

Location of the critical point from Lattice QCD

Christian Schmidt



HotQCD Collaboration:

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

[arXiv: [2403.09390](https://arxiv.org/abs/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](https://arxiv.org/abs/2405.10196)]

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

LBNL, May 20-24, 2024

Method:

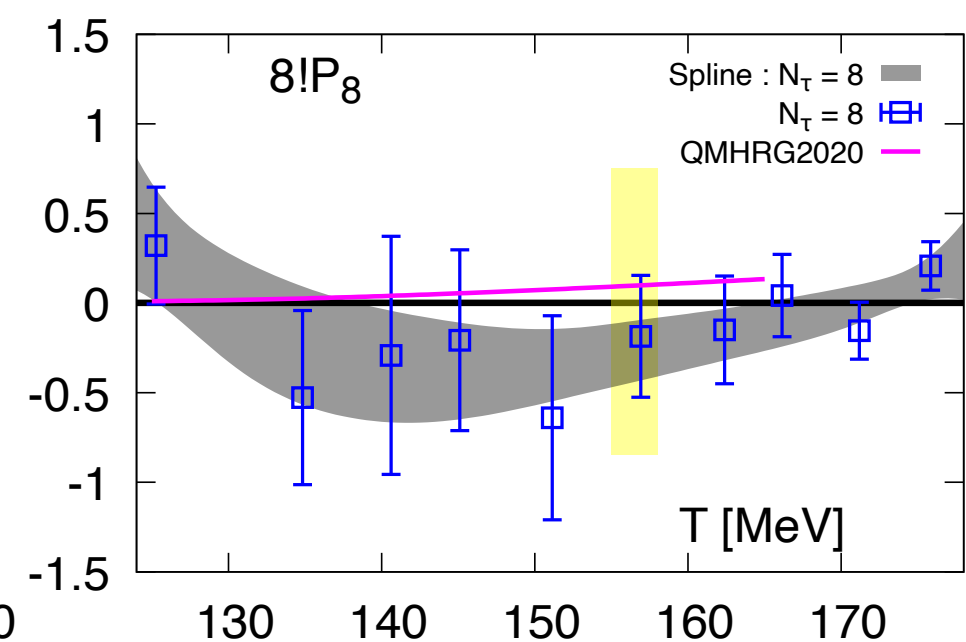
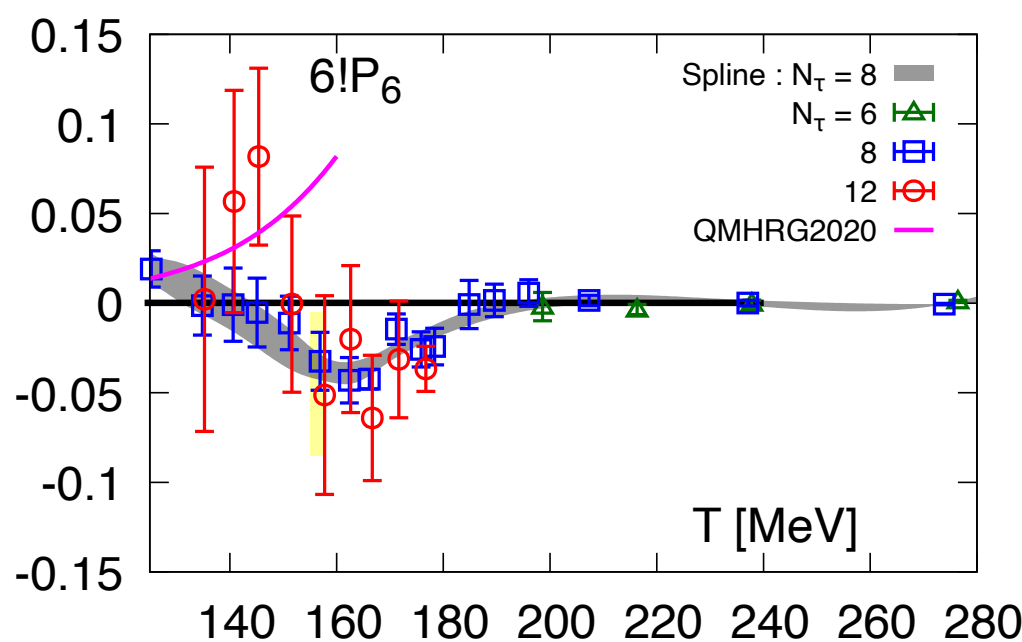
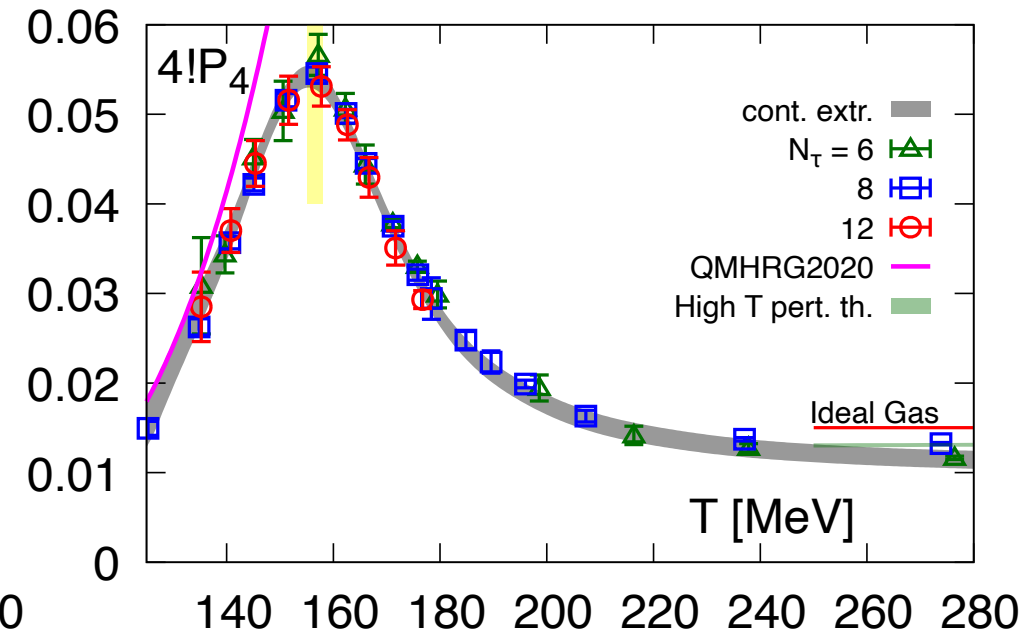
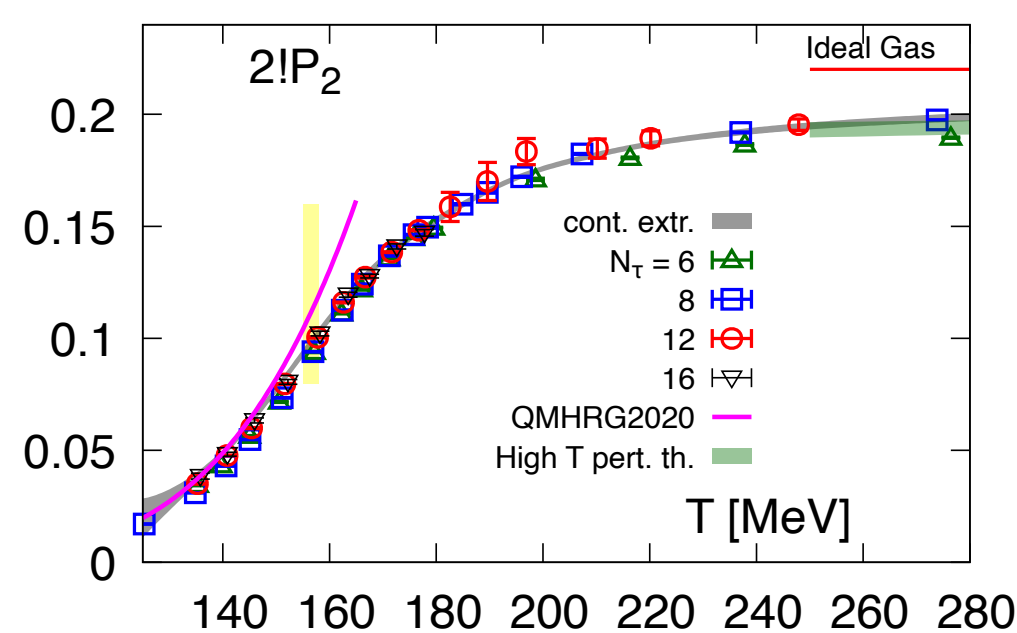
- * Estimate location of complex zeros of the partition function by multi-point Padé technique
- * Replace expensive calculation of sixth and eights order by many expansion points at imaginary chemical potential
- * Investigate the universal Lee-Yang scaling of the zeros
 - ➔ **determine location of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

This is not the final answer!

- * Lattice QCD is hindered by the infamous sign problem
 - ➔ **need to rely 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**

- * 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

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



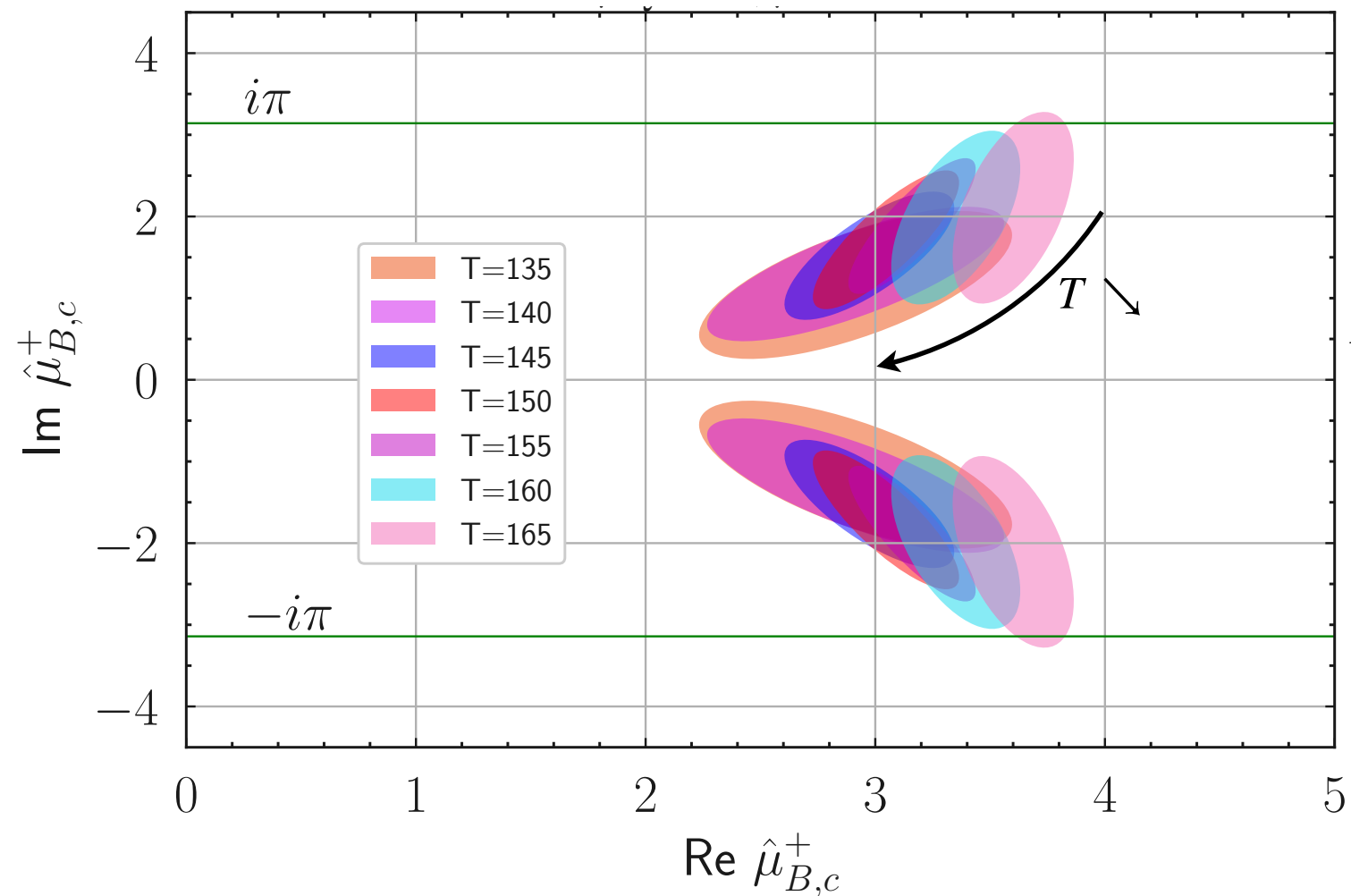
- * Construct [4,4]-Padé from 8th order Taylor Expansion

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

- * Calculate complex roots of the denominator

- * Find apparent approach to the real axis with decreasing temperature

- * Can also be combined with conformal maps
 \Rightarrow see talk by G. Basar on Friday



Code:

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

Simulation Parameters:

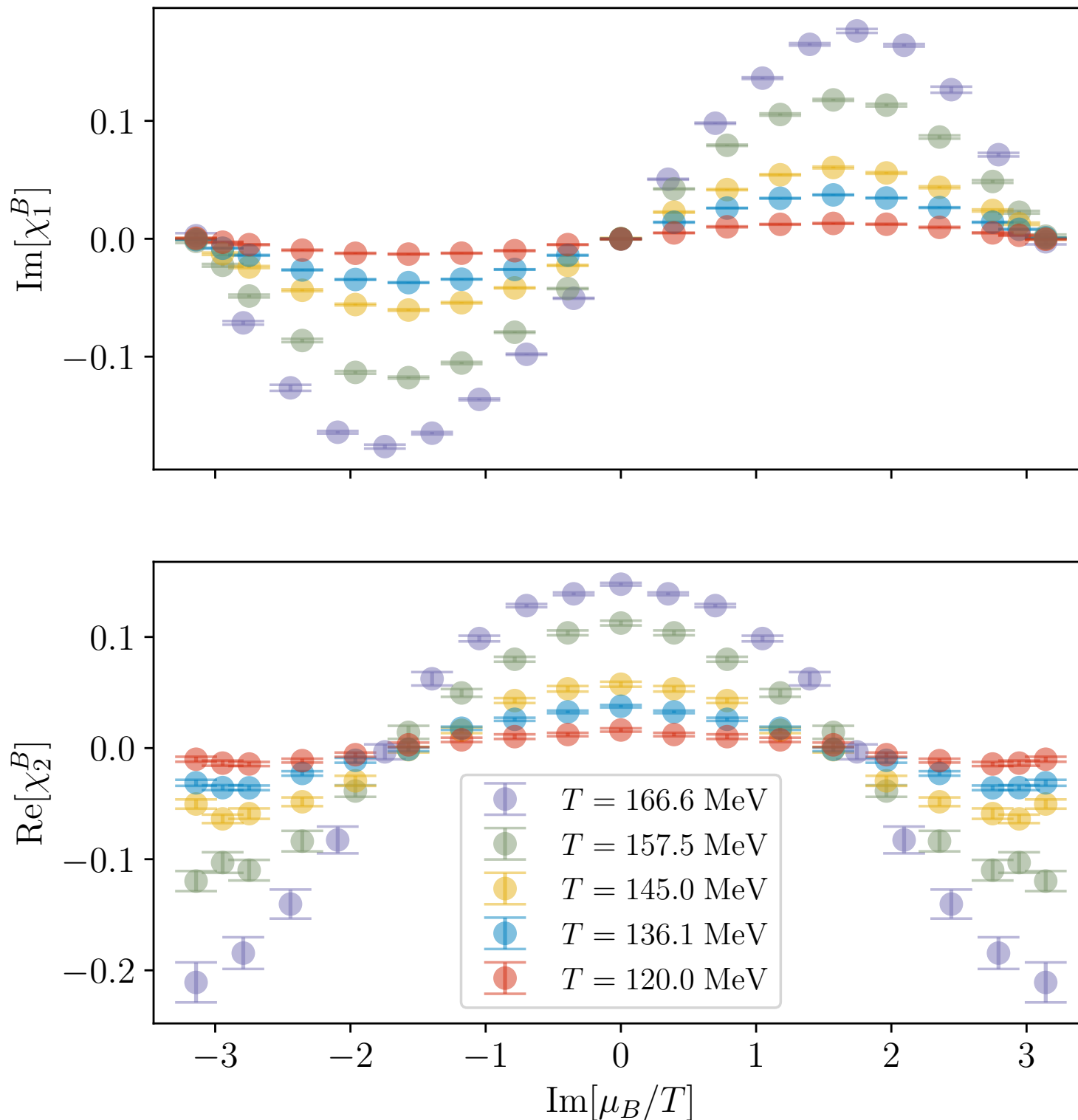
- * Use (2+1)-flavor of *Highly Improved Staggered Quarks* (HISQ) with physical masses ($m_l/m_s = 1/27$).
- * Lattice size: $36^3 \times 6$
- * Use *Line of Constant Physics* (LCP) and scale setting from HotQCD
- * Introduce non-zero imaginary chemical potential $\hat{\mu}_u = \hat{\mu}_d = \hat{\mu}_s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

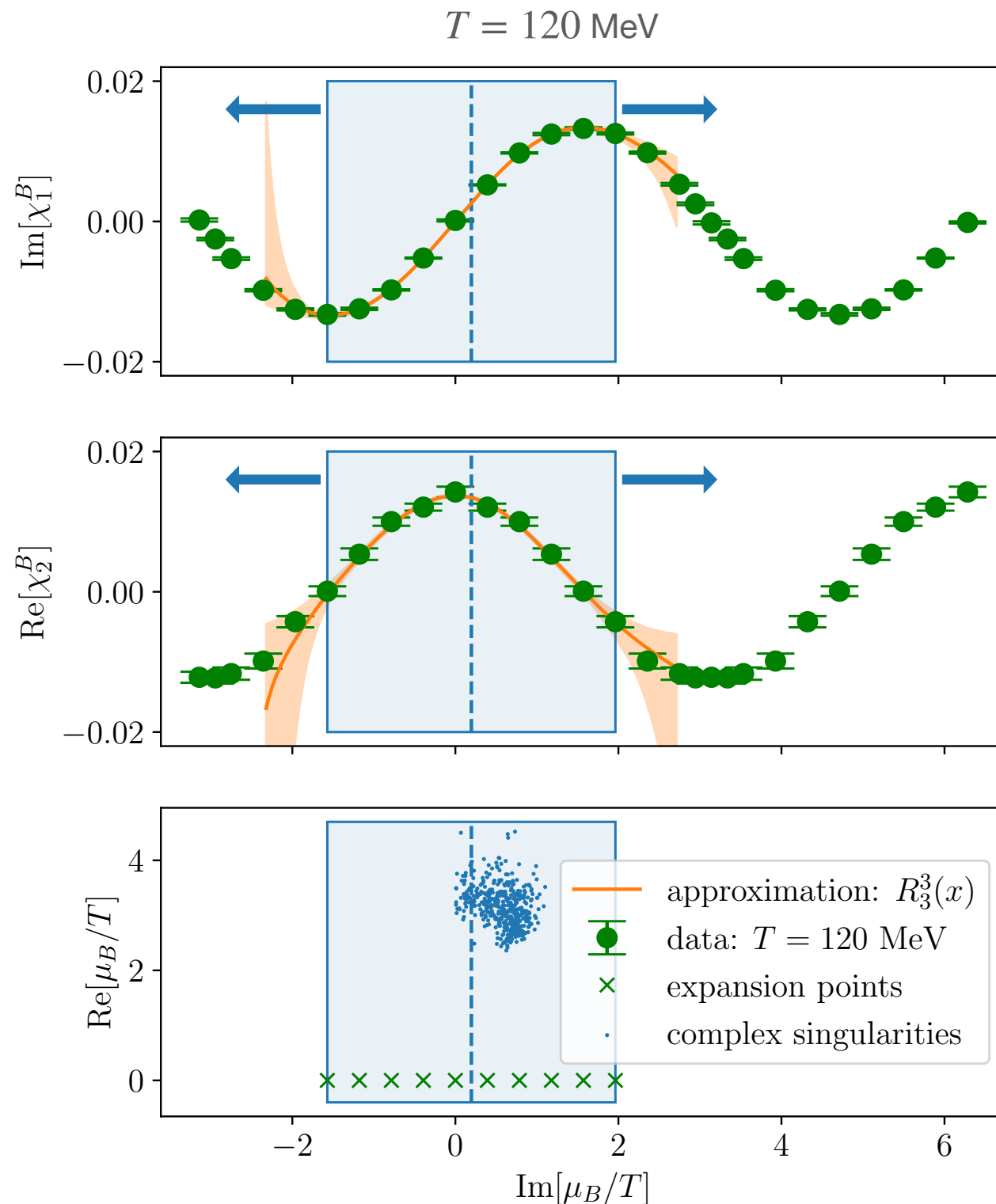
- * Juwels-Booster @ JSC
- * Marconi100 @ CINECA
- * Leonardo @ CINECA

Lattice size: $36^3 \times 6$ [arXiv: [2403.09390](https://arxiv.org/abs/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 $\hat{\mu}_B = i\theta$



[arXiv: [2403.09390](https://arxiv.org/abs/2403.09390)]

Procedure:

- * Perform simultaneous fits to χ_1^B and χ_2^B for each temperature
- * Use [3,3]-Padé
- * Vary 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.

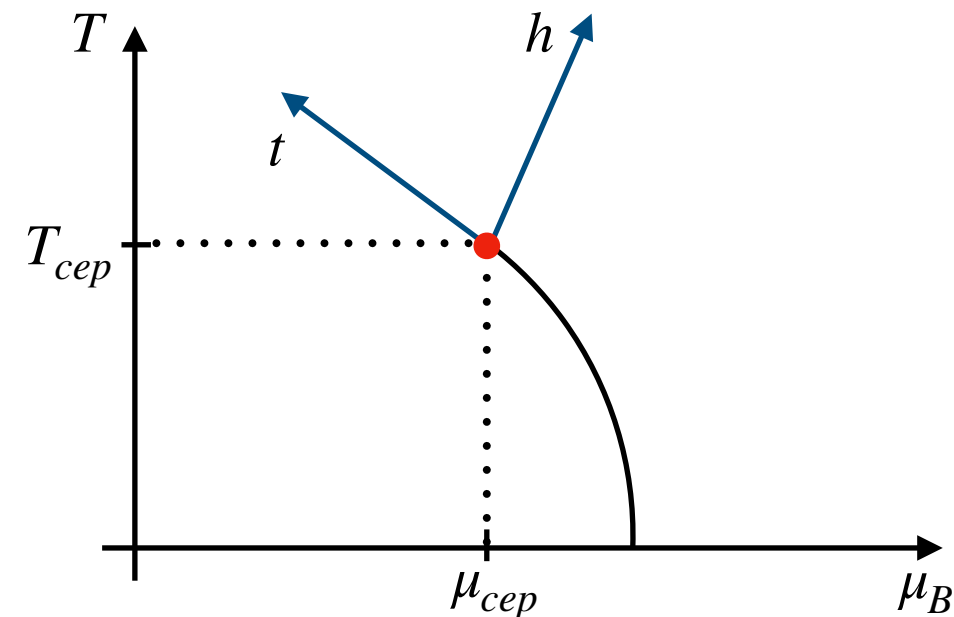
Mixing of scaling fields:

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

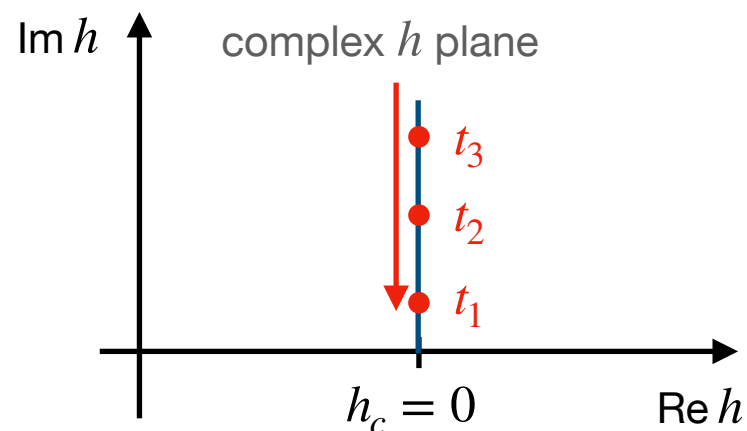
$$t = A_t \Delta T + B_t \Delta \mu_B,$$

$$h = A_h \Delta T + B_h \Delta \mu_B,$$

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



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

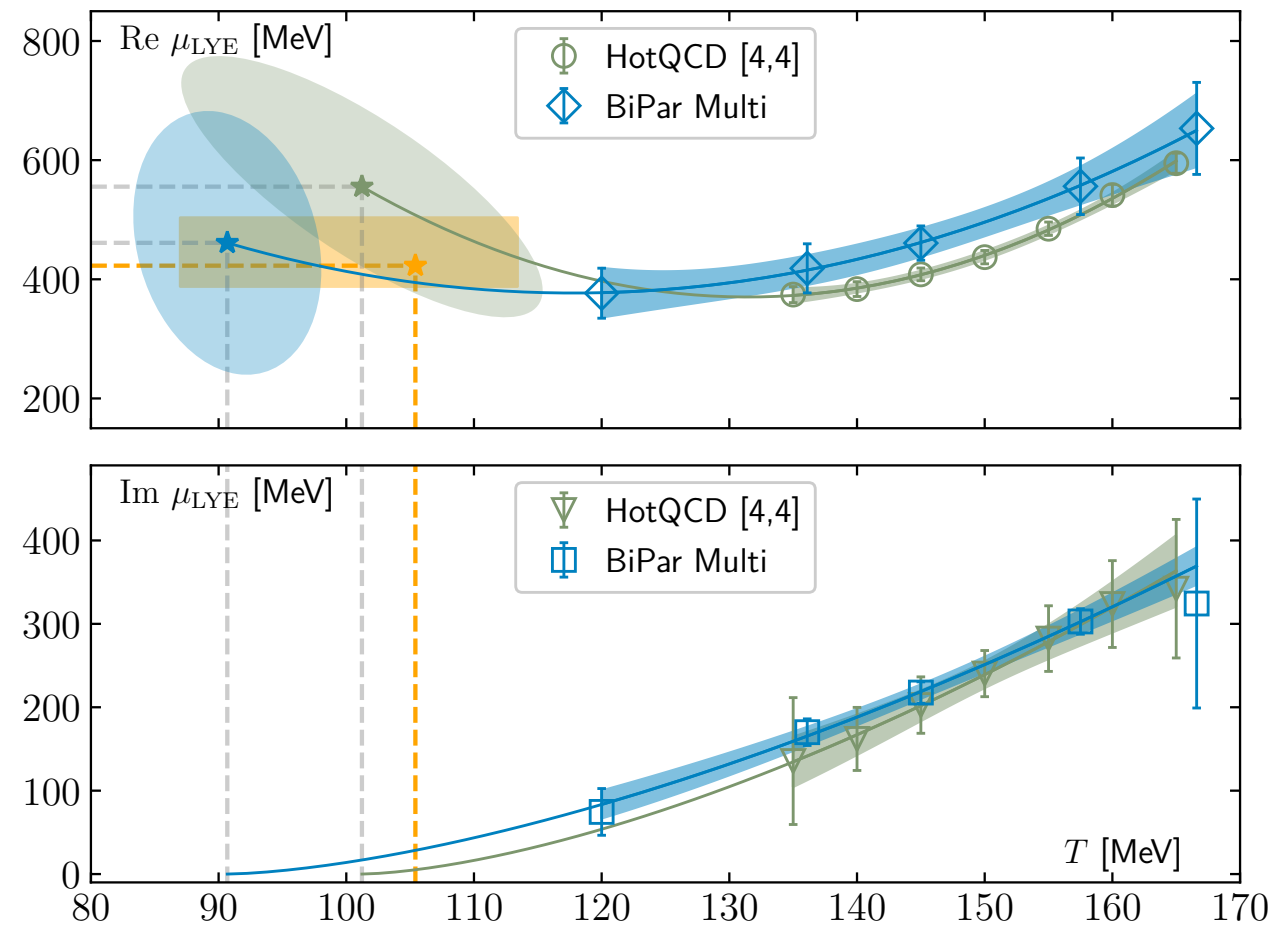
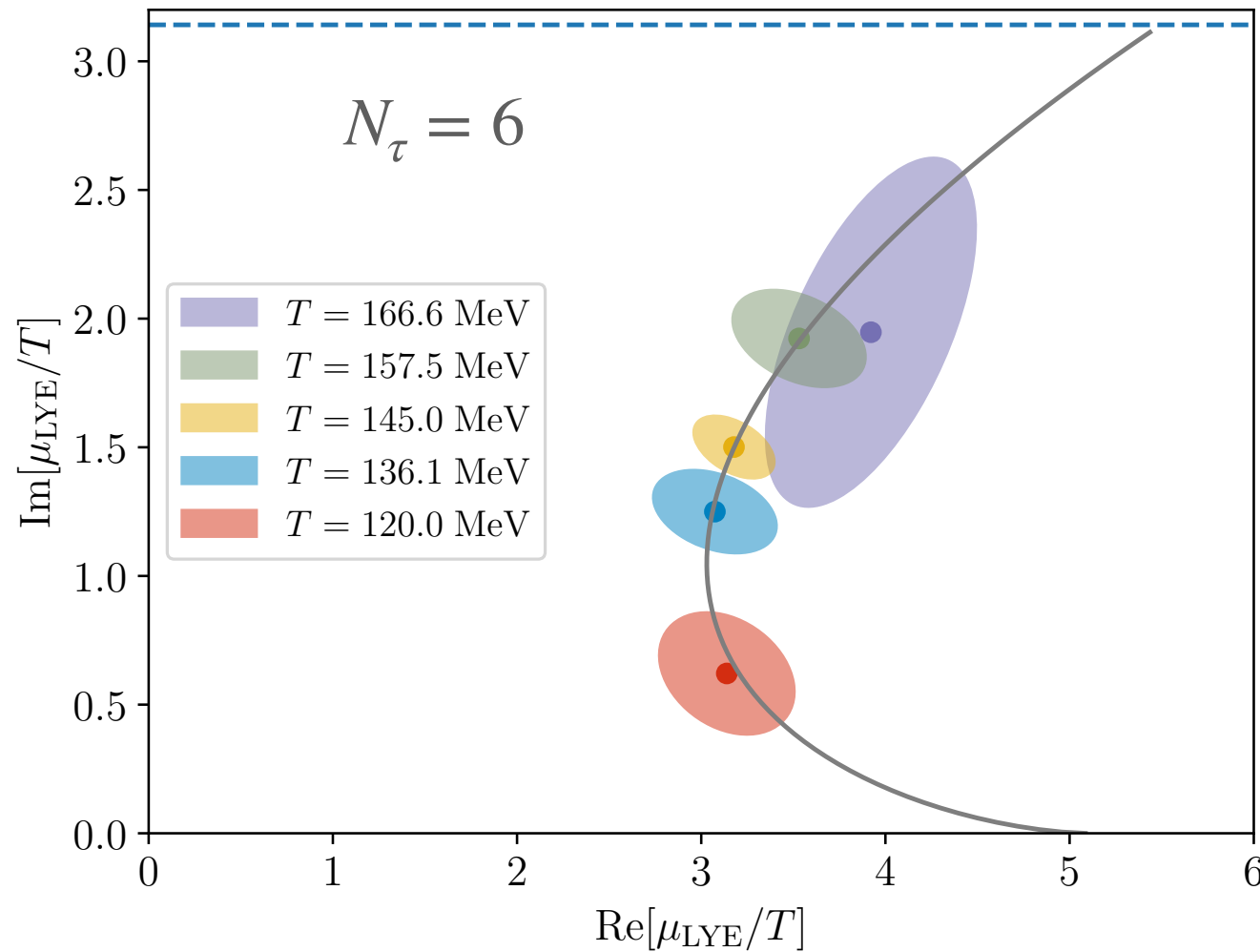
$$\text{Re}[\mu_{\text{LYE}}] = \mu_B^{\text{CEP}} + c_1 \Delta T + c_2 \Delta T^2 + O(\Delta T^3)$$

$$\text{Im}[\mu_{\text{LYE}}] = c_3 \Delta T^{\beta\delta},$$

[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: $c_1 = -A_h/B_h$

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



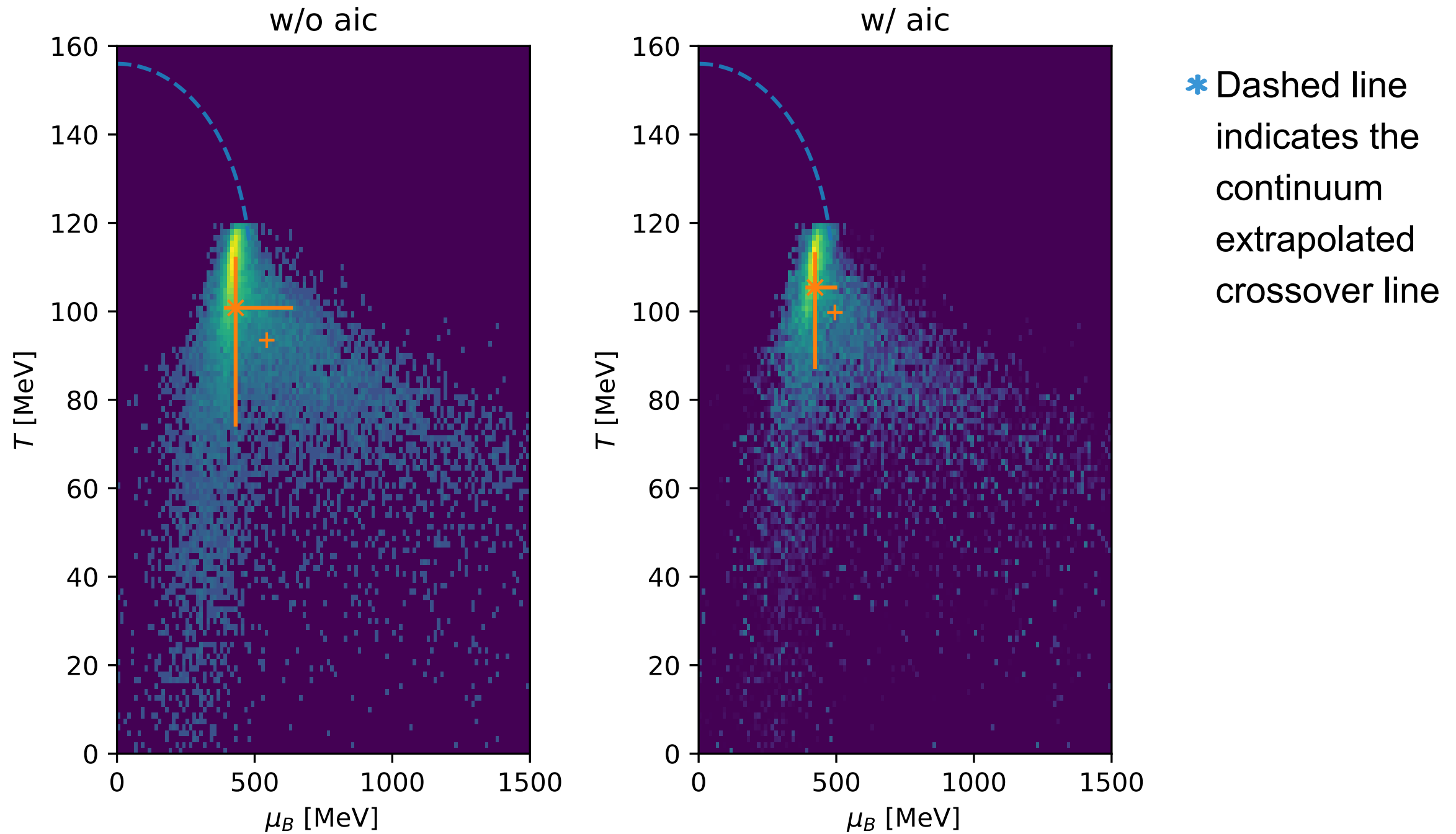
* Ellipses show 1σ confidence region, using the Pearson correlation coefficient

* $N_\tau = 6$ singularities show here are chosen on the basis of the χ^2 of the scaling fit (“best fit”)

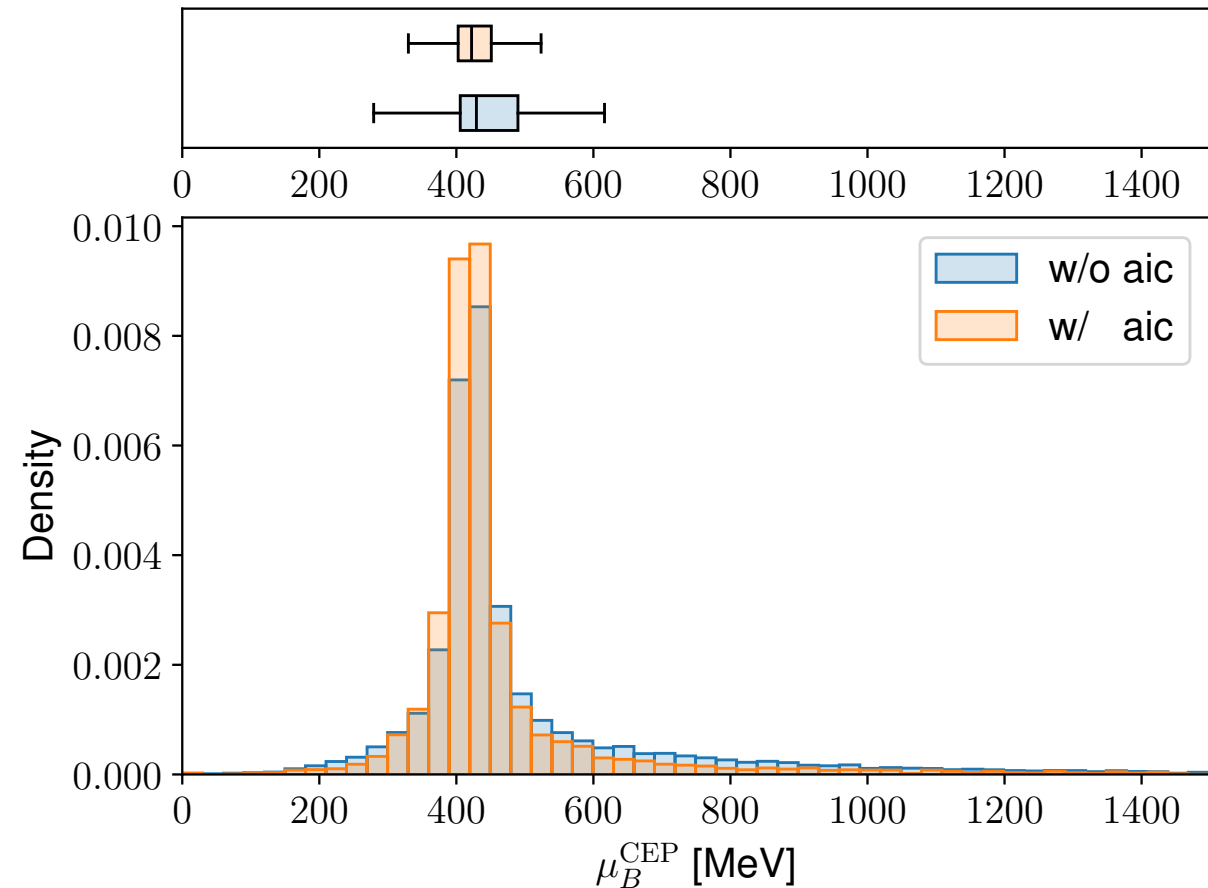
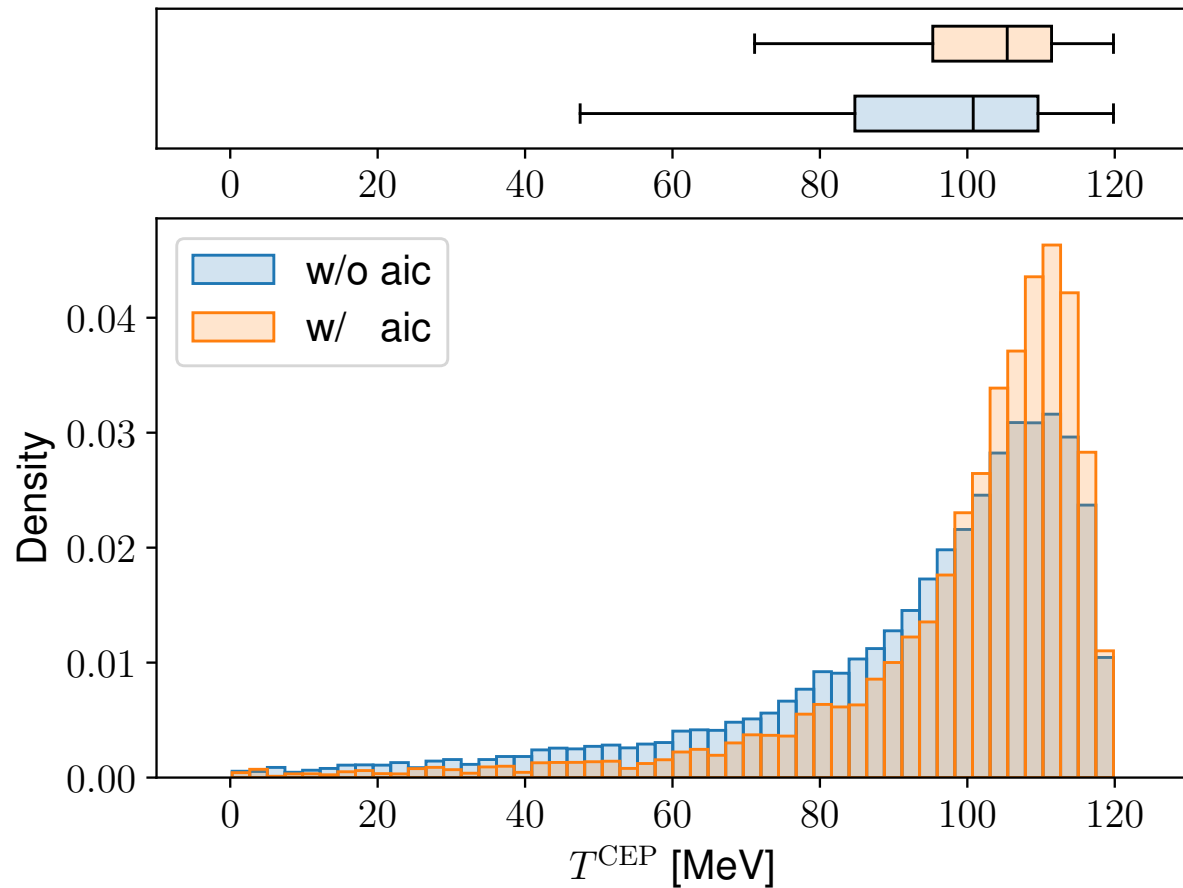
$$\text{Re}[\mu_{\text{LYE}}] = \mu_B^{\text{CEP}} + c_1 \Delta T + c_2 \Delta T^2$$

$$\text{Im}[\mu_{\text{LYE}}] = c_3 \Delta T^{\beta\delta},$$

* Orange box shows the AIC weighted result for $N_\tau = 6$, based on $\mathcal{O}(10^5)$ scaling fits



- * 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

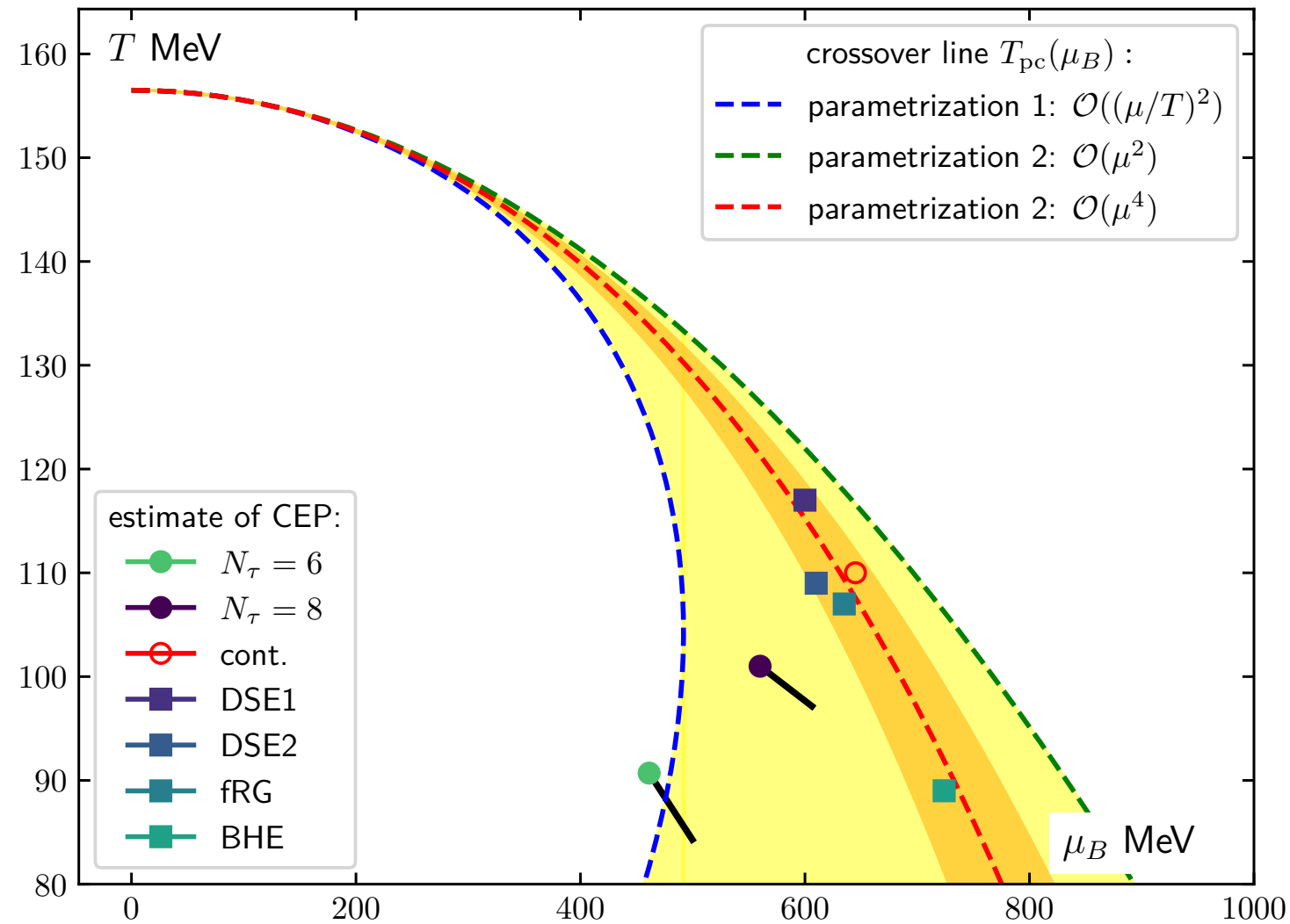


$N_\tau = 6$
multi-point Padé

$N_\tau = 8$
[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.)
$$T_{pc}(\mu_B) = T_{pc}(0) \left[1 + \kappa_2^B \left(\frac{\mu_B}{T} \right)^2 + \kappa_4^B \left(\frac{\mu_B}{T} \right)^4 \right]$$

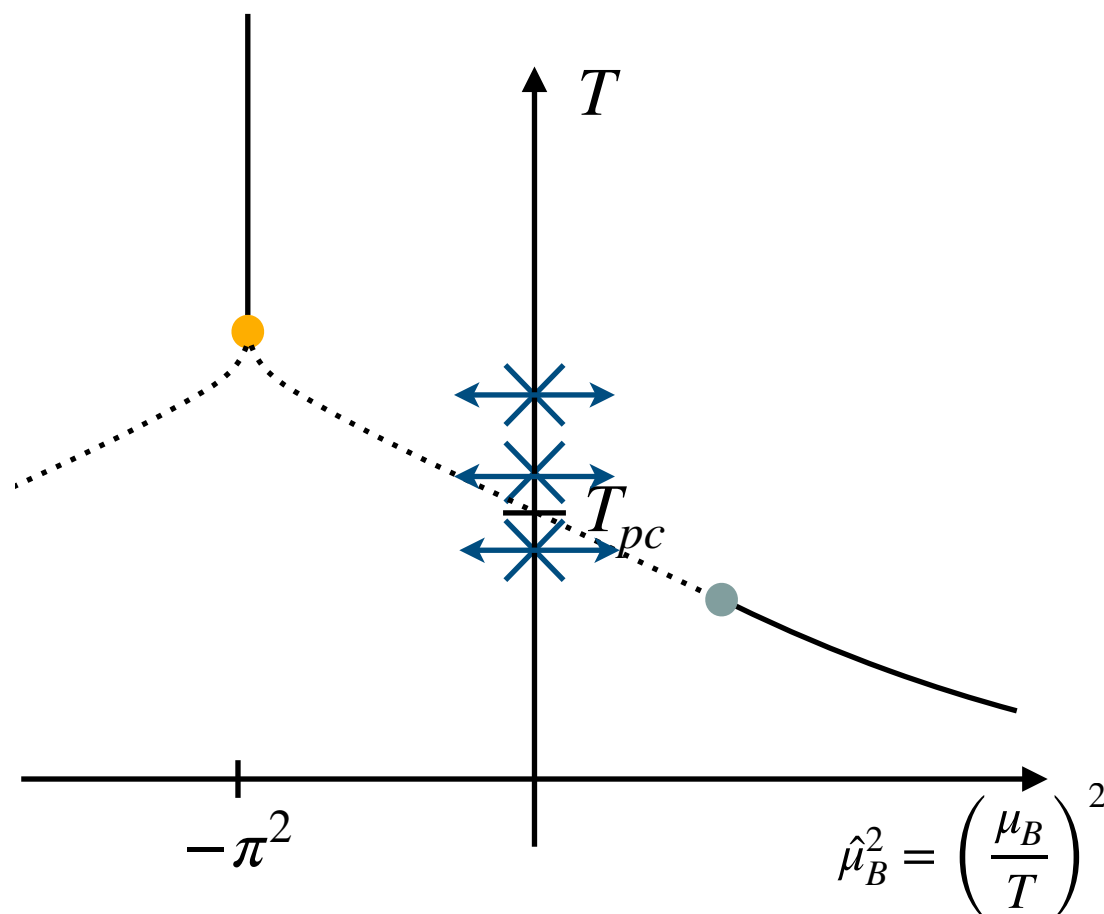
* 2.)
$$T_{pc}(\mu_B) = T_{pc}(0) \left[1 + \bar{\kappa}_2^B \left(\frac{\mu_B}{T_{pc}(0)} \right)^2 + \bar{\kappa}_4^B \left(\frac{\mu_B}{T_{pc}(0)} \right)^4 \right]$$

- * 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 $N_\tau = 6$: $(T^{\text{CEP}}, \mu_B^{\text{CEP}}) = (105_{-18}^{+8}, 422_{-35}^{+80}) \text{ MeV} .$
- * No continuum result yet
- * Current estimates of the cutoff effects increase μ_B^{CEP} towards $\mu_B^{\text{CEP}} \approx 650 \text{ MeV}$

Back Up Slides

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

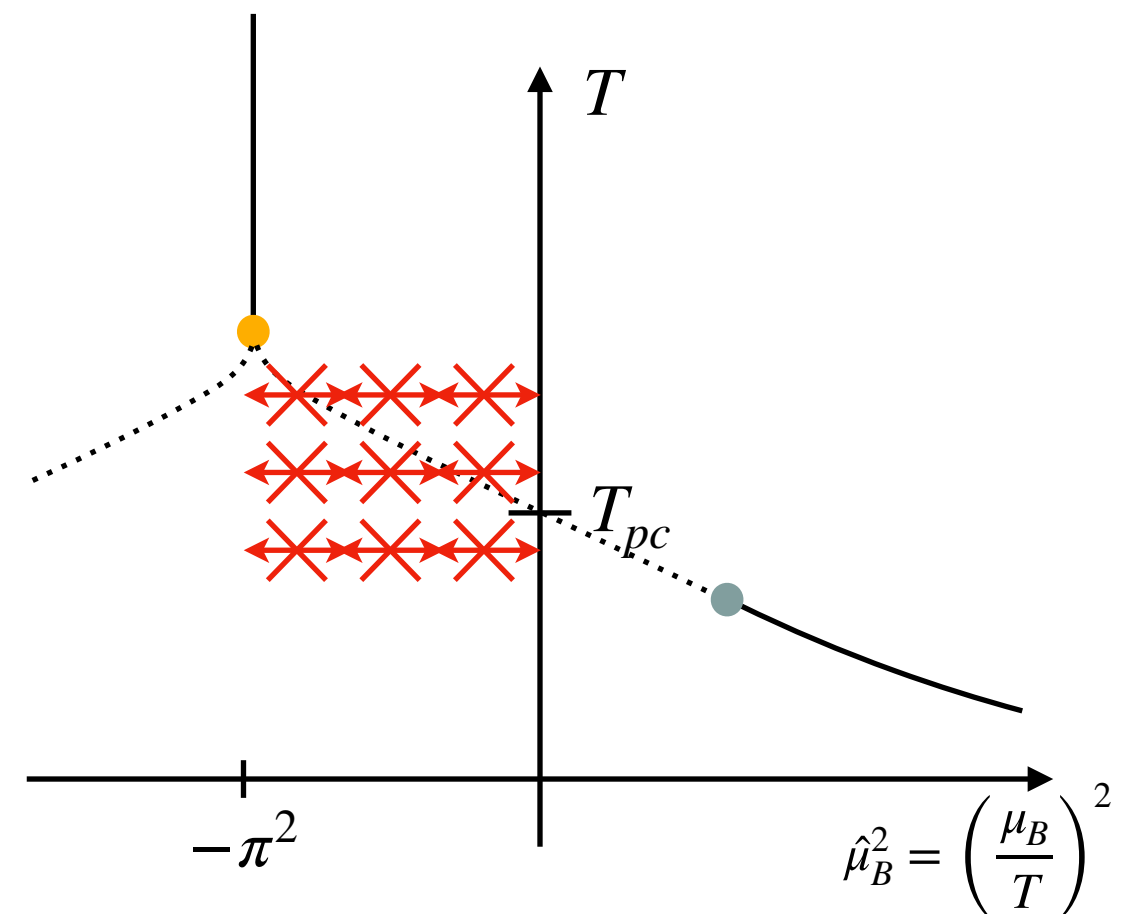
$(T, \mu_B = 0)$: Taylor expansion in μ_B^2



[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 Forcrand, 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

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

$$P'_m(0) - f'(0)Q_n(0) - f(0)Q'_n(0) = f'(0)$$

⋮

→ 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

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

$$P'_m(x_0) - f'(x_0)Q_n(x_0) - f(x_0)Q'_n(x_0) = f'(x_0)$$

⋮

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

$$P'_m(x_1) - f'(x_1)Q_n(x_1) - f(x_1)Q'_n(x_1) = f'(x_1)$$

⋮

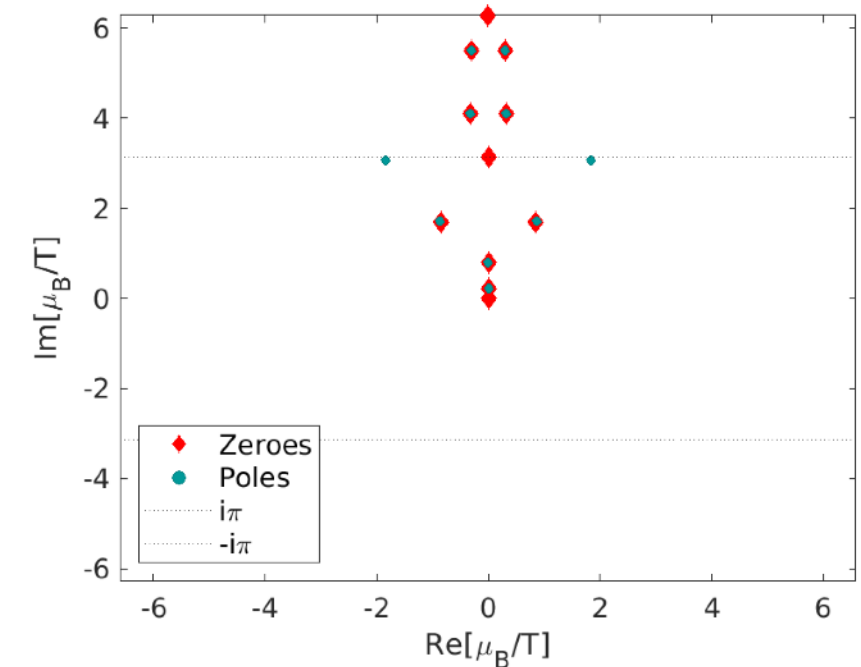
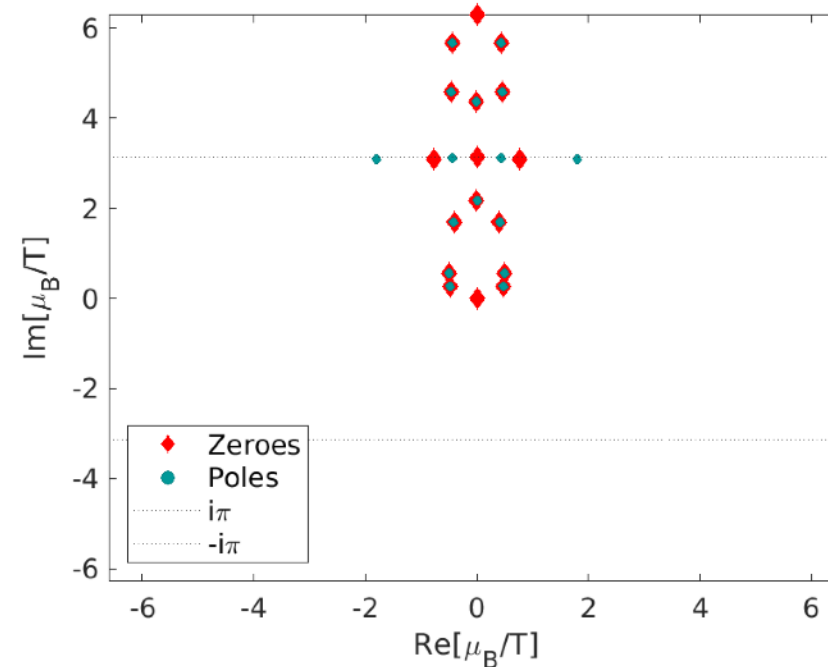
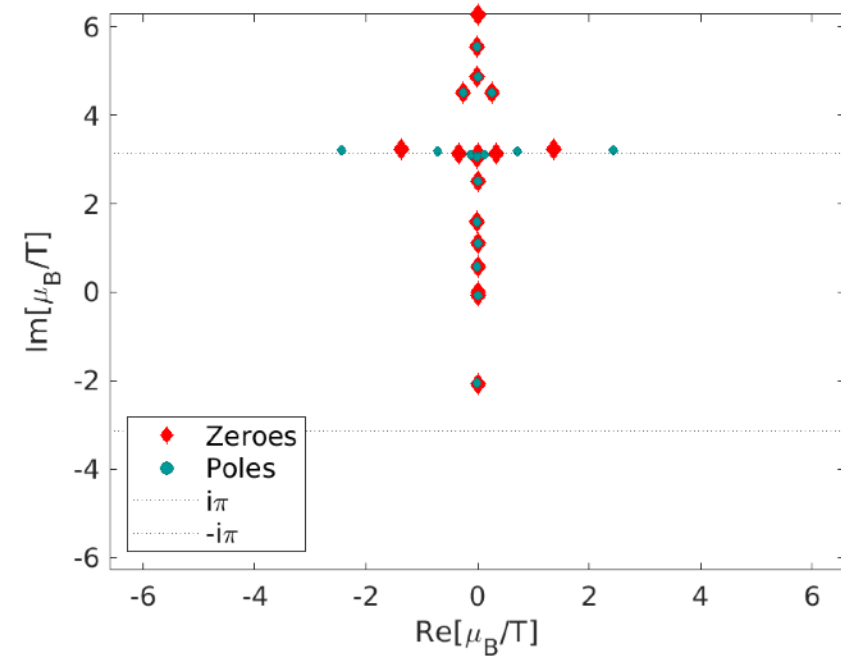
→ again a linear system of size $m + n + 1$, need much less derivatives, we have

$$m + n + 1 = \sum_k (L_k + 1)$$

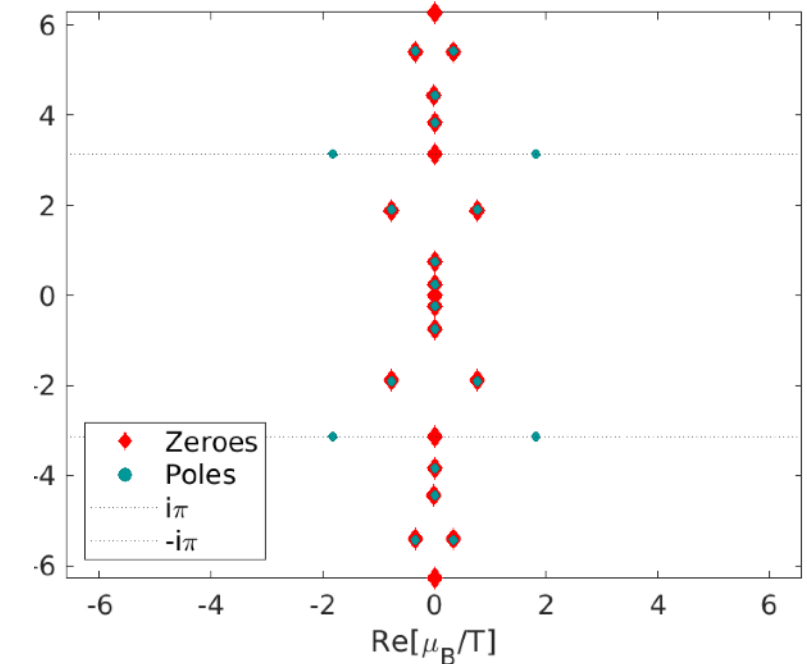
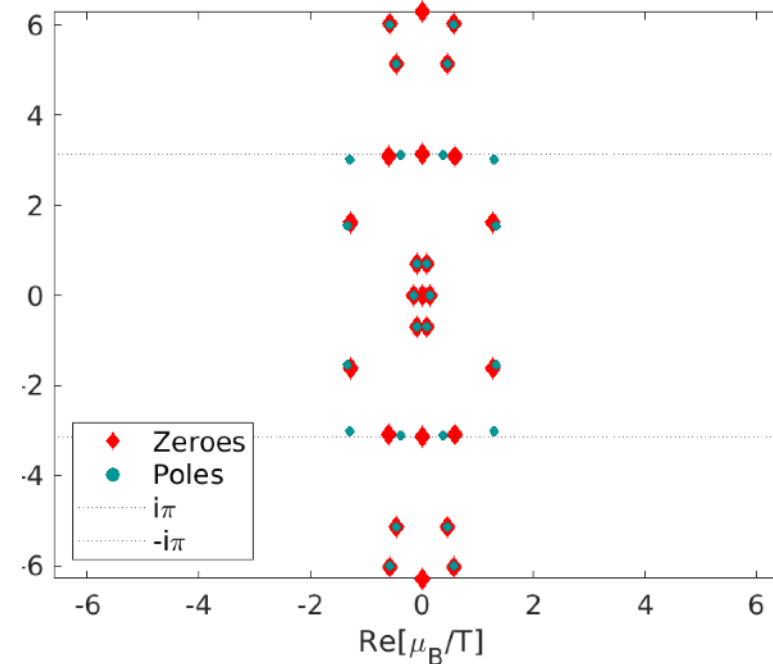
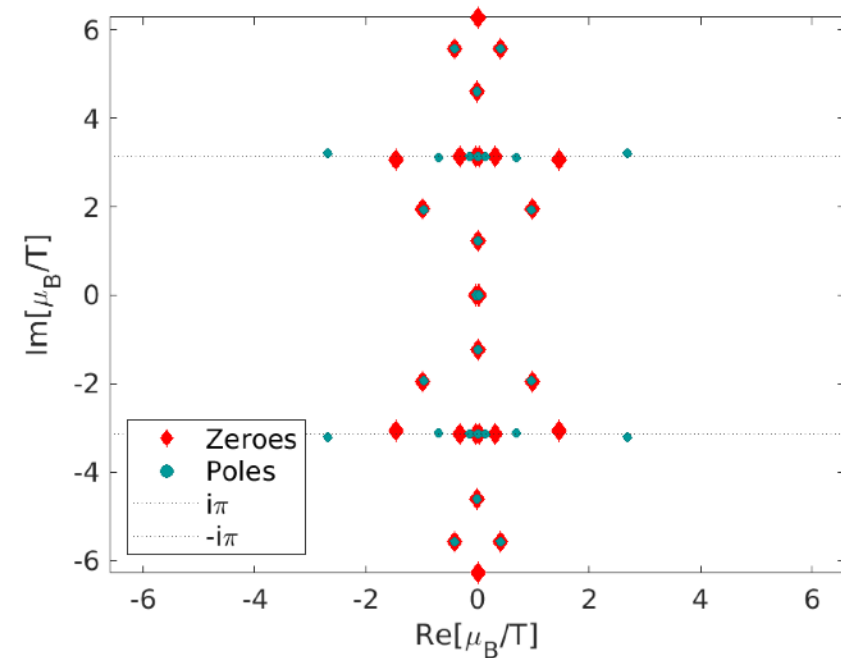
$T = 201 \text{ MeV} = T_{RW}$

$T = 186 \text{ MeV}$

$T = 167 \text{ MeV}$



(NS)

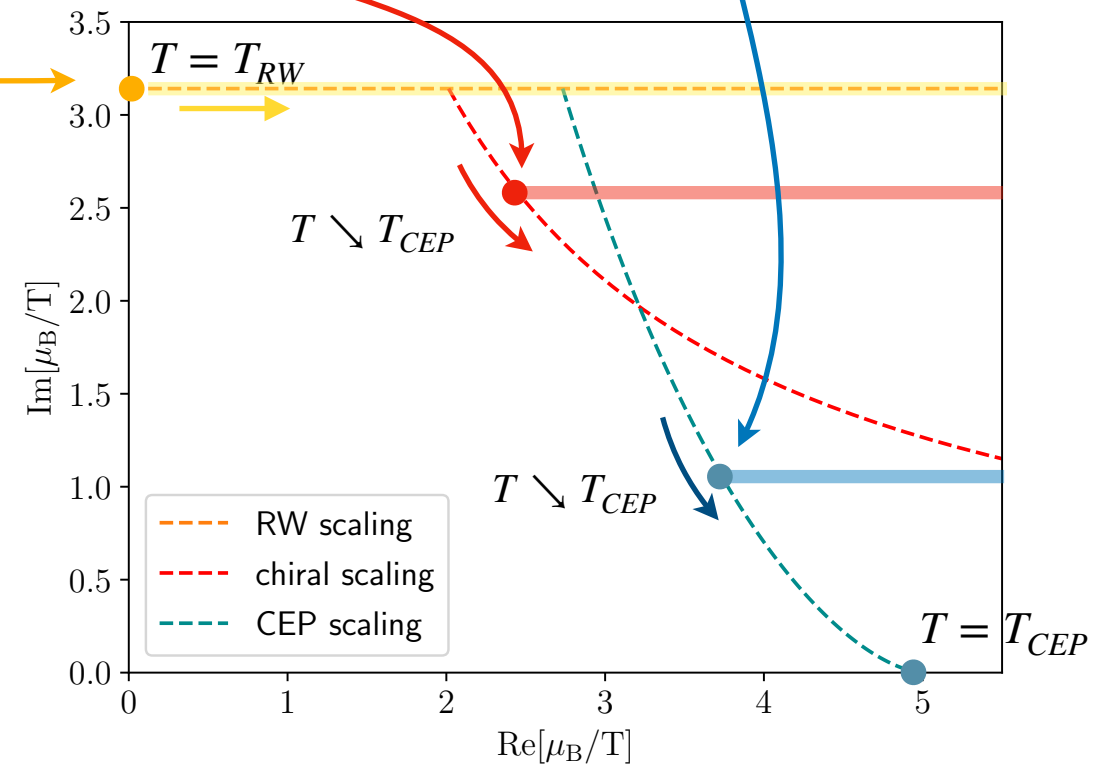
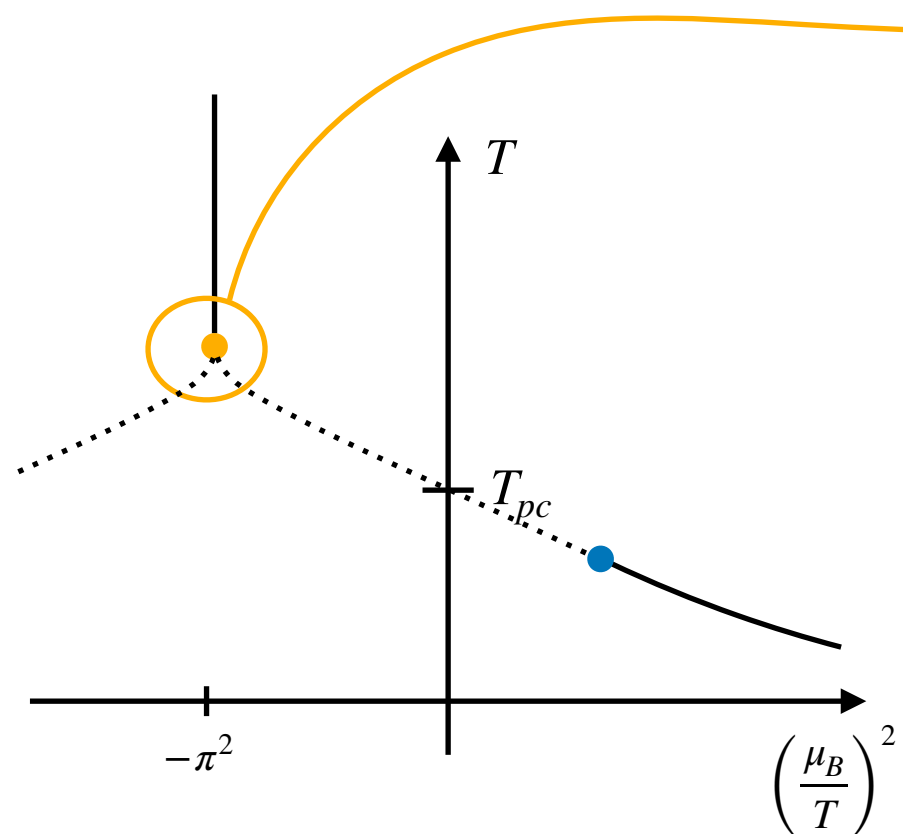
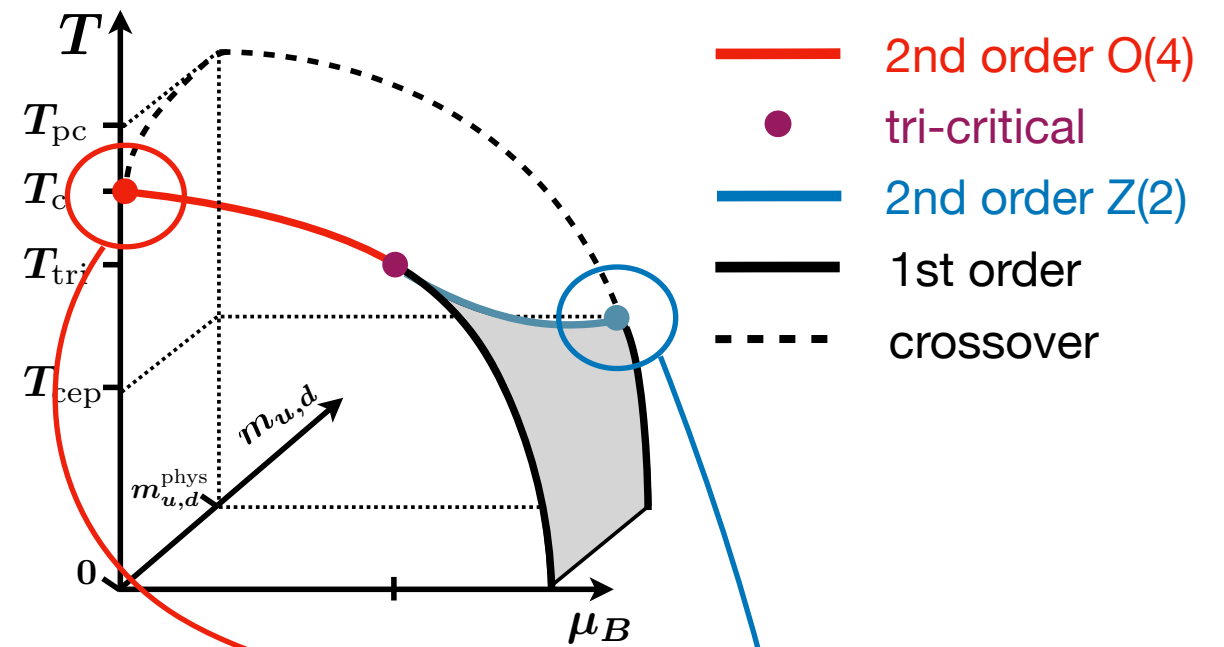


(S)

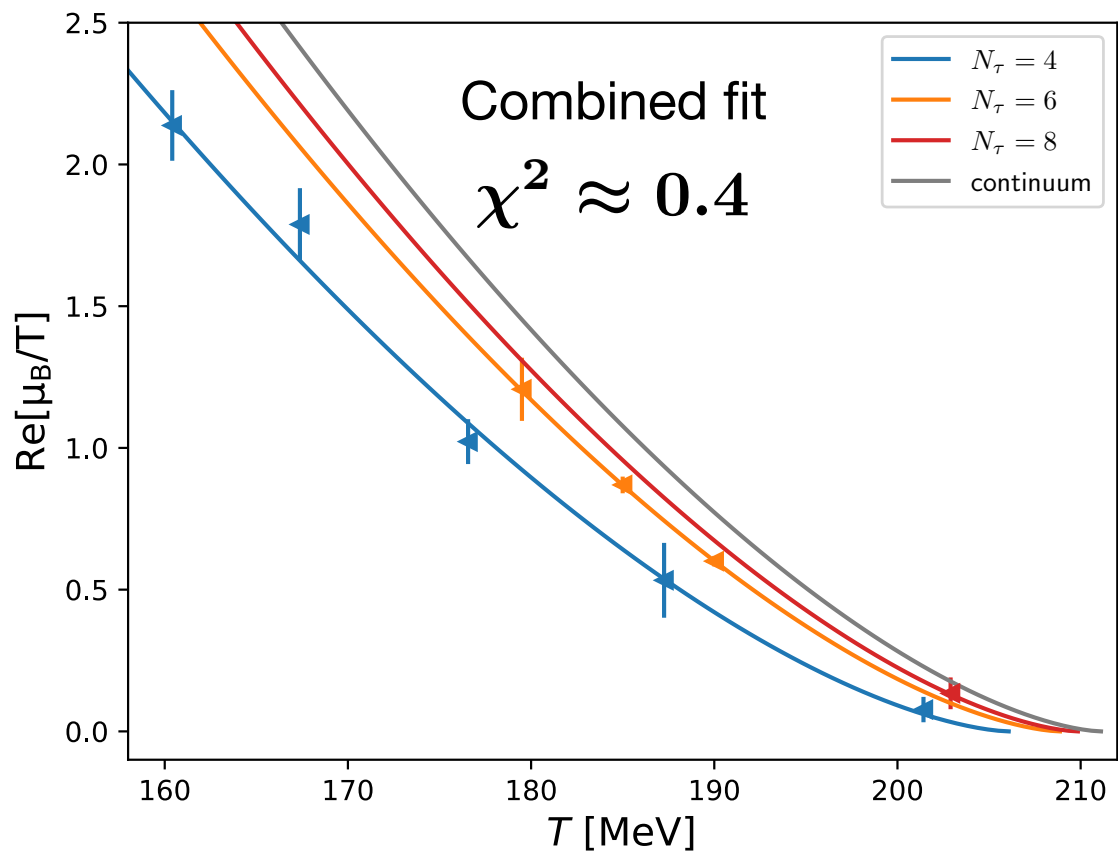
→ find almost perfect cancelation of many zeros and poles

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

- * 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



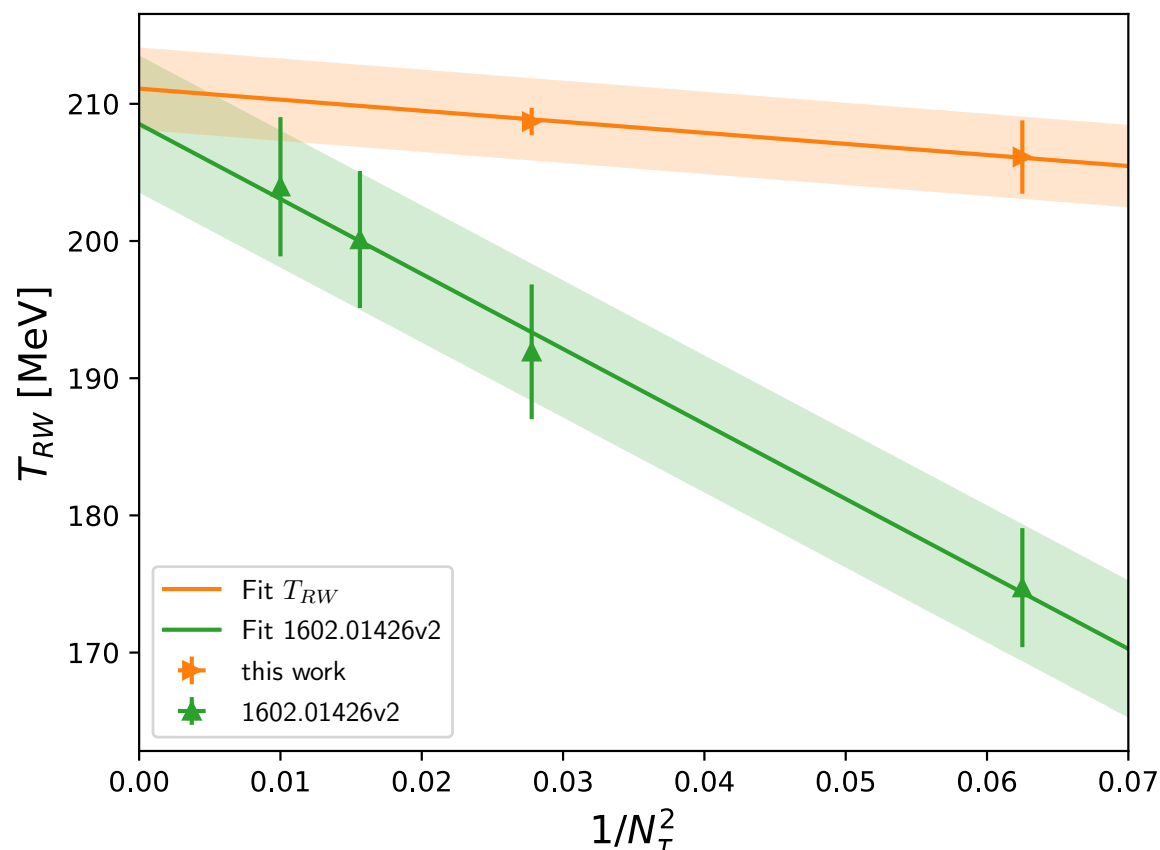
* The approach of the LY edge to the RW critical point: By solving $z = t/h^{1/\beta\delta} \equiv z_c$ we find

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

with $\hat{\mu}_{LY}^R = \text{Re}[\mu_B/T]$

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

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



* Obtain continuum result

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

⇒ in good agreement with previous results from the Pisa group

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

$$M = m_0 R^\beta \theta$$

$$t = R(1 - \theta^2)$$

$$h = h_0 R^{\beta\delta} h(\theta)$$

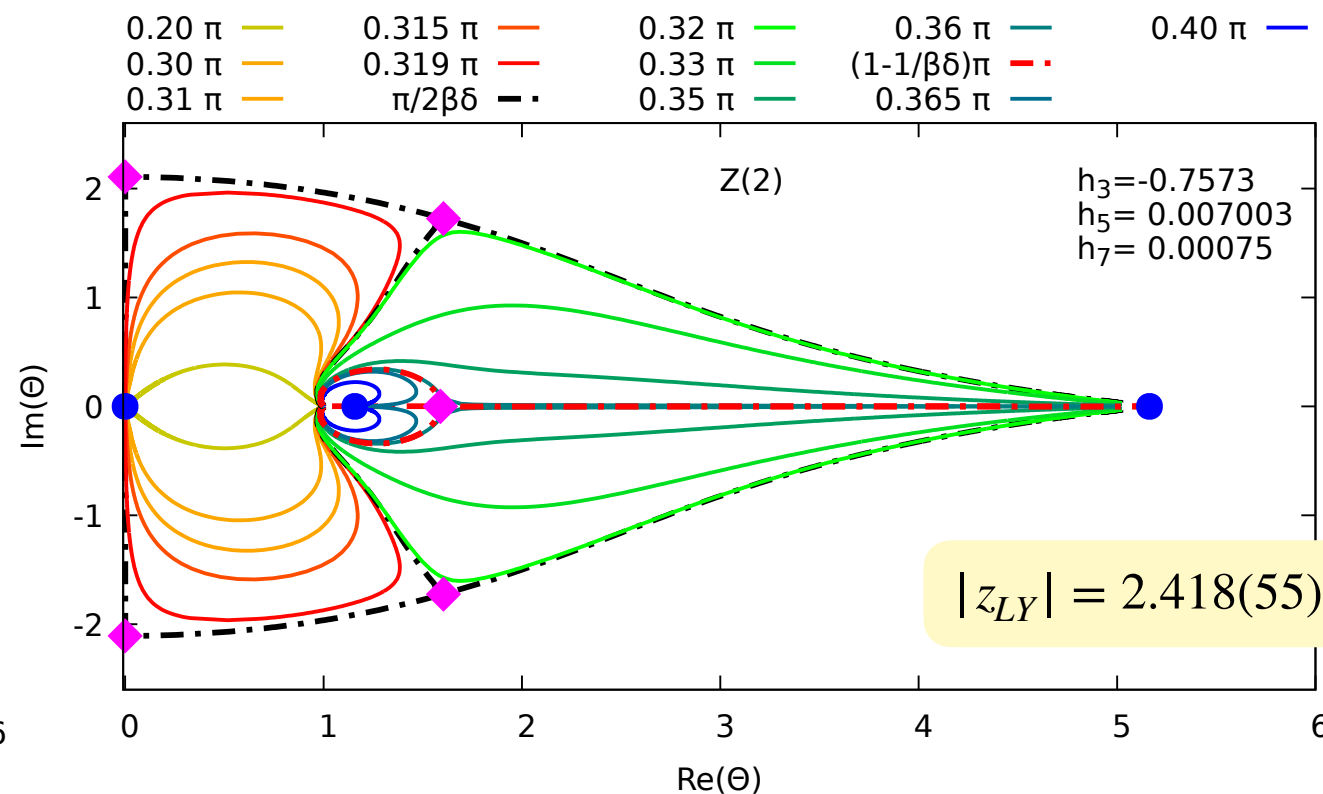
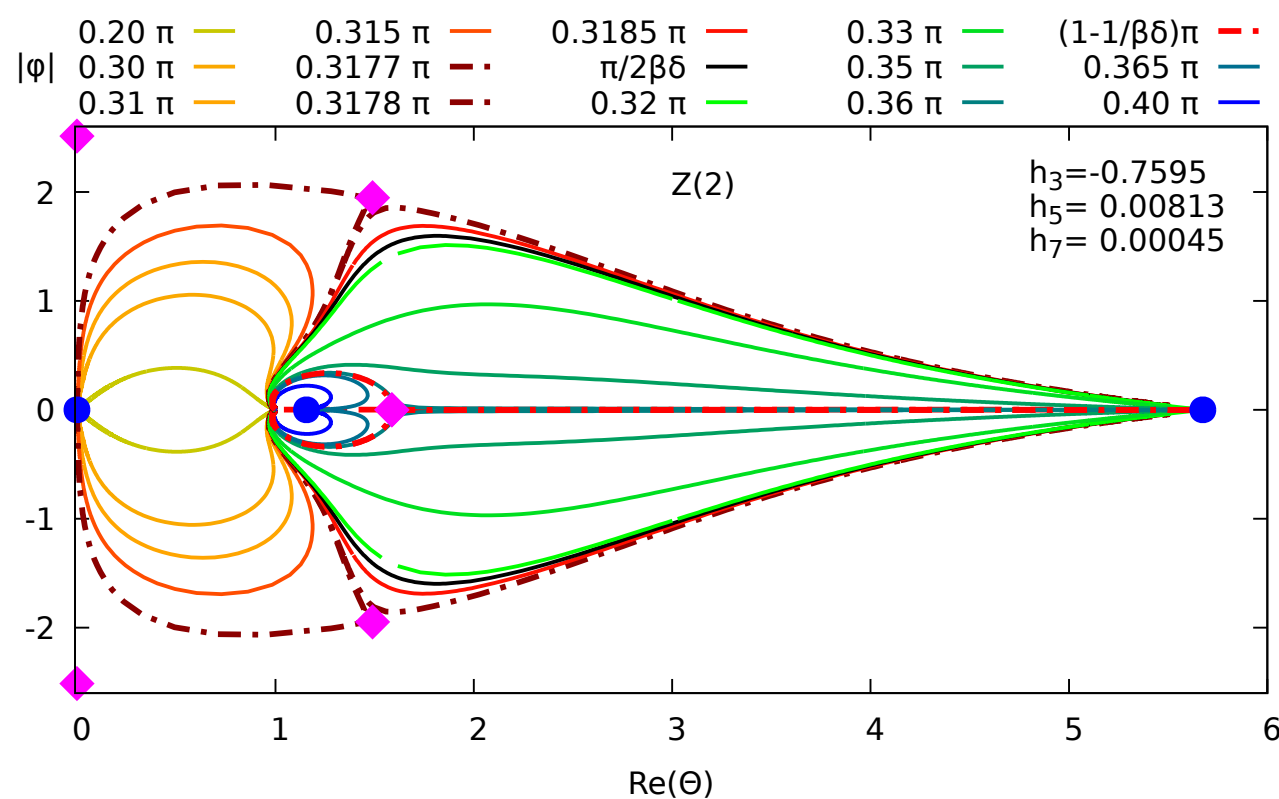
$$h(\theta) = \theta (1 + h_3 \theta^2 + h_5 \theta^4 + h_7 \theta^6 + \dots)$$

- 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]

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

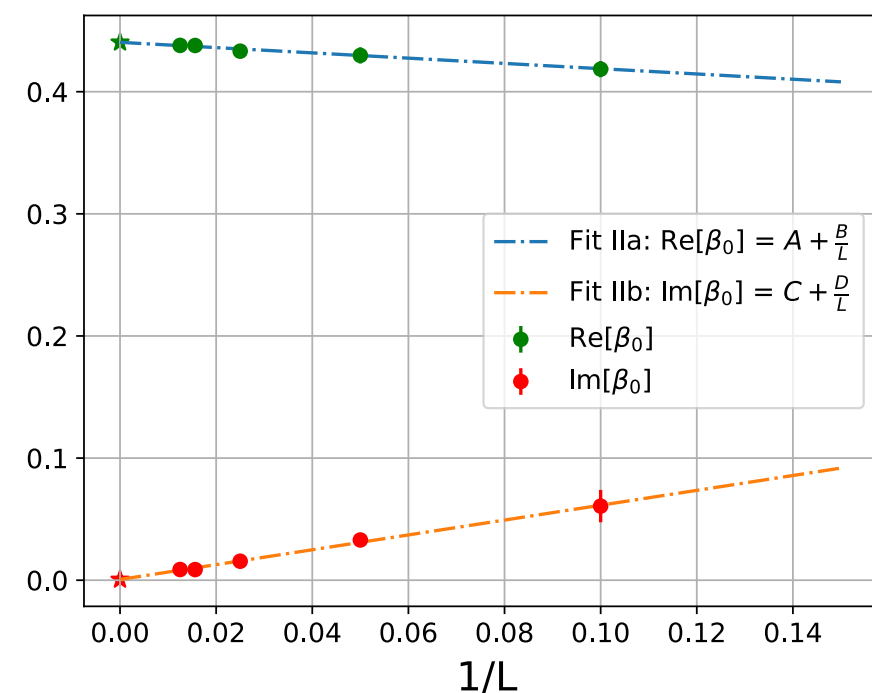
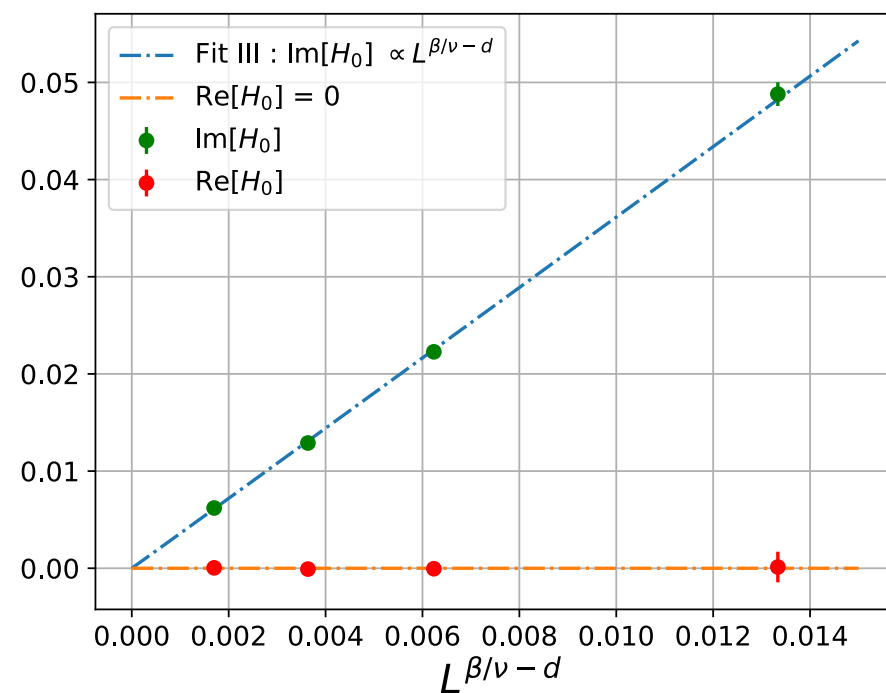
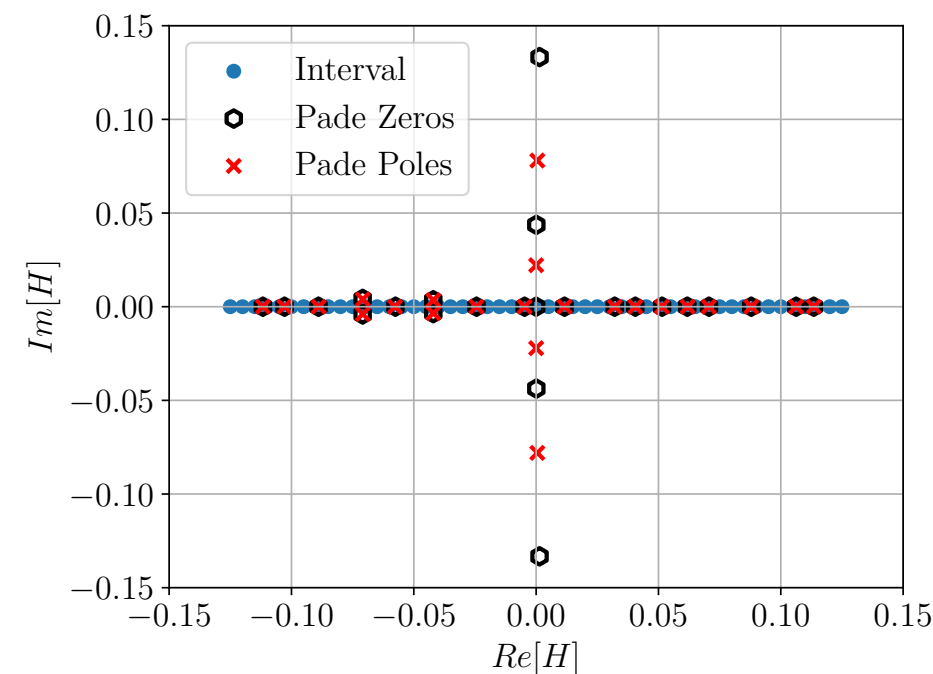
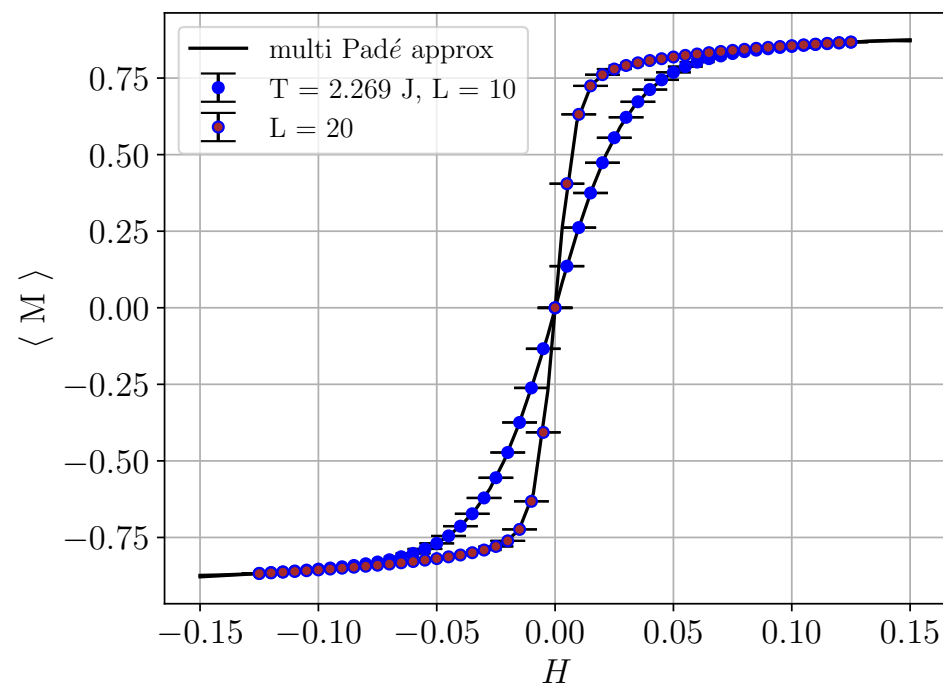


- the coefficient h_7 is not known precisely (zero within current precision)
- $h_7 \neq 0$ introduces an additional pair of singularities (imaginary if $h_7 > 0$, real if $h_7 < 0$)
- h_7 can be used to tune the phase of the LY edge singularity

[Karsch, CS, Singh, arXiv:2311.13530]

* The multi-point method works well in the Ising model when applied to the magnetisation or the specific heat.

* A finite size scaling analysis reproduces the transition temperature β_c and the critical exponents ν and $\beta\delta$



[Singh et al, *PRD* 109 (2024) 7, 07450, arXiv: [2312.03178](https://arxiv.org/abs/2312.03178)]