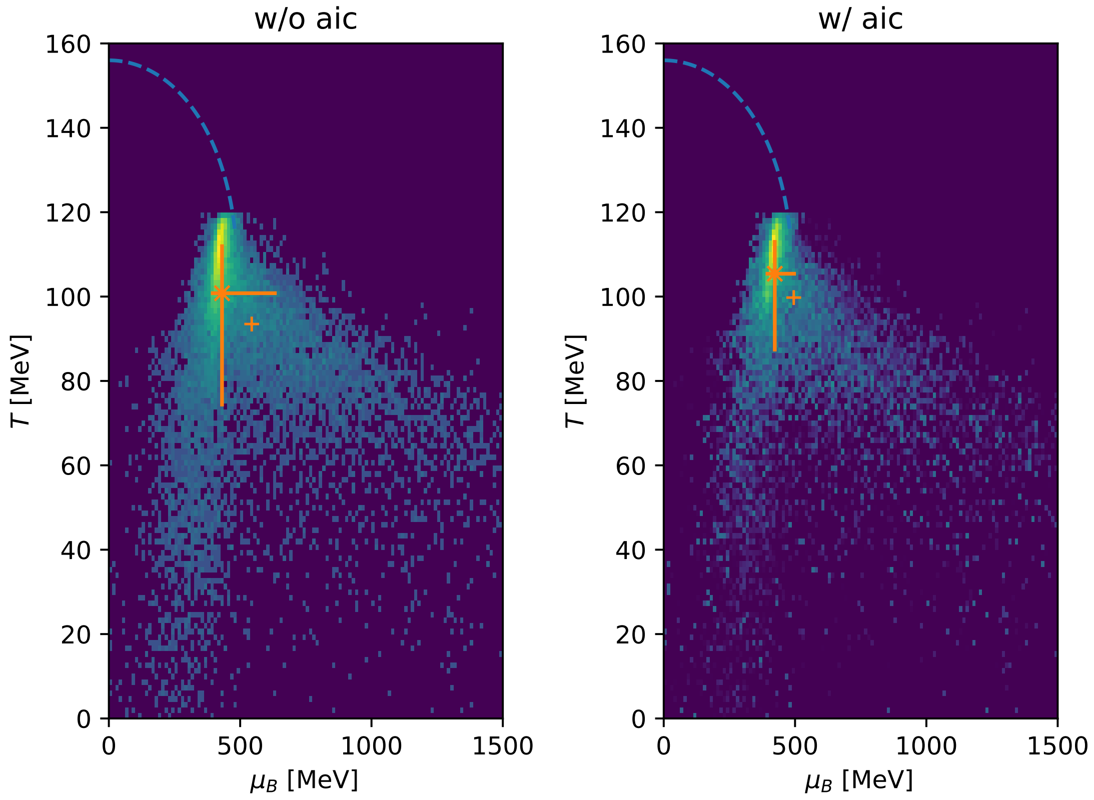
* Chiral Transition at $\mu_B = 0$: pseudo-critical temperature $T_{pc}(\mu_B, \mu_S, m_s)$
  ➡ Special case $n_S = 0$

[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]



* QCD critical end-point
  ➡ Lee-Yang edge singularity
  ➡ Metodoly: multi-point Pade vs Taylor expansion
  ➡ First results on the location of the CEP

[arXiv: 2405.10196]



Scaling fields

$$h = \frac{1}{h_0} H = \frac{1}{h_0} \frac{m_l}{m_s}$$

light quark mass (m_l)

strange quark mass (m_s)

$$t = \frac{1}{t_0} \left(\Delta T + \kappa_2^l \hat{\mu}_l^2 + \kappa_2^s \hat{\mu}_s^2 + 2\kappa_{11}^{ls} \hat{\mu}_l \hat{\mu}_s \right)$$

$$\Delta T = \frac{T - T_c}{T_c}$$

* chiral condensates couple to the temperature-like scaling field

Magnetic equation of state

$$M = h^{1/\delta} \left(f_G(z) - f_\chi(z) \right)$$

* $f_G(x)$ and $f_\chi(z)$ are universal function of a single scaling variable $z = t/h^{1/\beta\delta}$

Order parameter

$$M_l = \frac{m_s}{f_K^4} \frac{T}{V} \frac{\partial \ln Z}{\partial m_l}$$

Remove multiplicative UV divergences

$$\frac{\partial}{\partial m_l} = \frac{\partial}{\partial m_u} + \frac{\partial}{\partial m_d}$$

Magnetic susceptibility

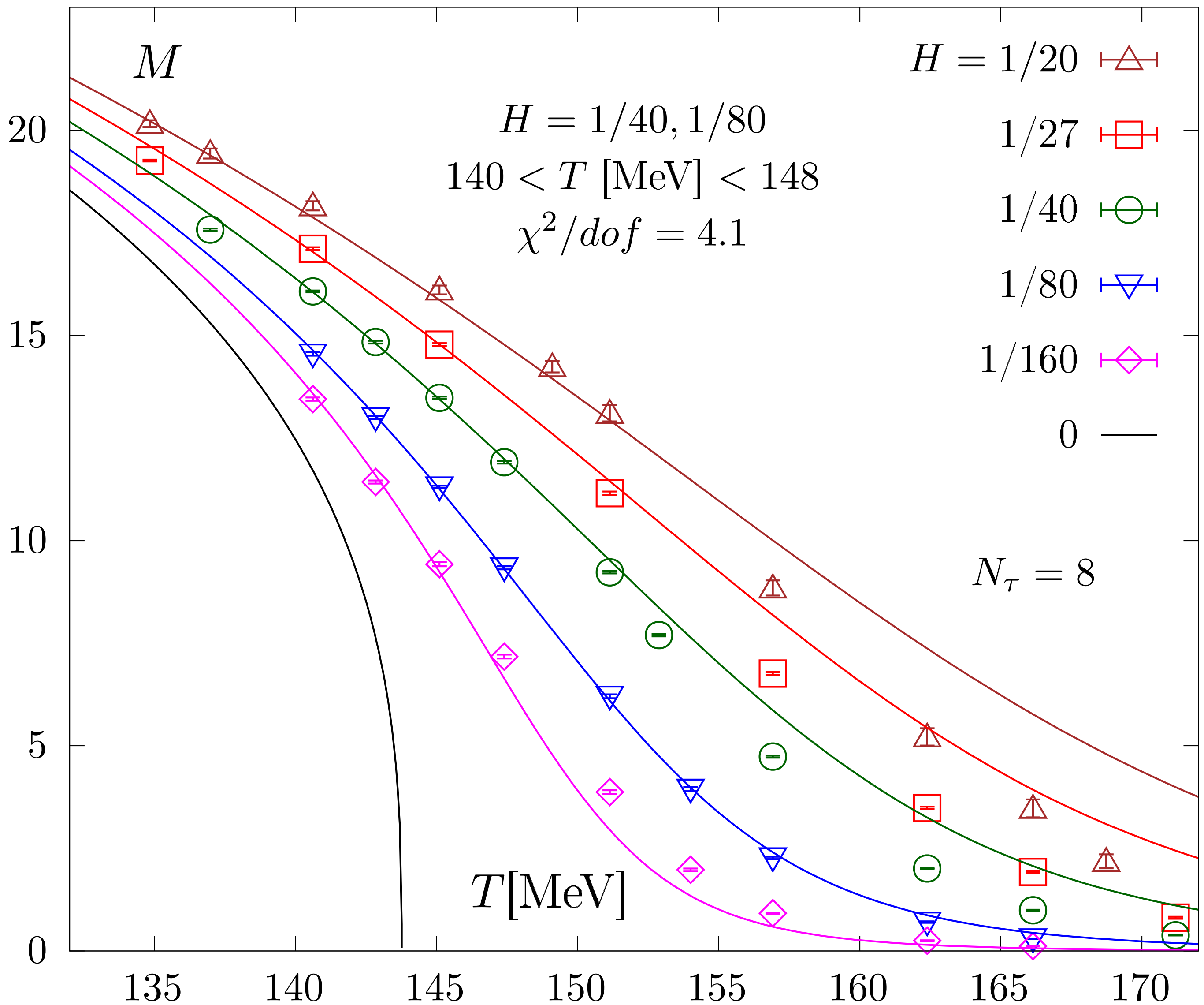
$$\chi_l = m_s \frac{\partial}{\partial m_l} M_l$$

"Improved" order parameter

$$M = M_l - H\chi_l$$

[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]

$$M = h_0^{-1/\delta} H^{1/\delta} \left(f_G(z) - f_\chi(z)\right)$$



[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]

- $N_\tau = 8$ (with updated statistics)
- Corresponding pion masses: $m_\pi \simeq$ 180 MeV, 140 MeV, 110 MeV, 80 MeV, 55 MeV.
- Use O(2) scaling functions and exponents due to staggered fermions
- Fit results for $N_\tau = 8$

$$T_c = 143.7(2)\ \mathrm{MeV}\ ,$$
$$z_0 = 1.42(6)\ ,$$
$$h_0^{-1/\delta} = 39.2(4)\ .$$

- Continuum estimate: $T_c = 132^{+2}_{-6}$ MeV

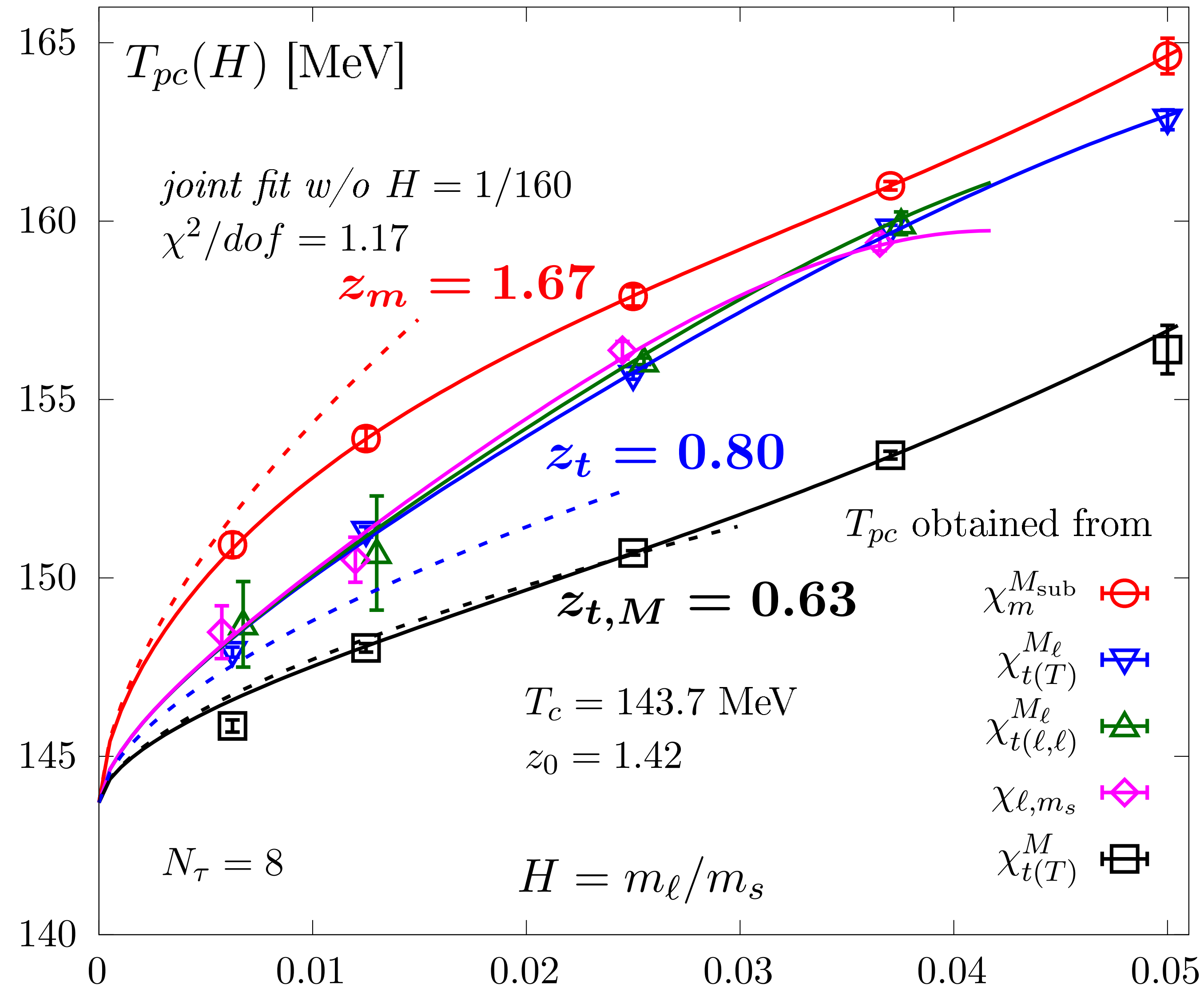
[PRL 123 (2019) 6, 062002, arXiv: 1903.04801]

* Temperature-like derivatives of the order parameter

$$\chi_{t(T)}^{M_\ell} = -T_c \frac{\partial M_\ell}{\partial T} ,$$

$$\chi_{t(f,f)}^{M_\ell} = -\frac{\partial^2 M_\ell}{\partial \hat{\mu}_f^2} ,$$

$$\chi_{t(\ell,s)}^{M_\ell} = -\frac{\partial^2 M_\ell}{\partial \hat{\mu}_\ell \partial \hat{\mu}_s} ,$$



[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]

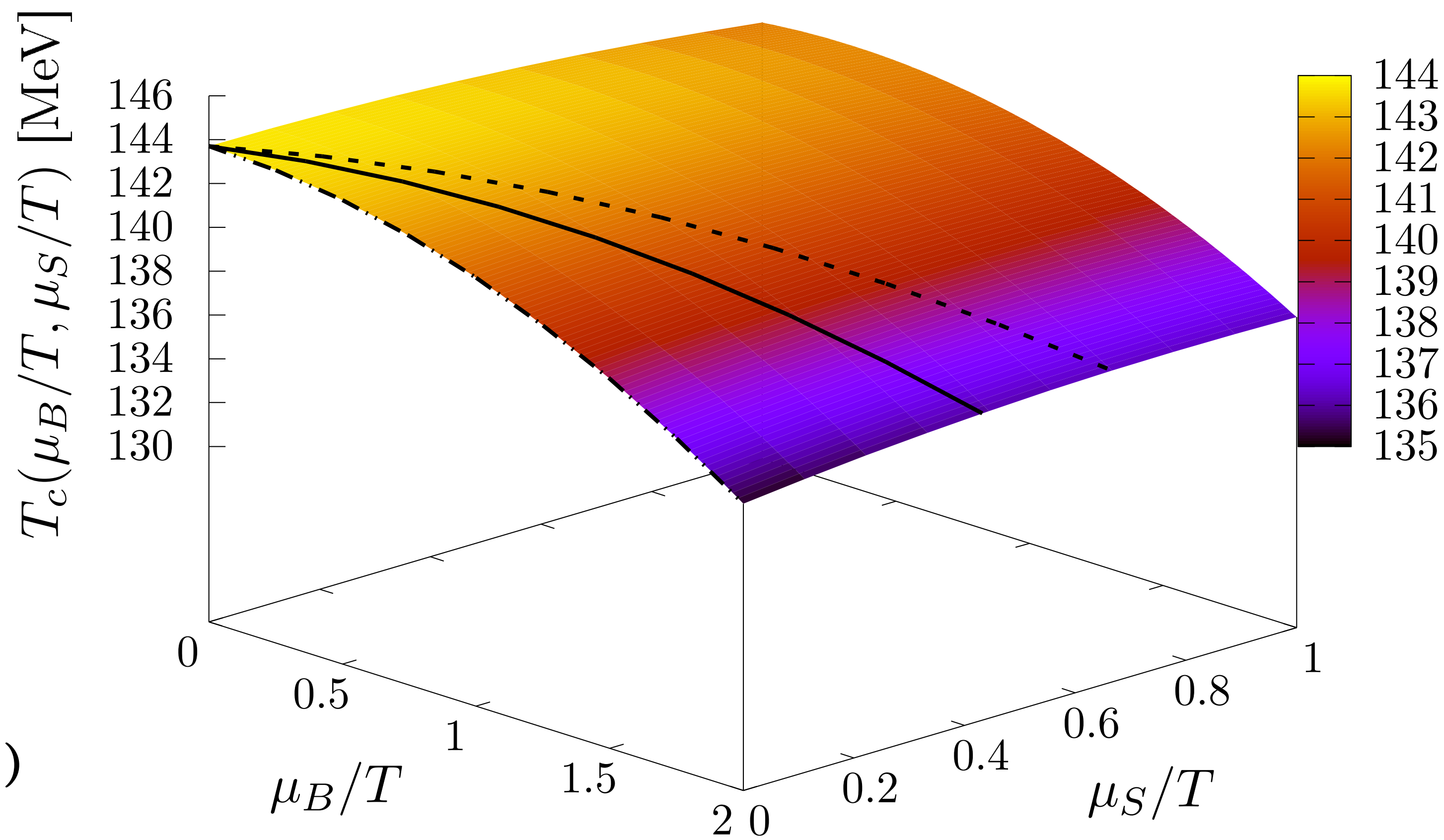
* Peak-position of susceptibilities determine a pseudo critical line (constant z_x)

$$T_{pc,x} = T_c \left(1 + \frac{z_x}{z_0} H^{1/\beta\delta} + \text{corrections to scaling}\right)$$

* Perform joined fit to peak positions of mixed susceptibilities, including corrections to scaling → results for T_c, z_0 are in good agreement with EoS fits.

- Remember:

$$t = \frac{1}{t_0}\left(\Delta T + \kappa_2^l \hat{\mu}_l^2 + \kappa_2^s \hat{\mu}_s^2 + 2\kappa_{11}^{ls}\hat{\mu}_l\hat{\mu}_s\right)$$



[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]

- Ratio of mixed susceptibilities are related to the curvature coefficients

$$\kappa_2^l = \frac{1}{2T_c}\left(\frac{\partial^2 M_l/\partial\hat{\mu}_l^2}{\partial M_l/\partial T}\right)\Bigg|_{(T=T_c,\vec{\mu}=0)}$$

$$\kappa_{11}^{ls} = \frac{1}{2T_c}\left(\frac{\partial^2 M_l/\partial\hat{\mu}_l\hat{\mu}_s}{\partial M_l/\partial T}\right)\Bigg|_{(T=T_c,\vec{\mu}=0)}$$

- results may be transformed to the hadronic basis

$$\kappa_2^{B,\hat{\mu}_S=0} \equiv \kappa_2^B = 0.015(1)$$

$$\kappa_2^{B,n_S=0} = 0.893(35)\kappa_2^B$$

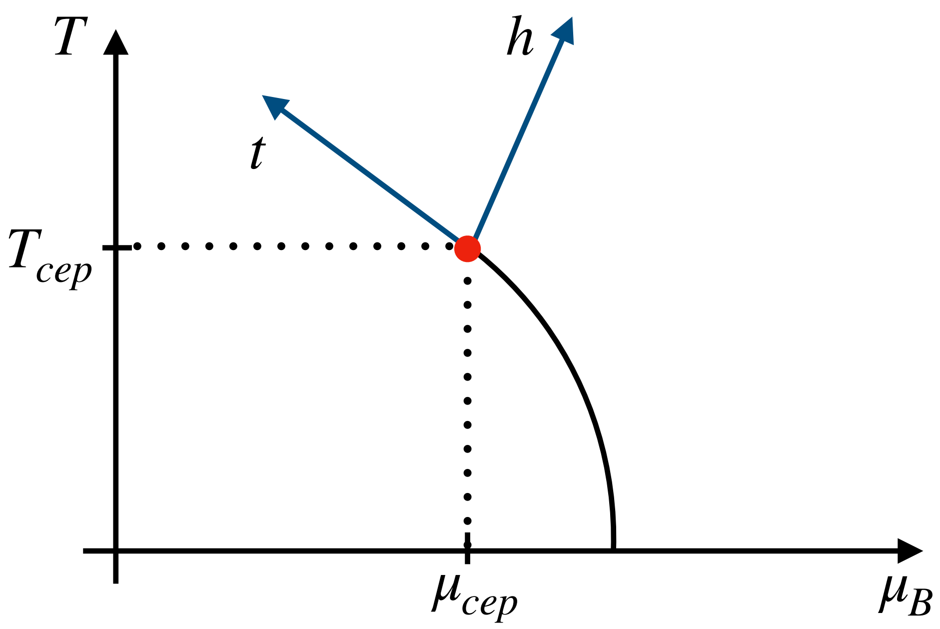
$$\kappa_2^{B,\hat{\mu}_s=0} = 0.968(23)\kappa_2^{n_S=0}$$

Mixing of scaling fields:

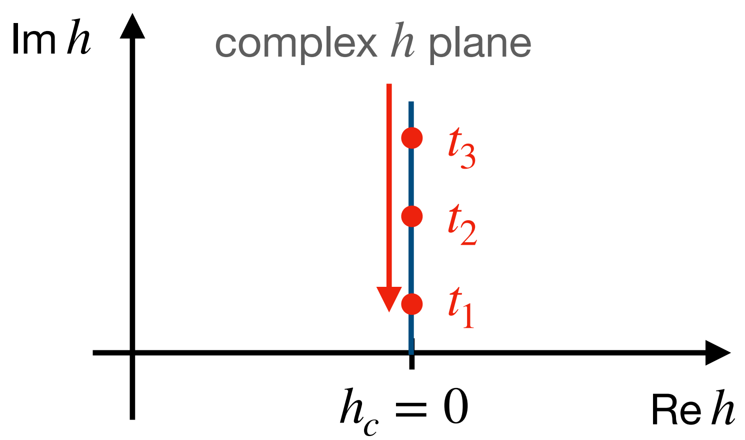
- Scaling fields are unknown, a frequently used ansatz is given by a linear mixing of T, μ_B

$$t = A_t \Delta T + B_t \Delta\mu_B,$$
$$h = A_h \Delta T + B_h \Delta\mu_B,$$

with $\Delta T = T - T^{\mathrm{CEP}}$ and $\Delta\mu_B = \mu_B - \mu_B^{\mathrm{CEP}}$



Lee-Yang edge:



- Poles approach critical point along imaginary h-axis **[Yang,Lee'59]**
- $t/h^{1/\beta\delta} = z_c$ is const. and universal

Fit Ansatz:

- For a constant $z = z_c$ we obtain

$$\mathrm{Re}[\mu_{\mathrm{LYE}}] = \mu_B^{\mathrm{CEP}} + c_1 \Delta T + c_2 \Delta T^2 + O(\Delta T^3)$$
$$\mathrm{Im}[\mu_{\mathrm{LYE}}] = c_3 \Delta T^{\beta\delta},$$

[Stephanov, Phys. Rev. D, 73.9, 094508 (2006)]

- The fit parameter c_1 gives the (inverse) slope of the 1st order line at the critical point: $c_1 = -A_h/B_h$

Method:

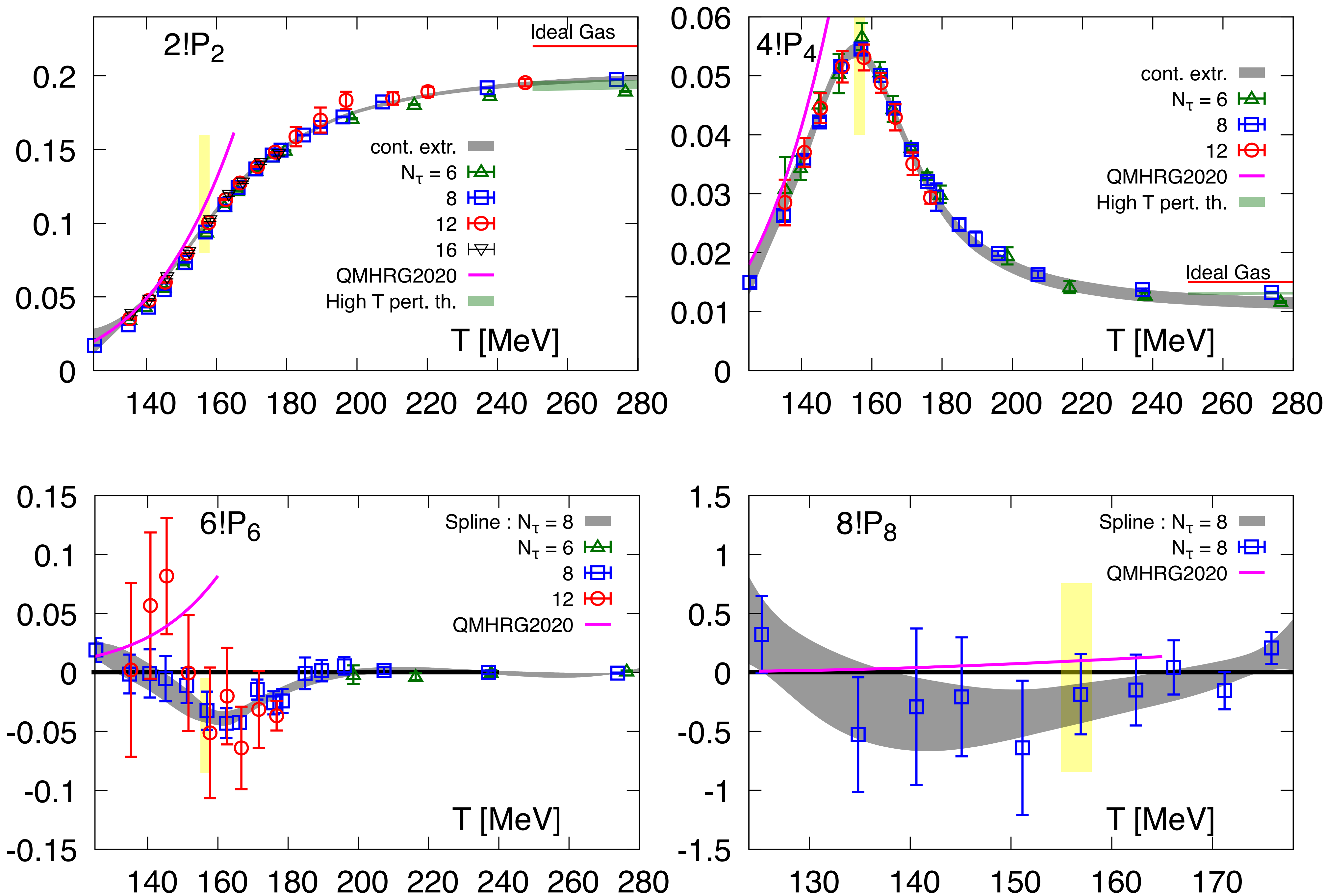
- Estimate location of complex zeros of the partition function by multi-point Padé technique
- Replace expensive calculation of sixth and eights order by many expansion points at imaginary chemical potential
- Investigate the universal Lee-Yang scaling of the zeros
  ➡ **determine location of the phase transition by extrapolation**

This is not the final answer!

- Lattice QCD is hindered by the infamous sign problem
  ➡ **need to relay on indirect methods**
- Use existing Taylor expansion around $\mu_B = 0$ and Padé resummation for $N_\tau = 8$, and multi-point Padé applied to calculations at imaginary μ_B for $N_\tau = 6$.
  ➡ **expect cutoff effects and systematic errors**

$$\Delta\hat{p} \equiv \frac{p(T,\mu_B)}{T^4} - \frac{p(T,0)}{T^4} = \sum_{k=1}^{\infty} P_{2k}(T)\hat{\mu}_B^{2k}$$

- Detecting phase transitions via Padé and post-Padé approximants has a long history in statistical and high energy physics
- They are often used in combination with perturbation theory
- QCD is non-perturbative in the vicinity of the phase
- The numerical calculation of the pressure series in μ_B is difficult

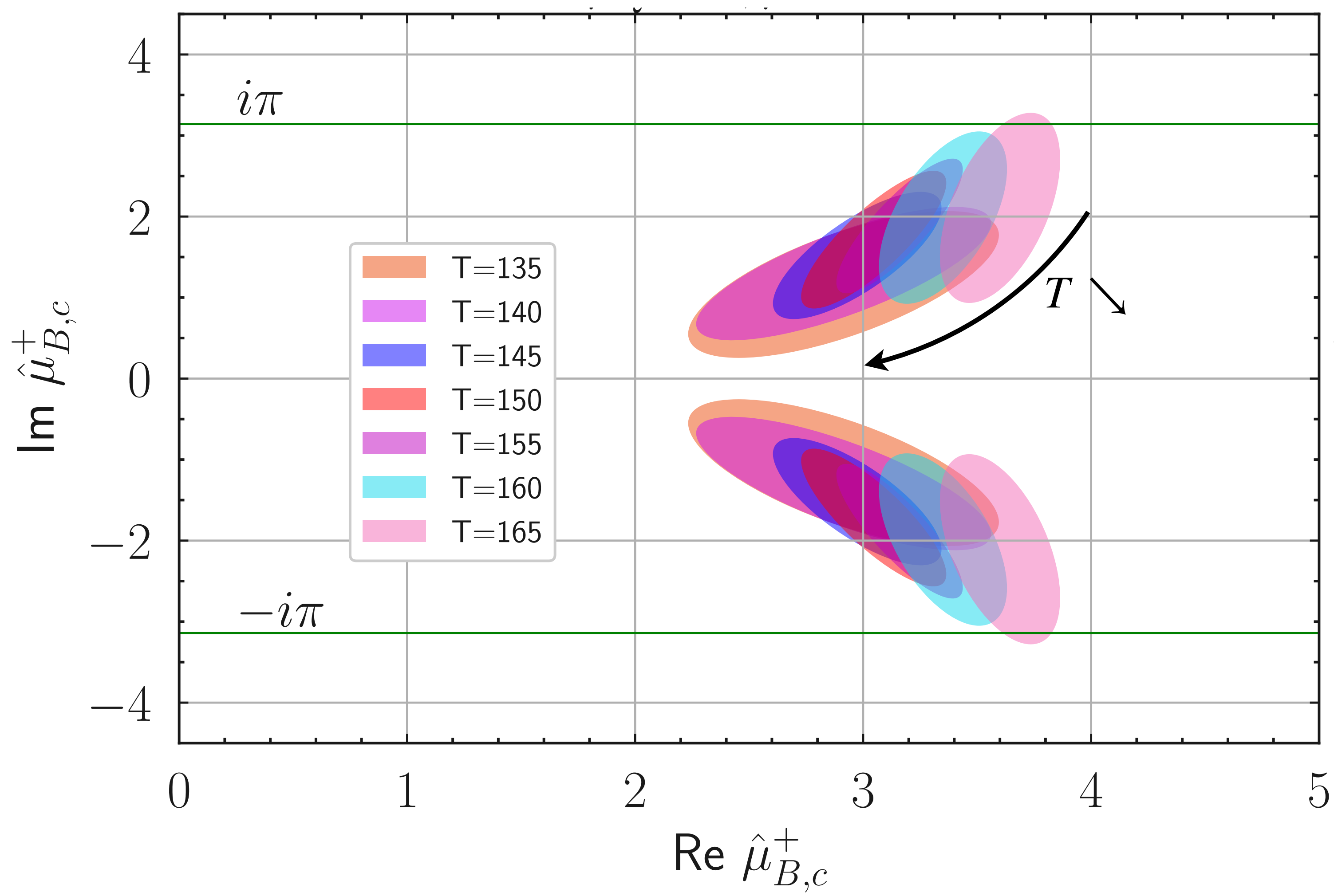


HotQCD, PRD 108 (2023) 1, 014510, arXiv: 2212.09043]

Padé resummation of the Taylor series about $\mu_B = 0$

- Construct [4,4]-Padé from 8th order Taylor Expansion
- Calculate complex roots of the denominator
- Find apparent approach to the real axis with decreasing temperature
- Can also be combined with conformal maps **[Basar, 2312.06952]**

$$P[4,4] = \frac{P_2\hat{\mu}_B^2 + (P_4 + (P_2^2 P_8)/P_4^2)\hat{\mu}_B^4}{1 + ((P_2 P_8)/P_4^2)\hat{\mu}_B^2 - (P_8/P_4)\hat{\mu}_B^4}$$



[PRD 105 (2022) 7, 074511, arXiv: 2202.09184]

Code:

- SIMULATeQCD by HotQCD **[Comp.Phys.Comm. 300 (2024) 109164]**

Simulation Parameters:

- Use (2+1)-flavor of *Highly Improved Staggered Quarks* (HISQ) with physical masses ($m_l/m_s = 1/27$).
- Lattice size: $36^3 \times 6$
- Use *Line of Constant Physics* (LCP) and scale setting from HotQCD
- Introduce non-zero imaginary chemical potential $\hat{\mu}_u = \hat{\mu}_d = \hat{\mu}_s = i\theta$, which corresponds to $\mu_B = 3\mu_u$ and $\mu_S = 0$

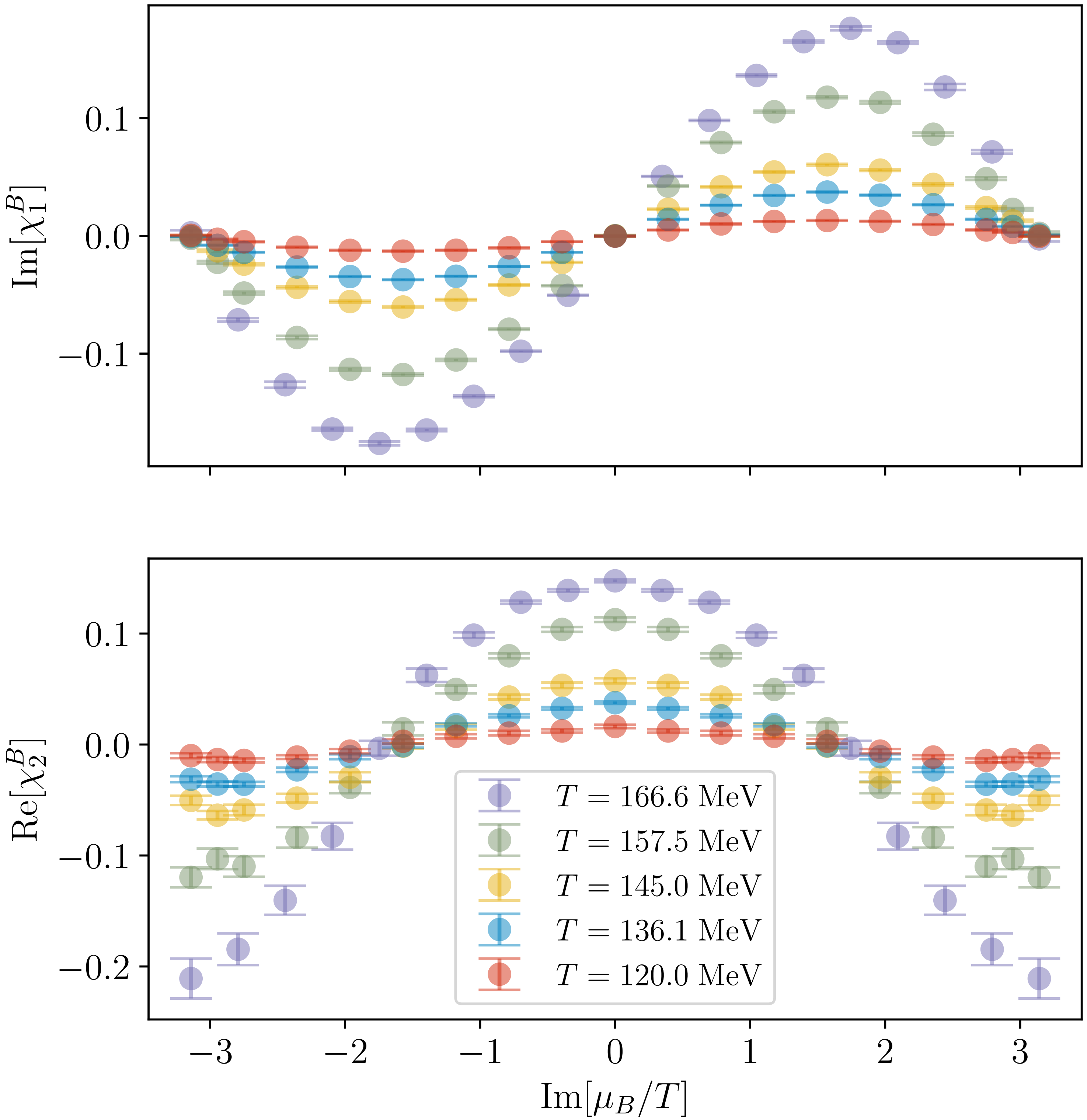
Statistics:

T [MeV]	N_μ	N_{conf}/N_μ
166.6	10	1800
157.5	10	4780
145.0	10	5300
136.1	10	6840
120.0	10	24000

Machines:

- Juwels-Booster @ JSC
- Marconi100 @ CINECA
- Leonardo @ CINECA

Lattice size: $36^3 \times 6$



[arXiv: 2403.09390]

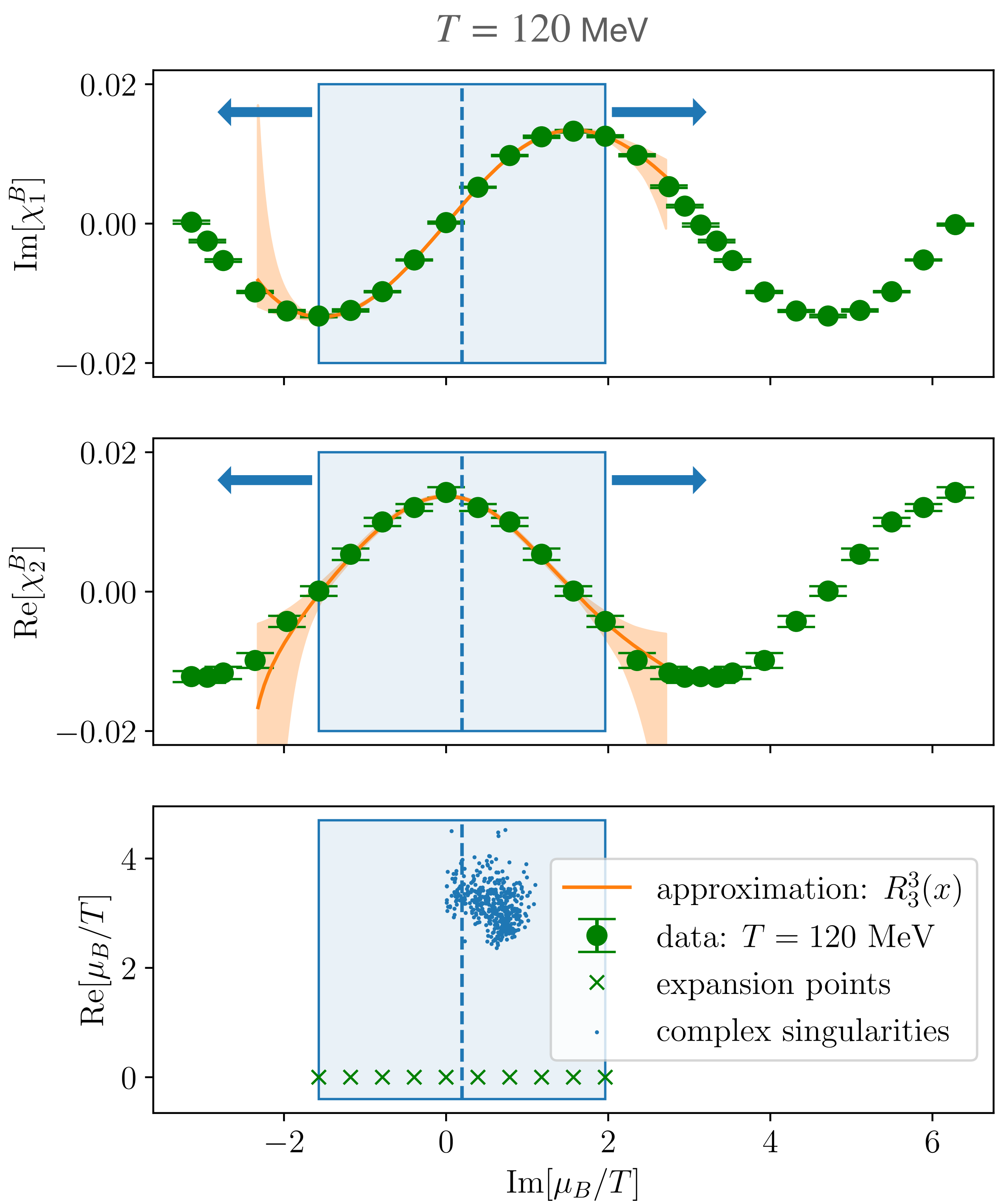
Observables:

- Derivatives of $\ln Z$, w.r.t $\hat{\mu}_B = \mu_B/T$

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

- $\ln Z$ is even in $\hat{\mu}_B = i\theta$ and periodic, with periodicity 2π
- Choose 10 equidistant $\hat{\mu}_B$-points in $[0, i\pi]$, all further points are obtained by periodicity and parity
- Odd (even) derivatives are imaginary (real) at $\hat{\mu}_B = i\theta$

Sliding Window Analysis



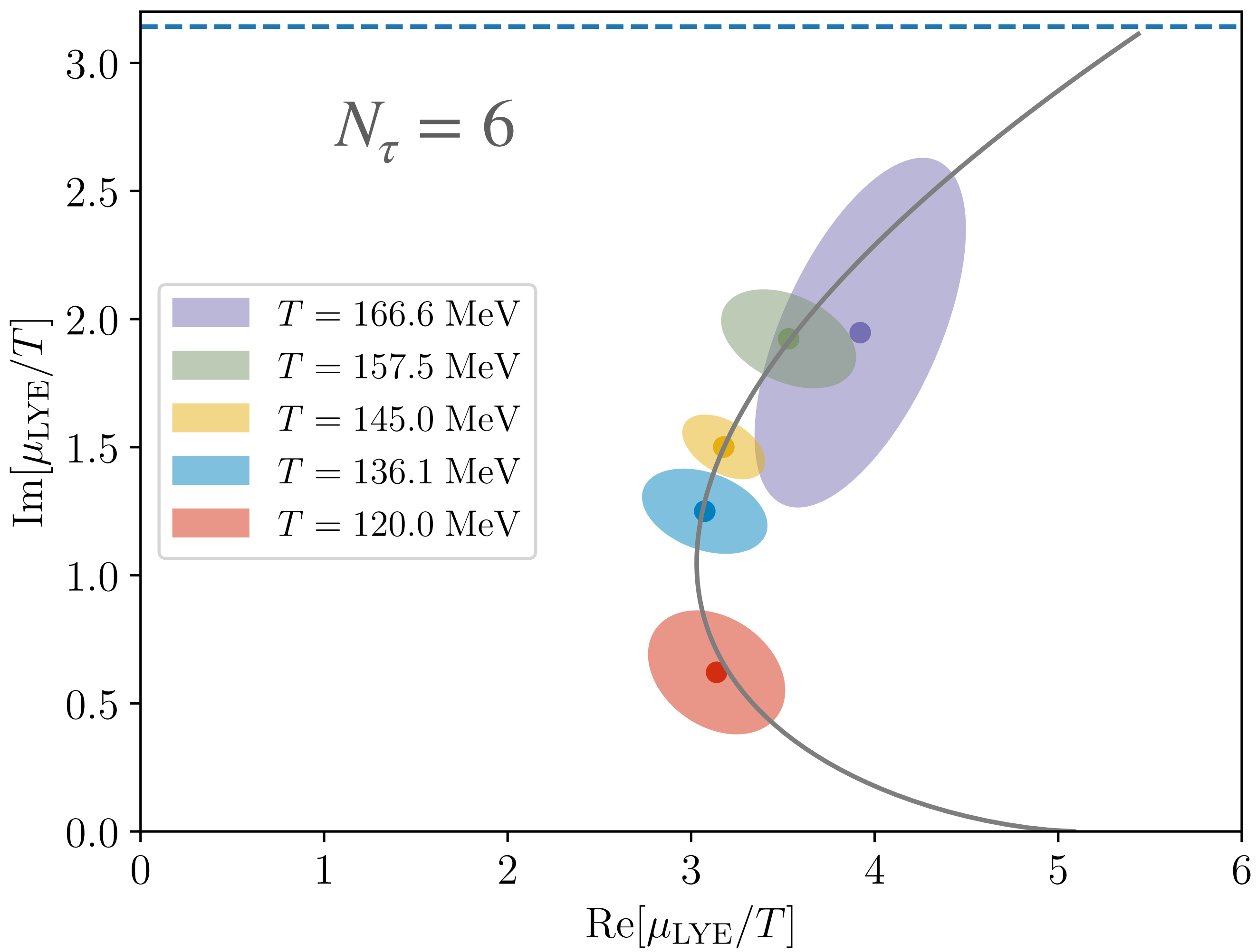
[arXiv: 2405.10196]

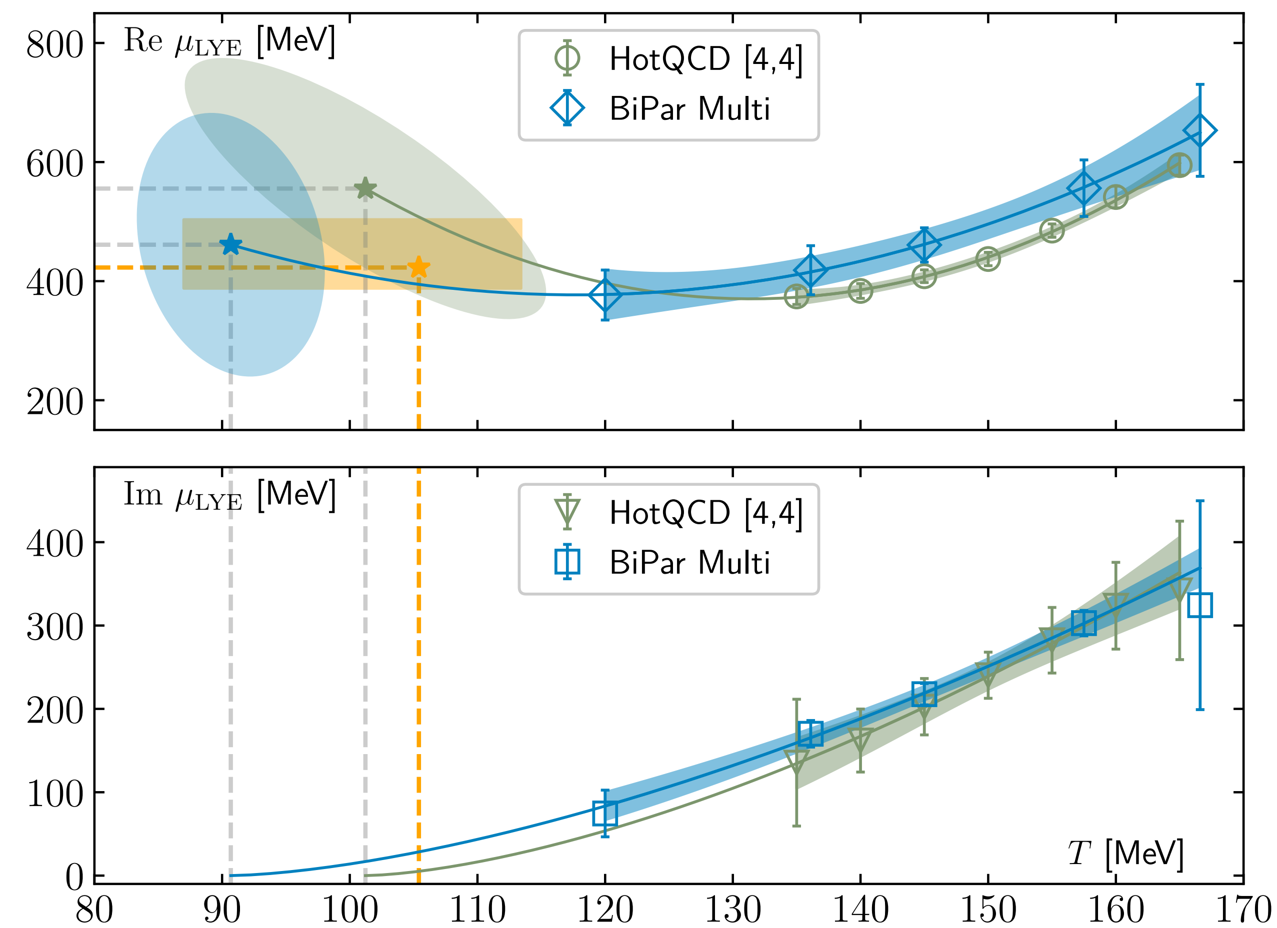
Procedure:

* Perform simultaneous fits to χ_1^B and χ_2^B for each temperature
* Use [3,3]-Padé
* Varry length of the fit interval in $[\pi, 2\pi]$ and the center of the interval in $[-\pi/2, +\pi/2]$
* bootstrap over the data by assuming independent and normal distributed errors
* Calculate roots of the denominator and keep only roots in the first quadrant
* Collect all the results for Lee-Yang scaling fits. We have 55 different intervals per temperature.

Fit results

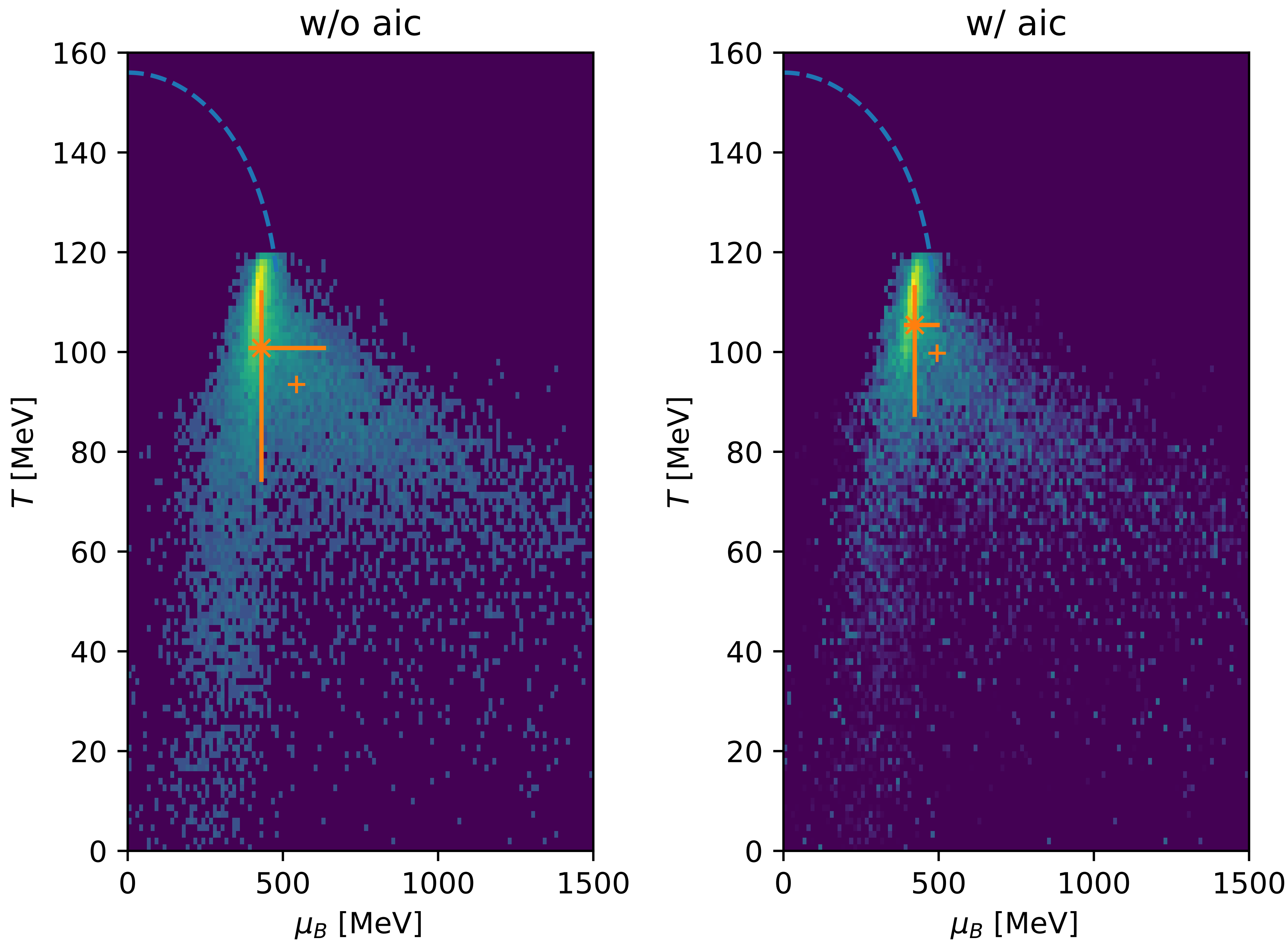
- Perform one fit for $N_\tau = 8$ and $\mathcal{O}(10^5)$ fits for $N_\tau = 6$





$$\mathrm{Re}[\mu_{\rm LYE}] = \mu_B^{\rm CEP} + c_1 \Delta T + c_2 \Delta T^2$$
$$\mathrm{Im}[\mu_{\rm LYE}] = c_3 \Delta T^{\beta\delta},$$

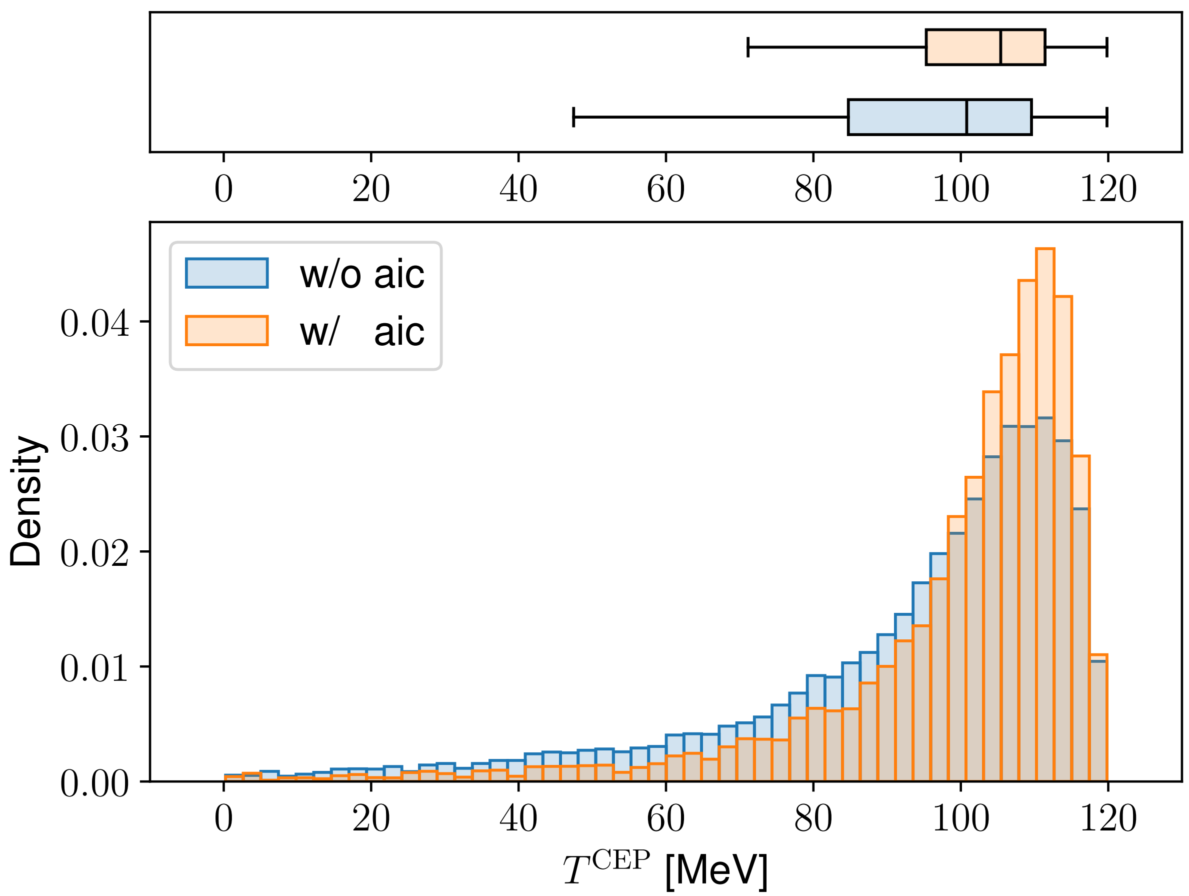
- Ellipses show 1σ confidence region, using the Pearson correlation coefficient
- $N_\tau = 6$ singularities show here are chosen on the basis of the χ^2 of the scaling fit (“best fit”)
- Orange box shows the AIC weighted result for $N_\tau = 6$, based on $\mathcal{O}(10^5)$ scaling fits

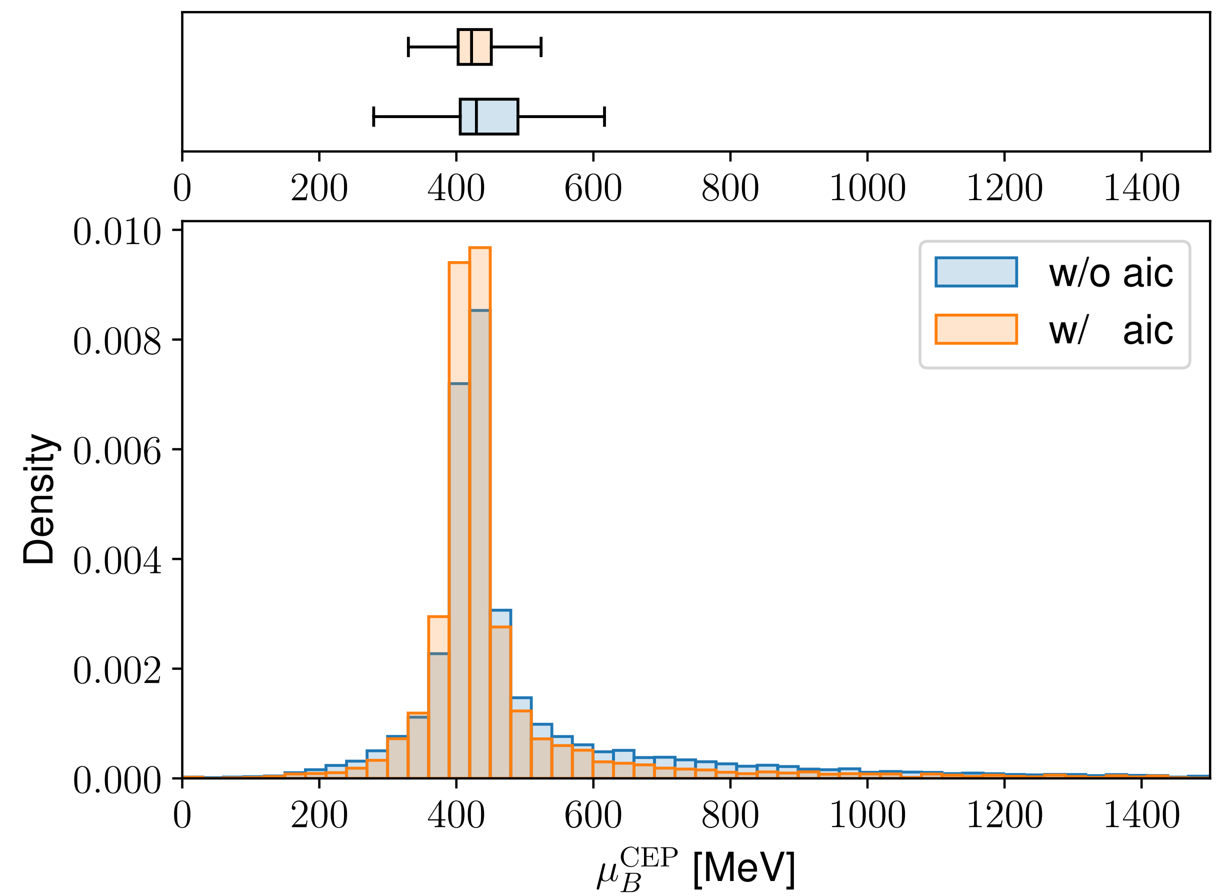


- Dashed line indicates the continuum extrapolated crossover line

- Histogram over the T^{CEP} and μ_B^{CEP} from the $\mathcal{O}(10^5)$ fits
- Error bars are based on the inner 68-percentile
- Observe interesting structure

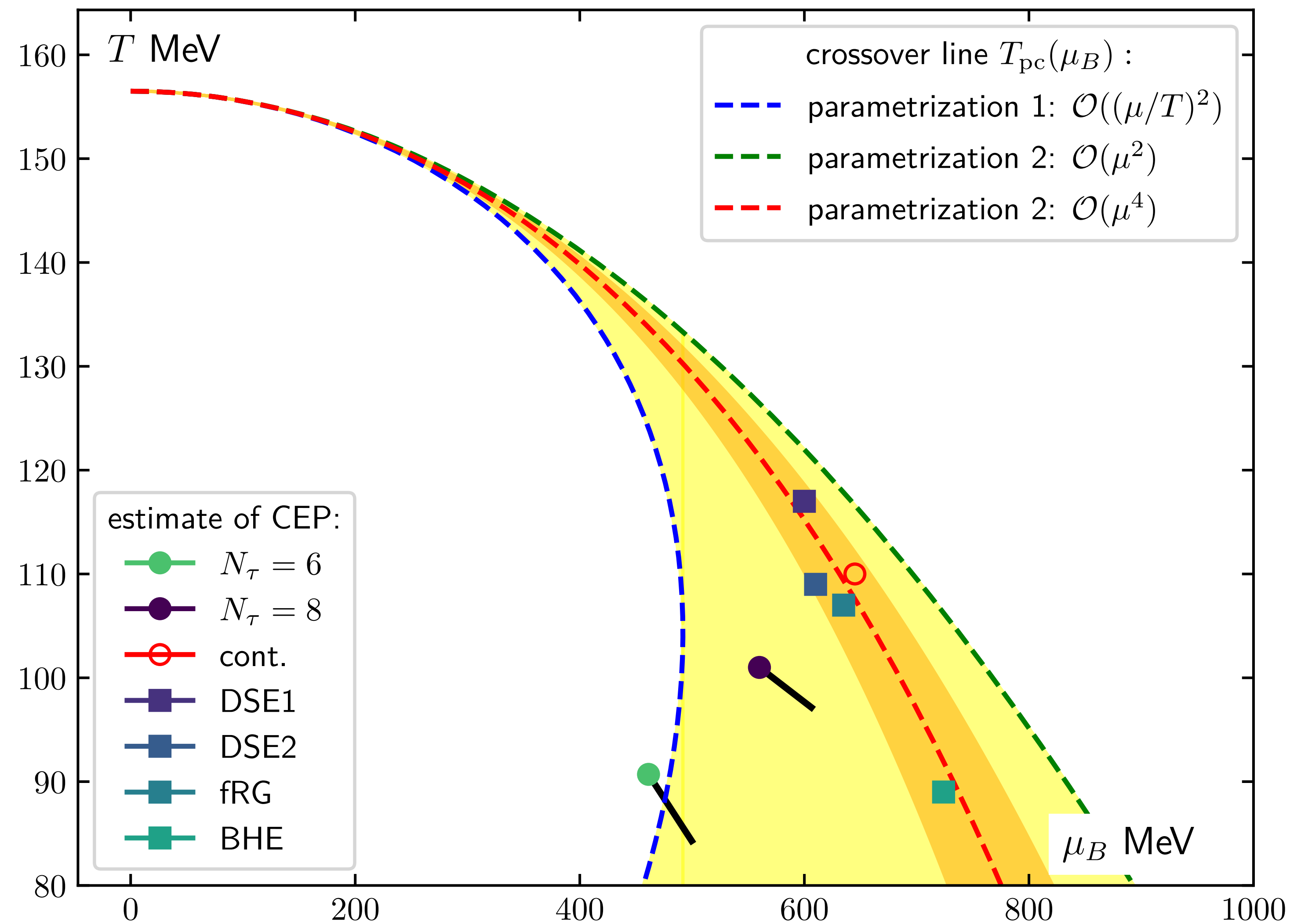
Statistical analysis of fits





	$\mathbf{N}_\tau = \mathbf{6}$ **multi-point Padé**			$\mathbf{N}_\tau = \mathbf{8}$ **[4,4]-Padé**		
	T^{CEP} [MeV]	μ_B^{CEP} [MeV]	μ_B/T	T^{CEP} [MeV]	μ_B^{CEP} [MeV]	μ_B/T
best fit	90.7 ± 7.7	461.2 ± 220	5.09 ± 0.68	101 ± 15	560 ± 140	5.5 ± 1.7
weight-1	$105.4 + 8.0 - 18.4$	$422.9 + 80.5 - 34.9$	$3.92 + 1.52 - 0.24$			
weight-2	$100.8 + 11.6 - 26.8$	$430.9 + 208.2 - 42.2$	$4.20 + 4.13 - 0.47$			
	c_1	c_2	c_3	c_1	c_2	c_3
best fit	-6.2 ± 9.2	0.115 ± 0.090	0.424 ± 0.086	-12.3 ± 8.1	0.203 ± 0.059	0.55 ± 0.25

* For $N_\tau = 8$: similar results by **[Basar, arXiv: 2312.06952]**



- Continuum estimate might suffer from large systematic effects (Padé vs multi-point Padé)
- $\kappa_2 = \bar{\kappa}_2 = -0.015(1)$
  [HotQCD, 2403.09390]
- Many results seem to favour a small $\bar{\kappa}_4 \approx -0.0002(1)$

Parametrizations of the crossover line:

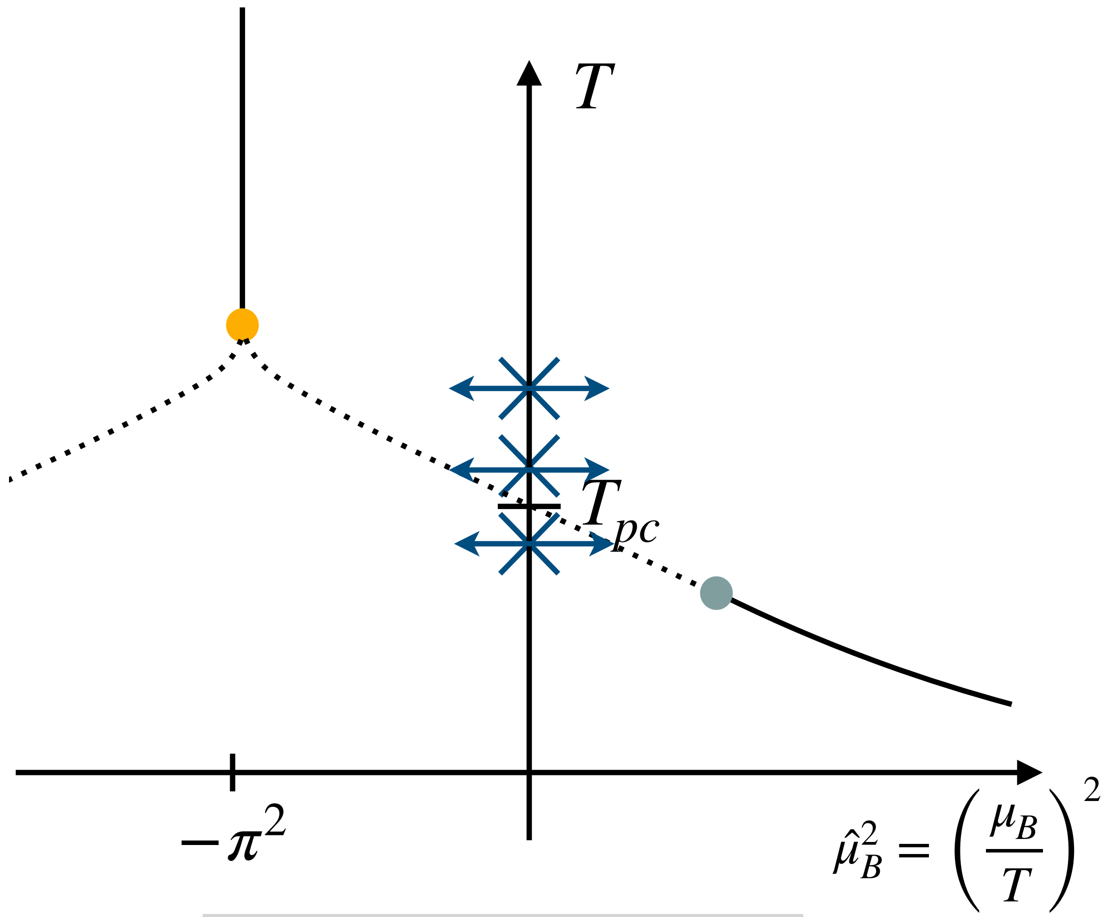
- 1.) $T_{\rm pc}(\mu_B) = T_{\rm pc}(0)\left[1 + \kappa_2^B \left(\frac{\mu_B}{T}\right)^2 + \kappa_4^B \left(\frac{\mu_B}{T}\right)^4\right]$
- 2.) $T_{\rm pc}(\mu_B) = T_{\rm pc}(0)\left[1 + \bar{\kappa}_2^B \left(\frac{\mu_B}{T_{\rm pc}(0)}\right)^2 + \bar{\kappa}_4^B \left(\frac{\mu_B}{T_{\rm pc}(0)}\right)^4\right]$

- Universal scaling is a very powerful tool if the scaling fields and the universality class are known.
- Transition temperate in the chiral limit, pseudo-critical line and curvature coefficients are obtained from scaling fits.
- Pseudo-critical lines correspond (asymptotically) to a constant real $z = t/h^{1/\beta\delta}$, the Lee-Yang edge to a universal complex z_c
- New Strategy: Determine the QCD critical point by the temperature scaling of the Lee-Yang edge singularity
- Technically this requires Pade or multi-point Pade analysis of $\ln Z$ derivatives. The later eliminates the need for the calculation of high order expansion coefficients but introduces some interval dependence.
- Find encouraging results for $N_\tau = 6$: $(T^{\mathrm{CEP}}, \mu_B^{\mathrm{CEP}}) = (105^{+8}_{-18}, 422^{+80}_{-35})$ MeV .
- No continuum result yet
- Current estimates of the cutoff effects increase μ_B^{CEP} towards $\mu_B^{\mathrm{CEP}} \approx 650$ MeV

Back Up Slides

* Calculate derivatives of the pressure $\frac{p}{T^4} = \frac{\ln Z}{VT^3}$

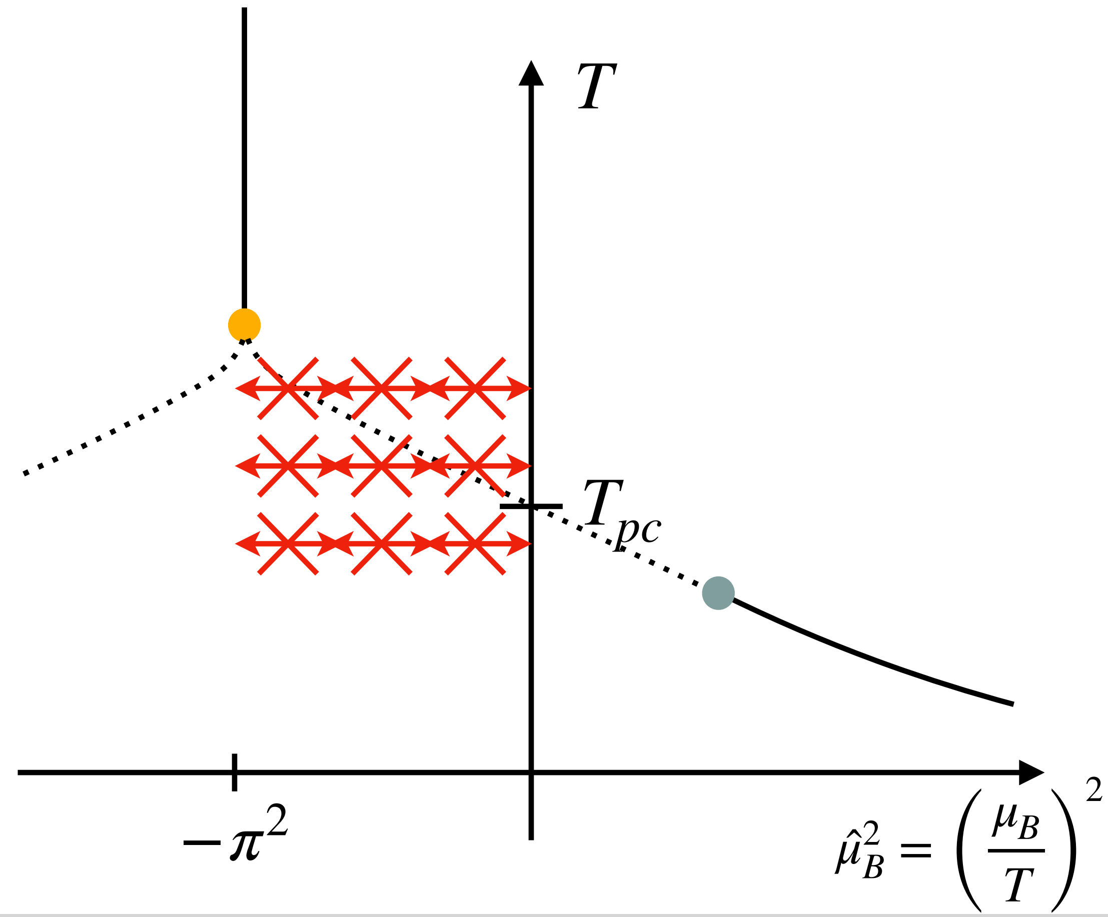
$(T, \mu_B = 0)$: **Taylor expansion in μ_B^2**



[Allton et al. PRD 66 (2002)]

⇒ perform a Padé resummation to obtain the complex singularity that limit the radius of convergence

$(T, \mu_B^2 < 0)$: **Taylor expansion in μ_B**



[De Frorcrand, Philipsen (2002); D'Elia, Lombardo (2003)]

⇒ obtain a rational approximation of the data (e.g. by the multi-point Padé) to obtain the closest singularity

⇒ alternatively, analyse the (asymptotic) behaviour of the Fourier coefficients

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

$$P_m(0) - f(0)Q_n(0) = f(0)$$

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

$$\vdots$$

→ 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

$$P_m(x_0) - f(x_0)Q_n(x_0) = f(x_0)$$

$$P_m'(x_0) - f'(x_0)Q_n(x_0) - f(x_0)Q_n'(x_0) = f'(x_0)$$

$$\vdots$$

$$P_m(x_1) - f(x_1)Q_n(x_1) = f(x_1)$$

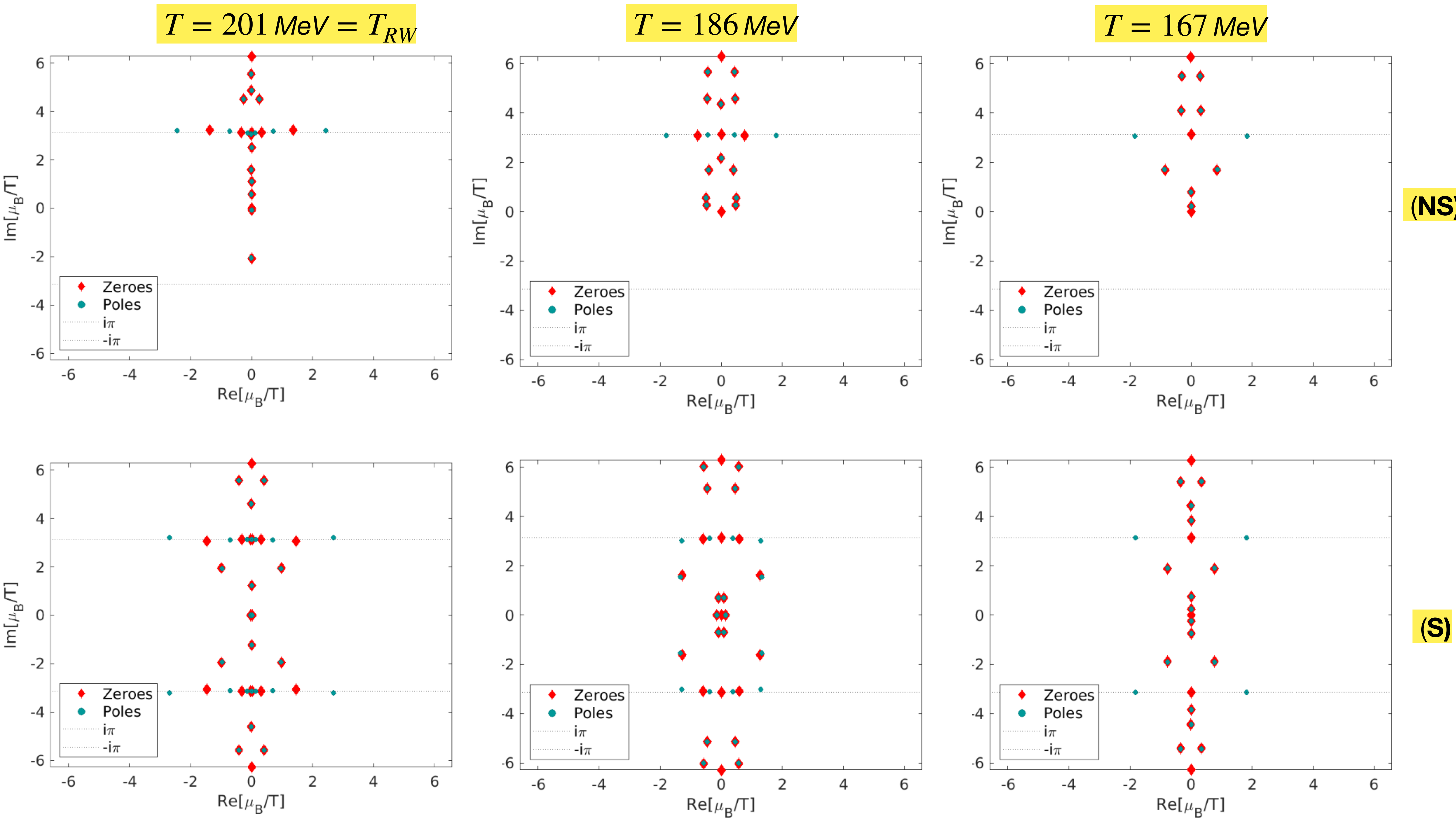
$$P_m'(x_1) - f'(x_1)Q_n(x_1) - f(x_1)Q_n'(x_1) = f'(x_1)$$

$$\vdots$$

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

[Dimpopoulos et al. Phys.Rev.D 105 (2022) 3, 034513]

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

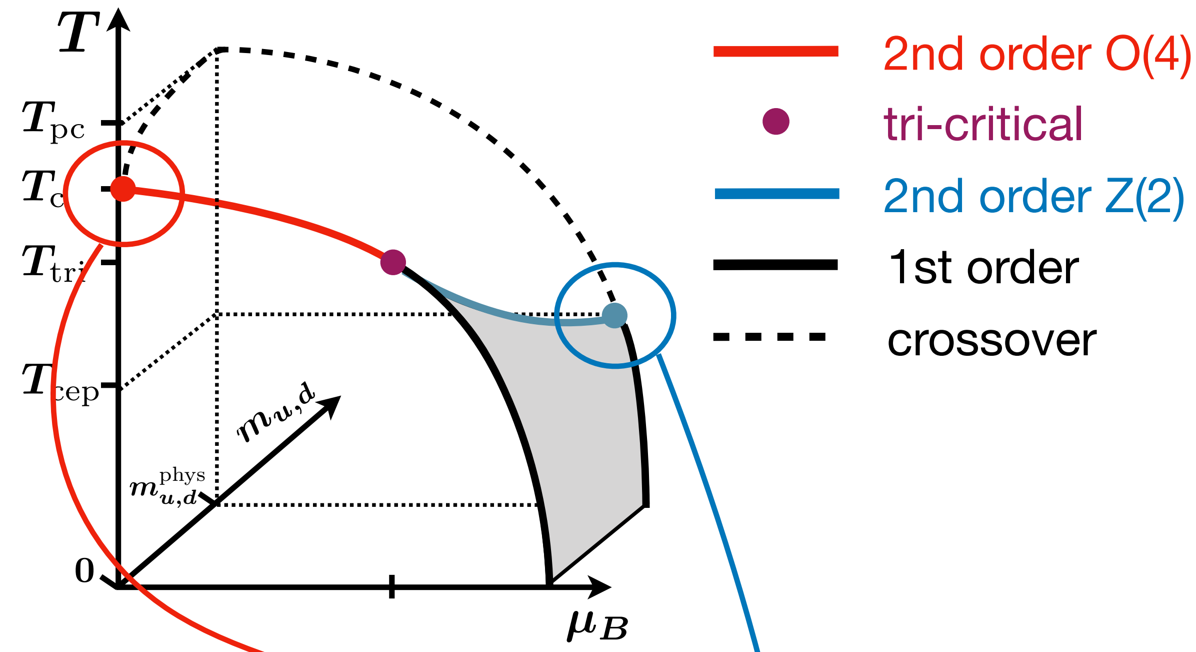


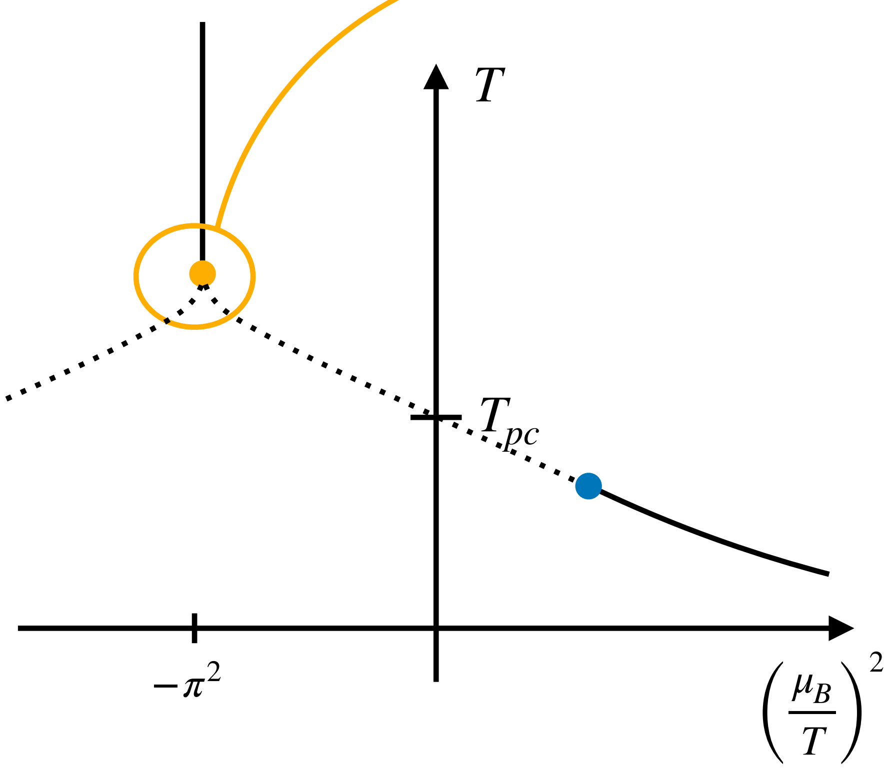
→ find almost perfect cancelation of many zeros and poles

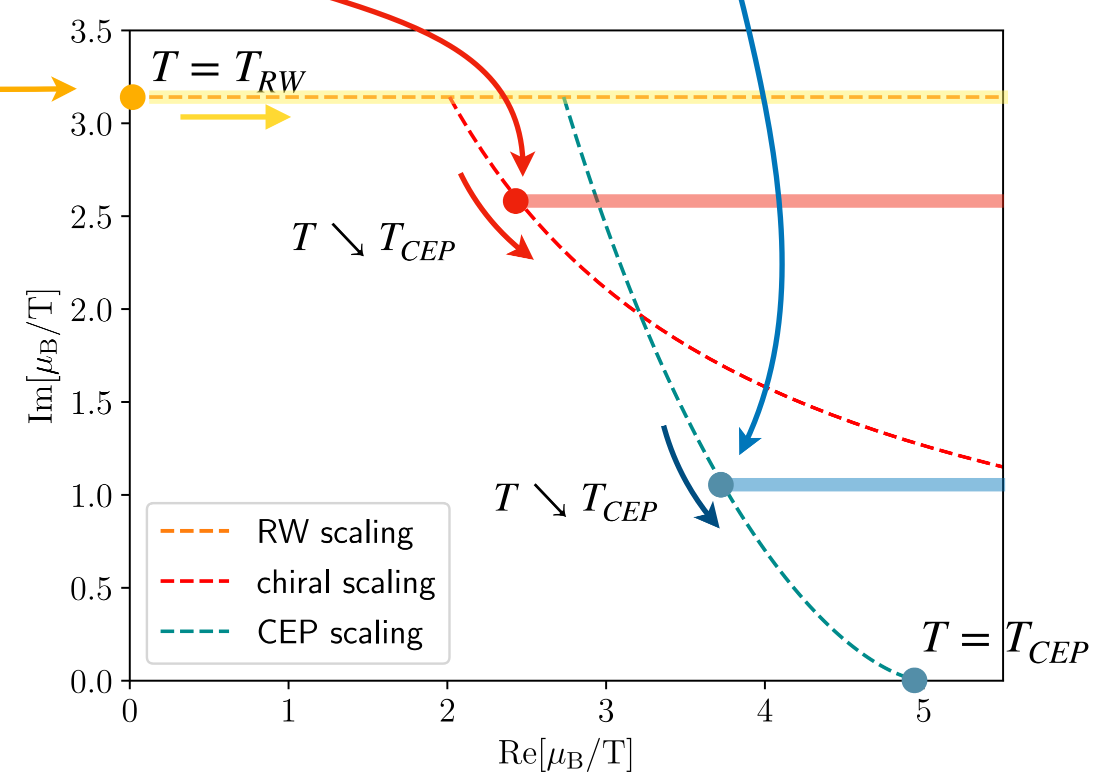
→ find signature for branch cut along $\mu_B/T = \mu_B^R \pm i\pi$ at $T = \{201, 186\}$ MeV

[Dimopoulos et al., *PRD* 105 (2022)]

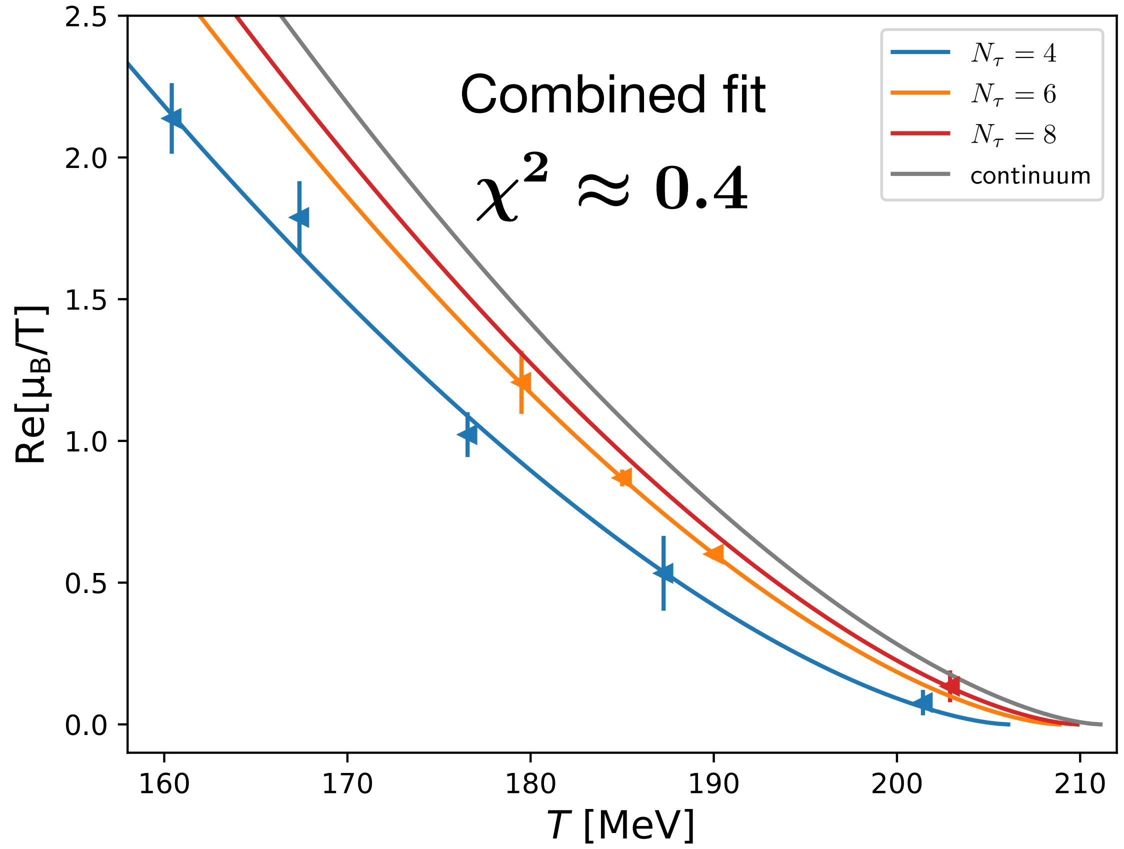
- Track Lee-Yang edge singularity in the complex $\frac{\mu_B}{T}$ -plane, as function of T
- We can think of three distinct critical points/ scaling regions: Roberge Weiss transition, chiral transition, QCD critical point
- Solve $t/h^{1/\beta\delta} \equiv z_{YL}$ for different scaling fields and non-universal constants.

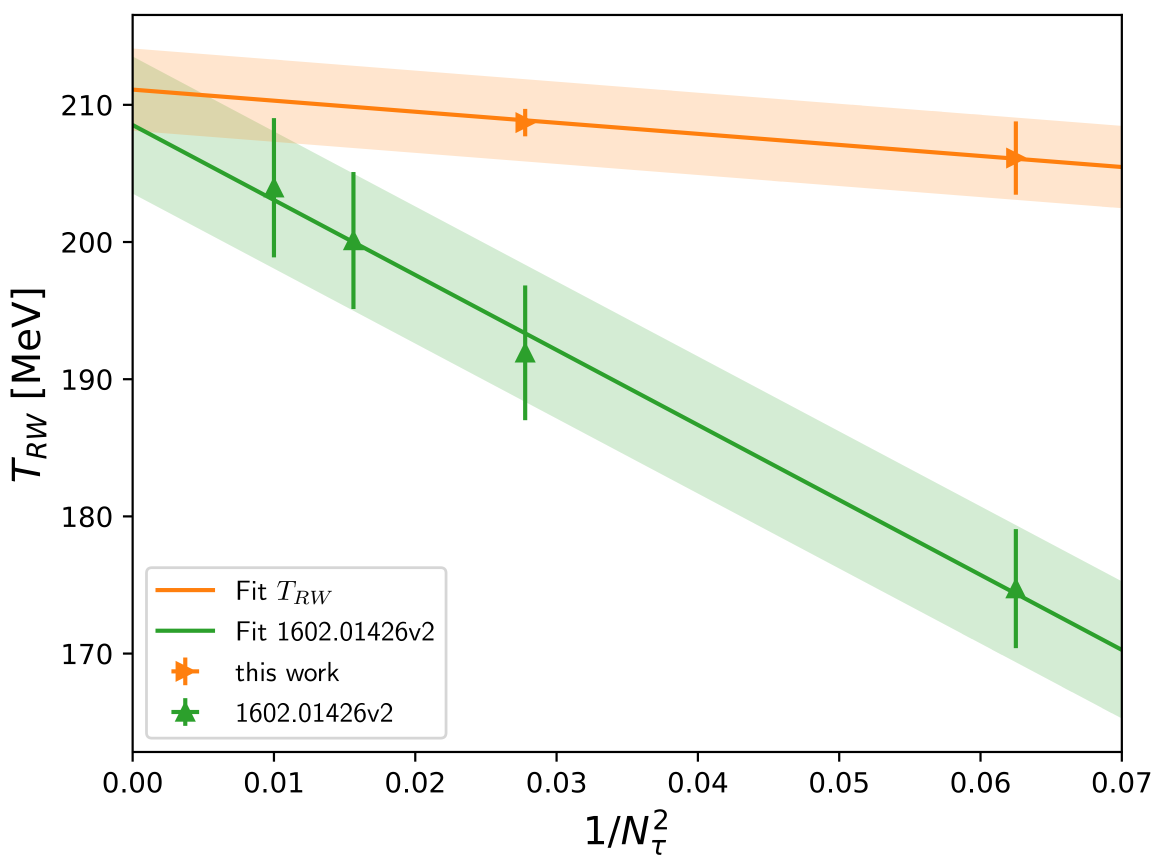






→ different temperature intervals are sensitive to different scaling of the Lee-Yang edge singularity





- The approach of the LY edge to the RW critical point: By solving $z = t/h^{1/\beta\delta} \equiv z_c$ we find

$$\hat{\mu}^R_{LY} = a(N_\tau) \left(\frac{T_{RW}(N_\tau) - T}{T_{RW}(N_\tau)} \right)^{\beta\delta}$$

with $\hat{\mu}^R_{LY} = \mathrm{Re}[\mu_B/T]$

We assume $T_{RW} = T^{(0)}_{RW} + T^{(2)}_{RW}/N_\tau^2$

$$a = a^{(0)} + a^{(2)}/N_\tau^2$$

- Obtain continuum result

$$T^{(0)}_{RW} = 211.1 \pm 3.1 \text{ MeV}$$

⇒ in good agreement with previous results from the Pisa group

[Bonati et al., PRD 93 (2016) 074504]

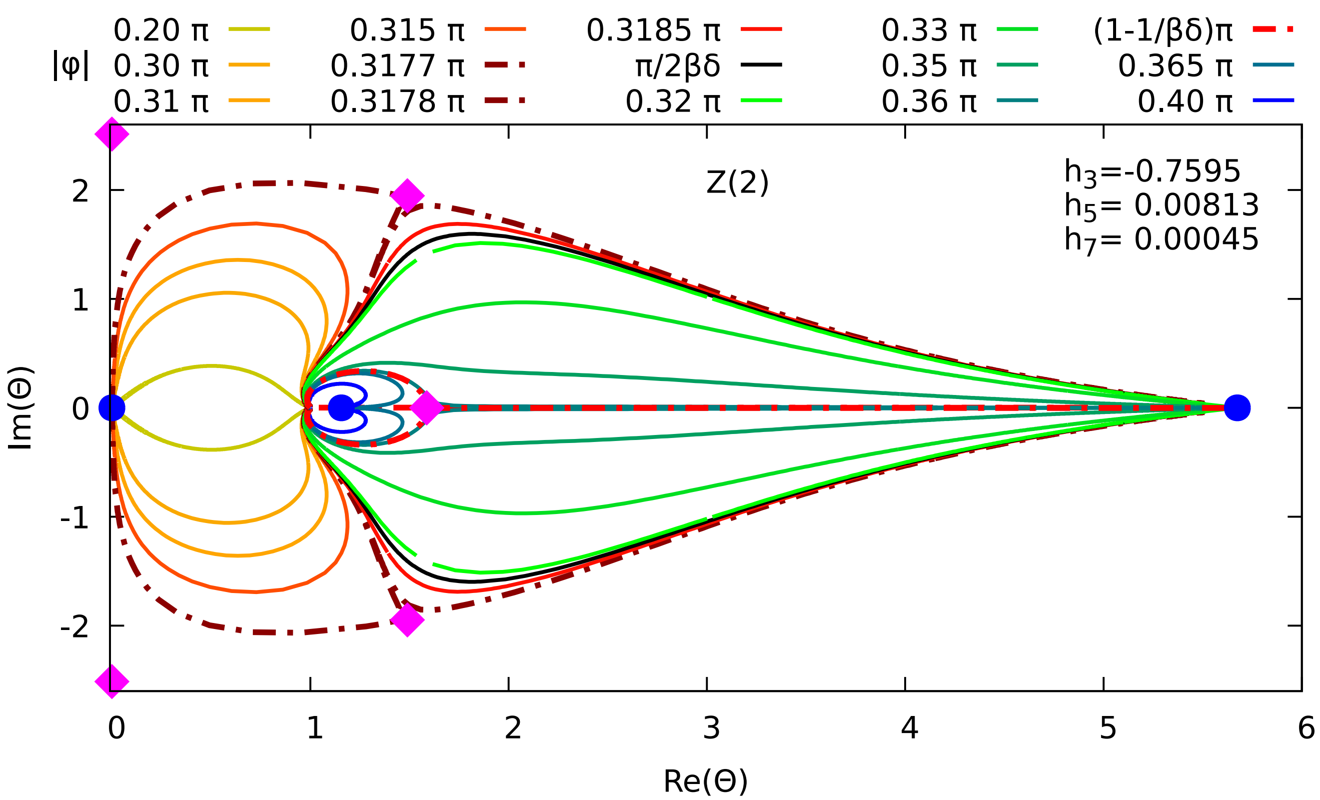
$$\begin{cases} M = m_0 R^{\beta} \theta \\ t = R(1-\theta^2) \\ h = h_0 R^{\beta\delta} h(\theta) \end{cases}$$

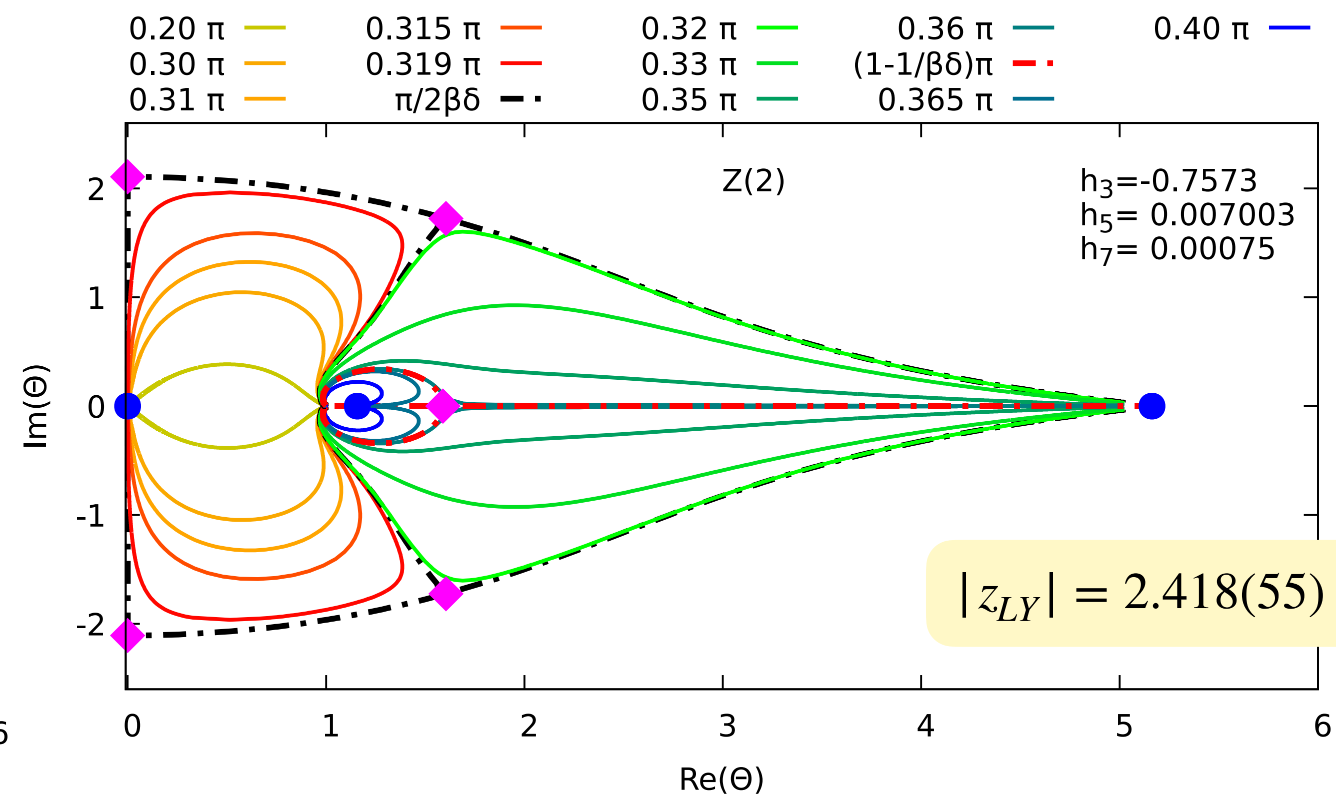
$$h(\theta) = \theta \left(1 + h_3\theta^2 + h_5\theta^4 + h_7\theta^6 + \cdots\right)$$

$$z(\theta) = \frac{1-\theta^2}{\theta_0^2 - 1}\theta_0^{1/\beta}\left(\frac{h(\theta)}{h(1)}\right)^{-1/\beta\delta}$$

- The coefficients h_3, h_5 can be determined perturbatively and non-perturbatively

[Guida, Zinn-Justin, NPB 489 (1997)]
[Karsch et al. PRD 108 (2023) 014505]





$|z_{LY}| = 2.418(55)$

- the coefficient h_7 is not known precisely (zero within current precision)
- $h_7 \neq 0$ introduces an additional pair of singularities (imaginary if $h_7 > 0$, real if $h_7 < 0$)
- h_7 can be used to tune the phase of the LY edge singularity

[Karsch, CS, Singh, arXiv:2311.13530]