

Exploring the Critical Points in QCD with Multi-Point Padè and Machine Learning Techniques in (2+1)-flavor QCD

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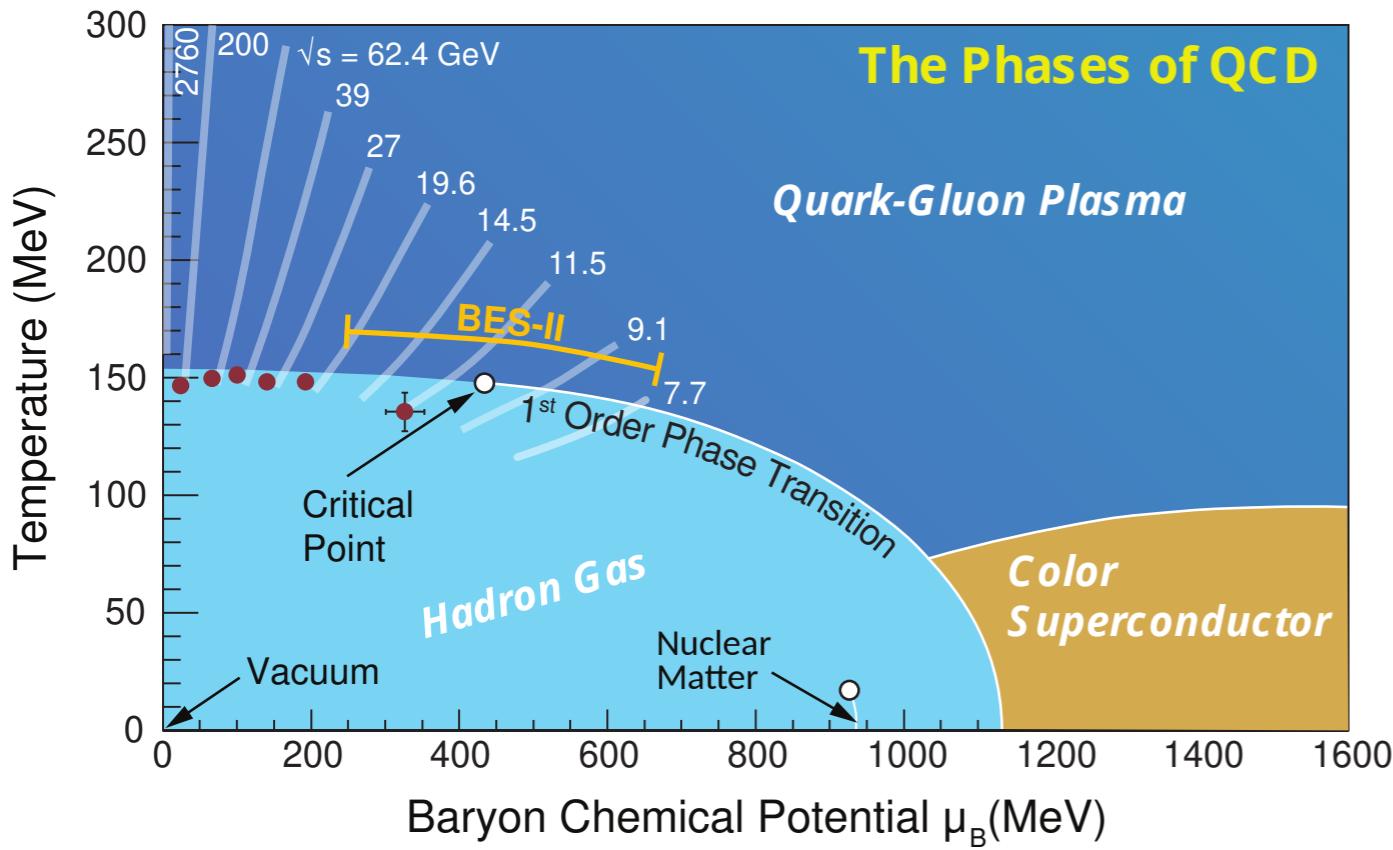
**With D. Clarke, P. Dimopoulos, F. Di Renzo, G. Nicotra,
C. Schmidt, S. Singh and K. Zambello**

[Bielefeld-Parma collaboration]

Houston, Texas, 06/09/2023



QCD Phase diagram



“Mapping the Phases of Quantum Chromodynamics with Beam Energy Scan”, Bzdak et al., Phys. Rept. ‘20

Multi point Padé approximant :
Simulations with multiple
imaginary chemical potential values
and
construct multi-point Padé
approximant.

P. Dimopoulos et al, Phys.Rev.D 105 (2022) 3, 034513

- Sign Problem :**
Two production level method :
- (I) Taylor expansion at $\mu = 0$.
D. Clarke 06/09, 14:40
 - (II) Analytical continuation from imaginary chemical potential.
P. Parotto, 05/09, 16:30
A. Pasztor, 04/09, 16:00

Expectation : CEP will exist at a lower temperature than T_{chiral} (~ 130 MeV)

[Halasz et al, arXiv: hep-ph/9804290](#)

Padé approximant : Possible extension of the Taylor series for exploring the low temperature and high density part of the QCD phase diagram.

EoS : [D. Bollweg et al\(HotQCD coll.\), Phys.Rev.D 108 \(2023\), JG \(HotQCD coll.\), PoS LATTICE2022 \(2023\) 149, JG QM2022](#)

Searching for CEP using Padé approximants

We only have finite number
of Taylor coefficients.

$$f(x) = \sum_{i=0}^n c_i x^i$$

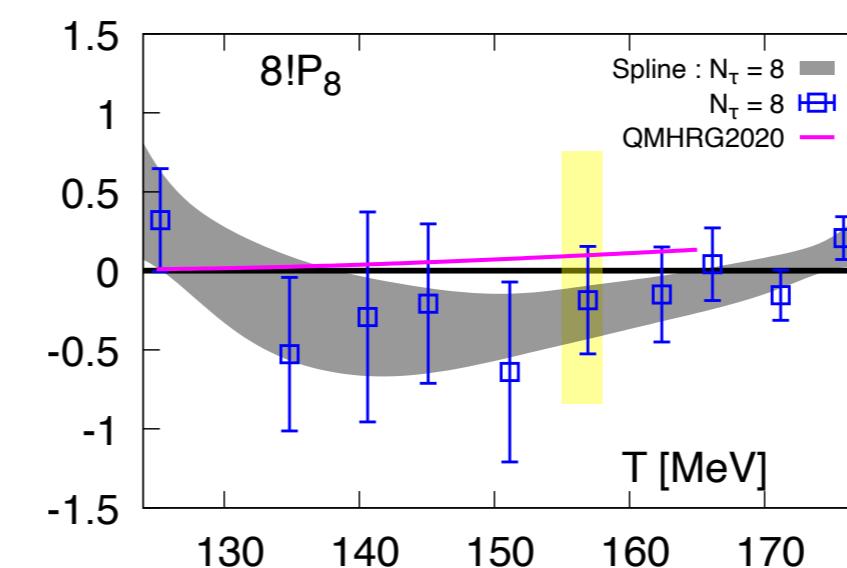
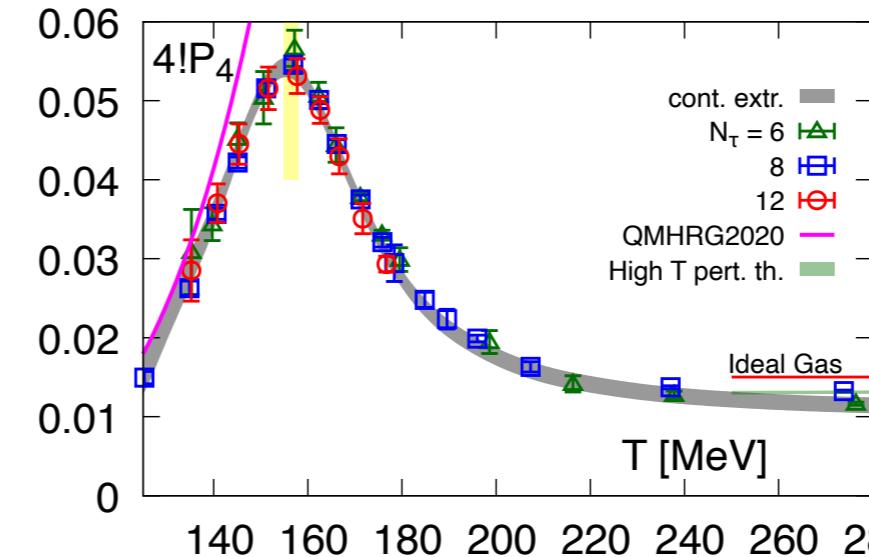
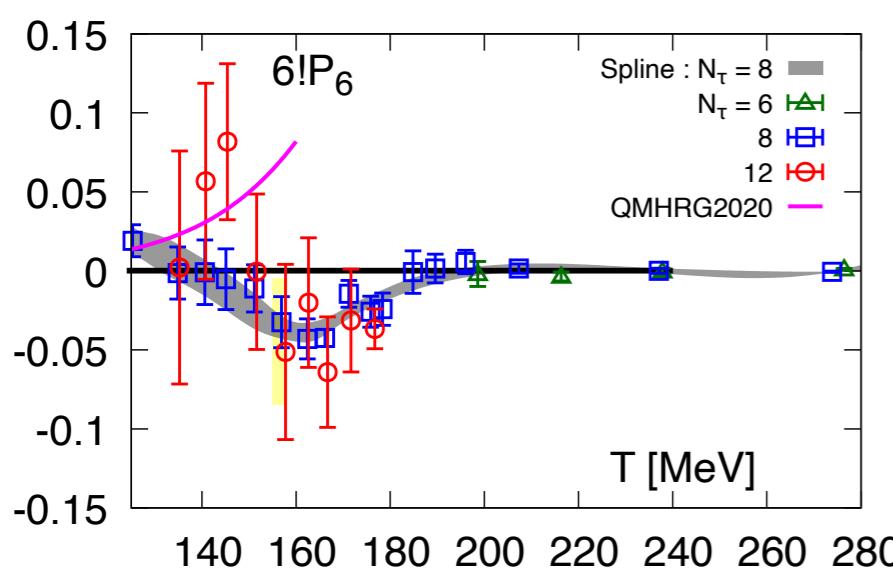
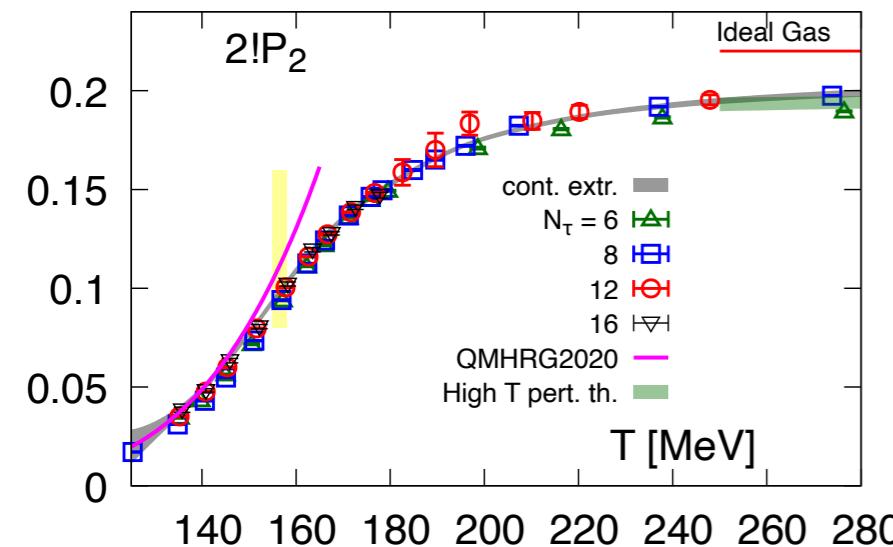
- Lee Yang : Phase transitions are related to singularities of the Taylor series on the real axis.
- Padé approximants : Rational functions of the form, $f(x) = \frac{\sum_{i=0}^a c_i x^i}{1 + \sum_{j=1}^b d_j x^j}$,
- Singularities : Solving the denominators.
- Furthermore, LYE singularities exhibit universal scaling behavior near a critical point

Complex zeros of the partition function



Investigate the universal scaling
of the zeros of the partition
function.

Expansion coefficient for the Taylor series



$$\Delta P(T, \mu_B/T)/T^4 = \frac{P(T, \mu_B/T) - P(T, 0)}{T^4} = \sum_{n=1}^4 P_{2n}(T) (\mu_B/T)^{2n}$$

$$\Delta P(T, \mu_B/T)/T^4 = \frac{\sum_{m=0}^2 c_{2m}(T) (\mu_B/T)^{2m}}{1 + \sum_{n=1}^2 d_{2n}(T) (\mu_B/T)^{2n}}$$

[4,4]-Padè approximant

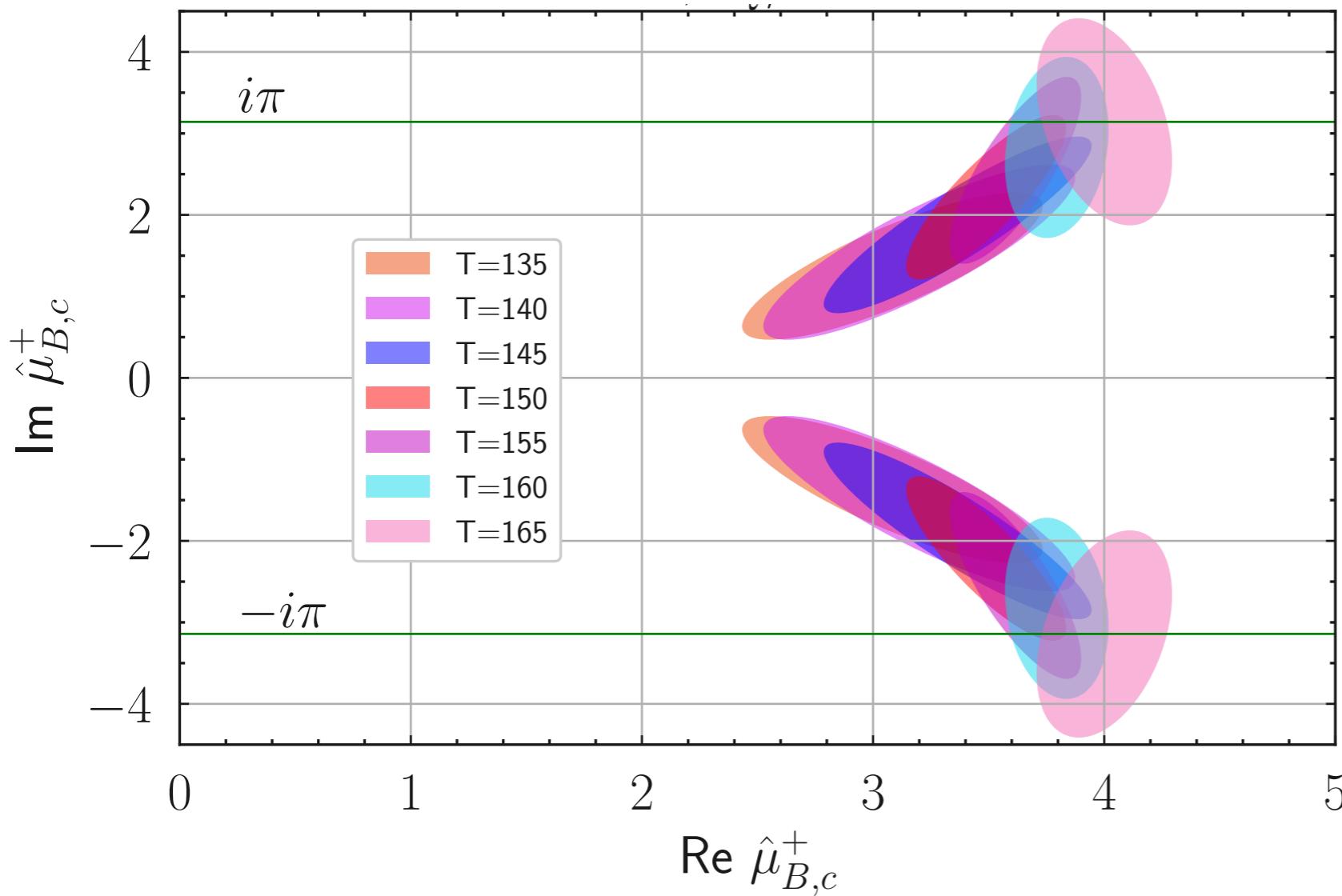
Almost 1.5-2 million gauge configuration

for $N_\tau = 8$ close to T_{pc} .

For, P_6 and P_8 we have used the $N_\tau = 8$.

8-th order Taylor series

Location of the critical point at finite μ_B ??



D. Bollweg et. al (HotQCD collaboration), Phys.Rev.D 105 (2022) 7, 074511,
J. G et. al (HotQCD collaboration), Acta Phys.Polon.Supp. 16 (2023) 1, 76

Singularity of the pressure series using a [4,4] padè constructed from 8th order Taylor series

Expectation :
 $T_{CEP} < T_{chiral}$
 $(T_{chiral} \sim 130 \text{ MeV})$

H.T. Ding et al,
Phys.Rev.Lett. 123 (2019) 6, 062002

Bound for CEP :

$T^{CEP} < 135 \text{ MeV}, \hat{\mu}_B/T \geq 2.5$

- **Lee-yang theorem:** Singularity in the real axis is a hint for a critical point.
- We find no indication of a CEP in almost the entire beam energy (\sqrt{s}) range covered by BESII in collider mode.

Multi-point Padé approximations

Lattice QCD calculations: HISQ (2+1)-flavor, fixed temperature , several imaginary chemical potentials

$$f(x) = \sum_{i=0}^L c_i x^i = \frac{P_m(x)}{1 + Q_n(x)} = \frac{\sum_{i=0}^m a_i x^i}{1 + \sum_{i=0}^n b_i x^i}$$

Standard Padé approximant:

Mathematica: `PadeApproximant[f, x, x0, {m, n}]`

$$m + n + 1 = L$$

Multipoint Padé approximant:

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

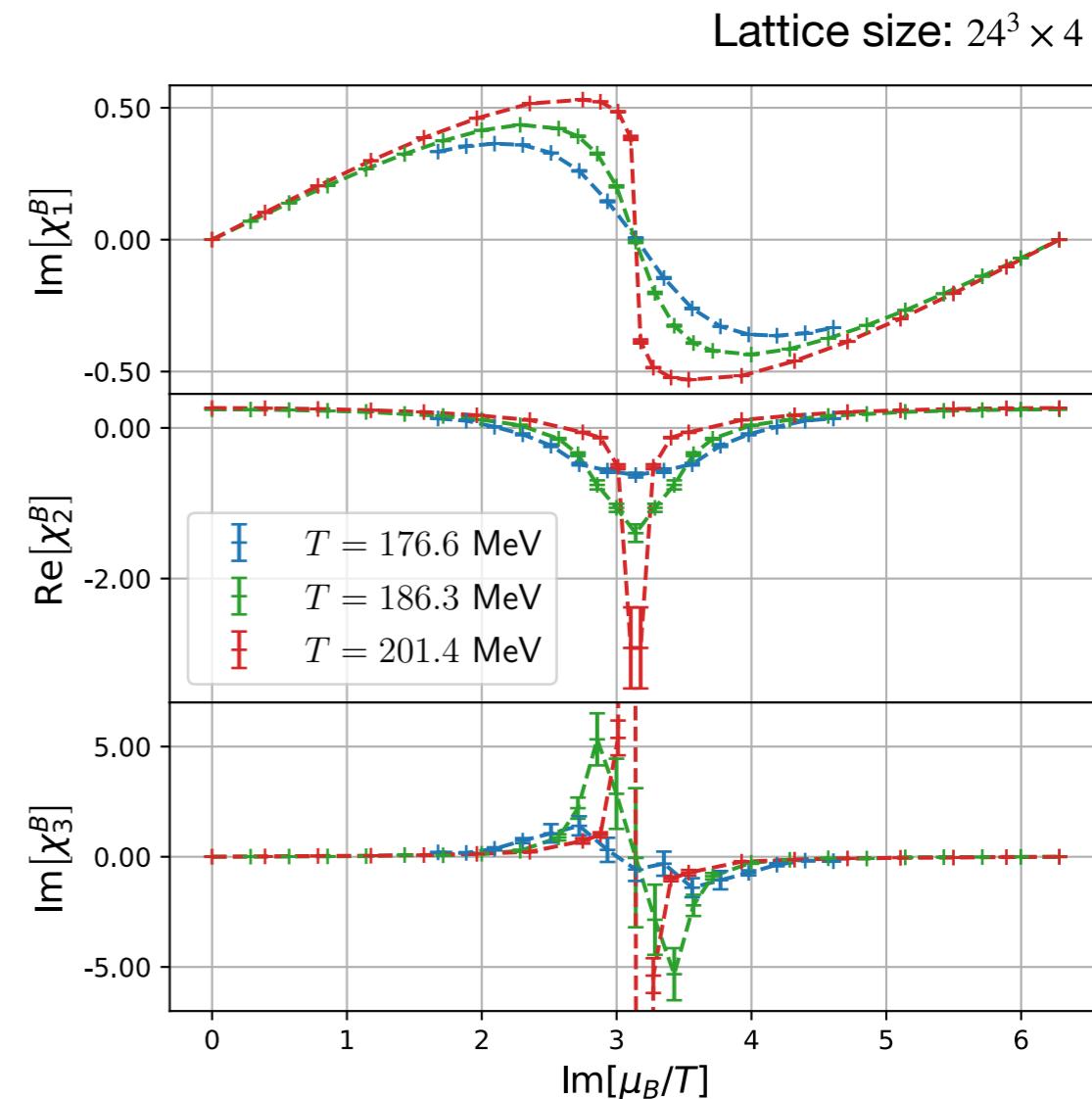
$$P'_m(x_0) - f'(x_0)Q_n(x_0) - f(x_0)Q'_n(x_0) = f'(x_0)$$

⋮

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

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

⋮



$x_k, k = 1, 2, 3 \dots N$ are the simulation points.

$$n + m + 1 = \sum_{i=1}^N (L_i + 1)$$

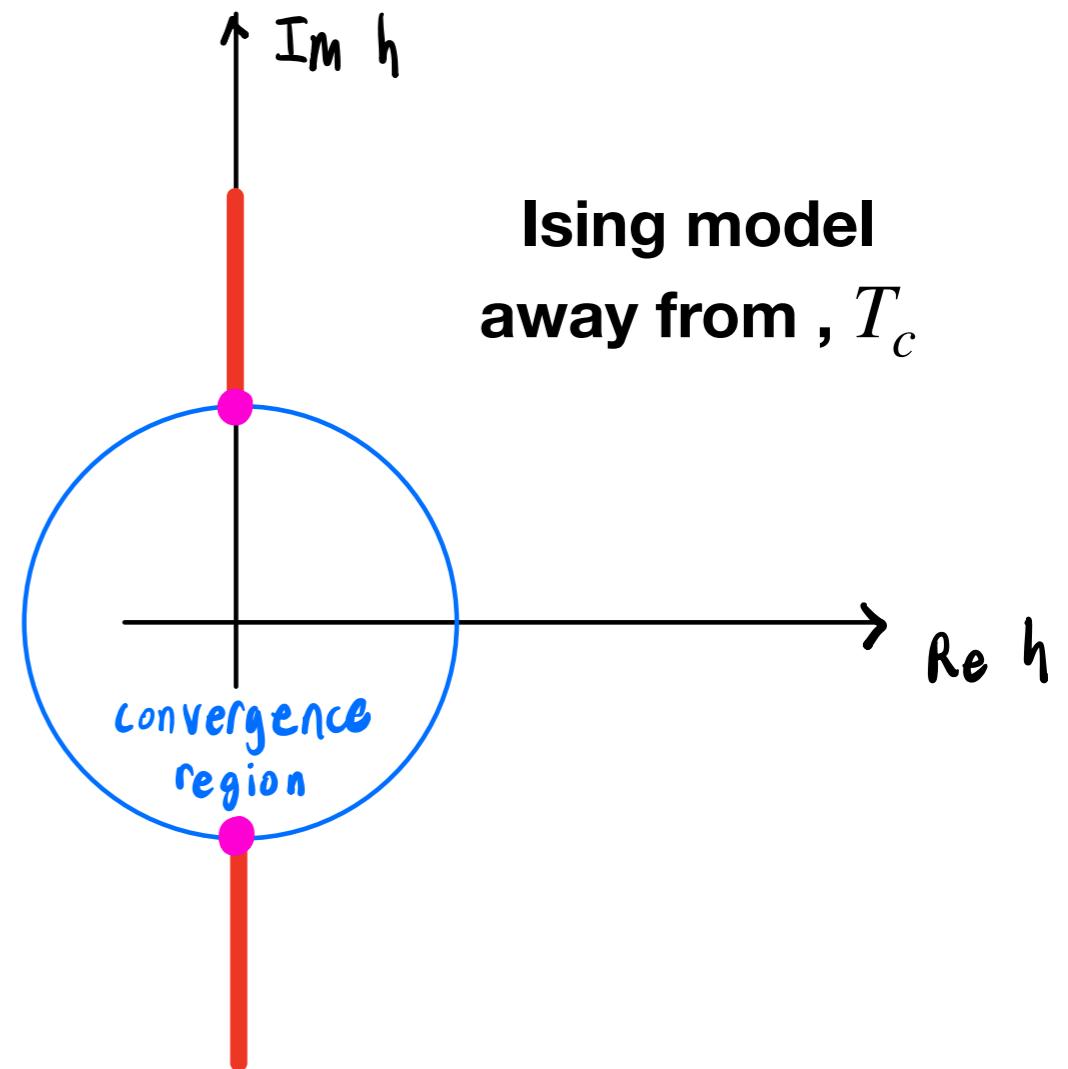
LeeYang Edge singularities (LYEs)

LeeYang Edge (LYEs): The singularities closest to real axis away from the critical temperature.

Position of the LYES:

$$z_c = |z_c| e^{\pm i\pi/2\beta\delta}$$

$z = t/h^{1/\beta\delta}$, β, δ are critical exponents



Extended analyticity conjecture: LYES are the nearest singularity to the origin.

LYEs from universal scaling functions

The universal scaling function for 2nd order phase transition, $t = (T - T_c)/T_c$,

$$t \rightarrow 0, h \rightarrow 0$$

$$f = b^{-d} f_s(b^{y_t} t, b^{y_h} h) + \text{regular}$$

$$f \sim h^{\frac{2-\alpha}{\beta}} f_s(z) + \text{regular}, z \rightarrow t/h^{1/\beta\delta}$$

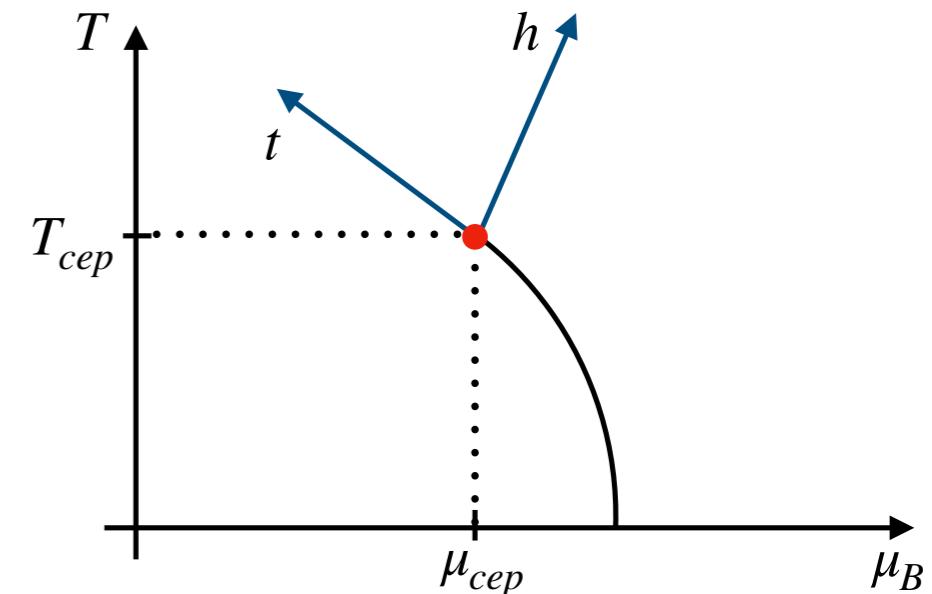
Lee Yang Edge singularities (LYEs) can be obtained by solving, $z = z_c = |z_c| e^{\pm i\pi/2\beta\delta}$

A linear mapping,

For CEP Z(2),

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

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



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

LYEs with many unknown parameters,

$$\mu_{LY} = \mu_{cep} - c_1(T - T_{cep}) + i c_2 |z_c|^{-\beta\delta} (T - T_{cep})^{\beta\delta}$$

Real part : linear in T Imaginary part : Power law in T

At, $\mu_{LY} \rightarrow \mu_{cep}$, imaginary part vanishes.

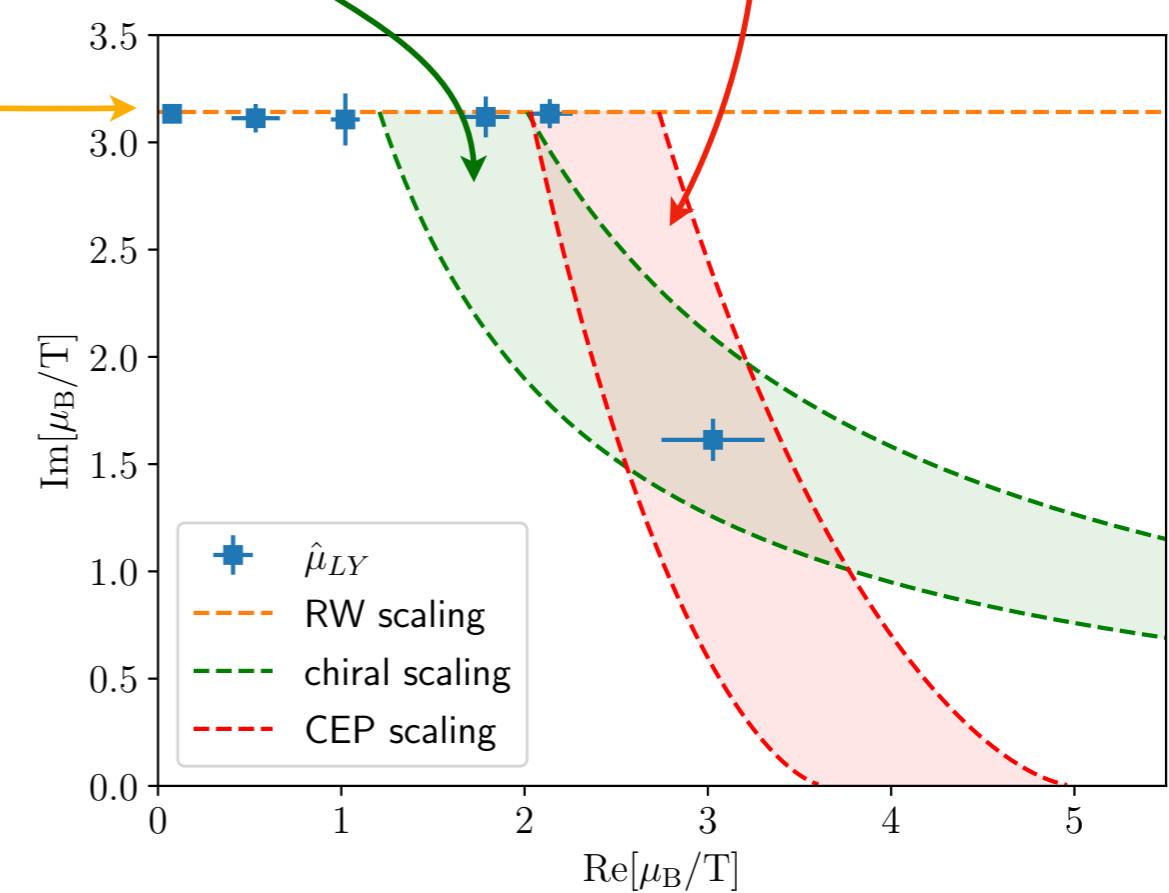
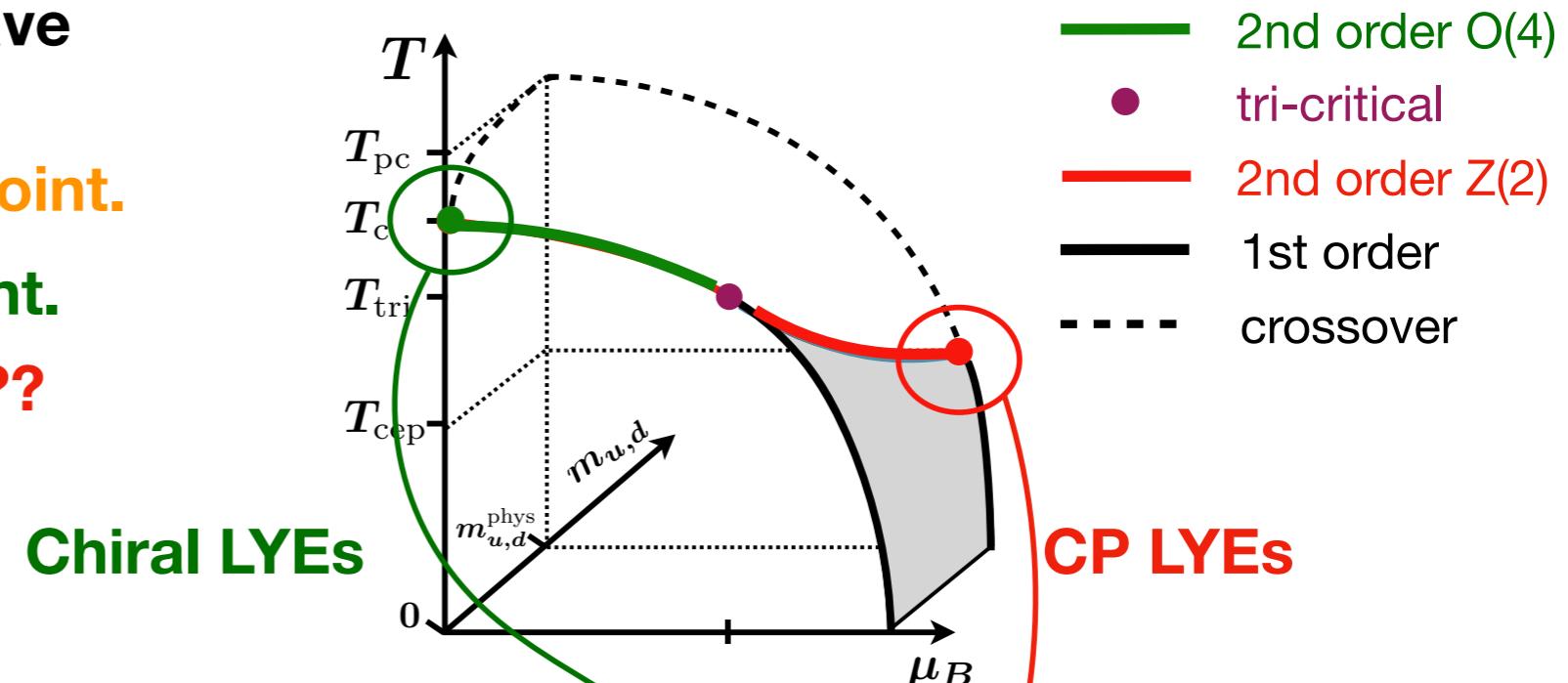
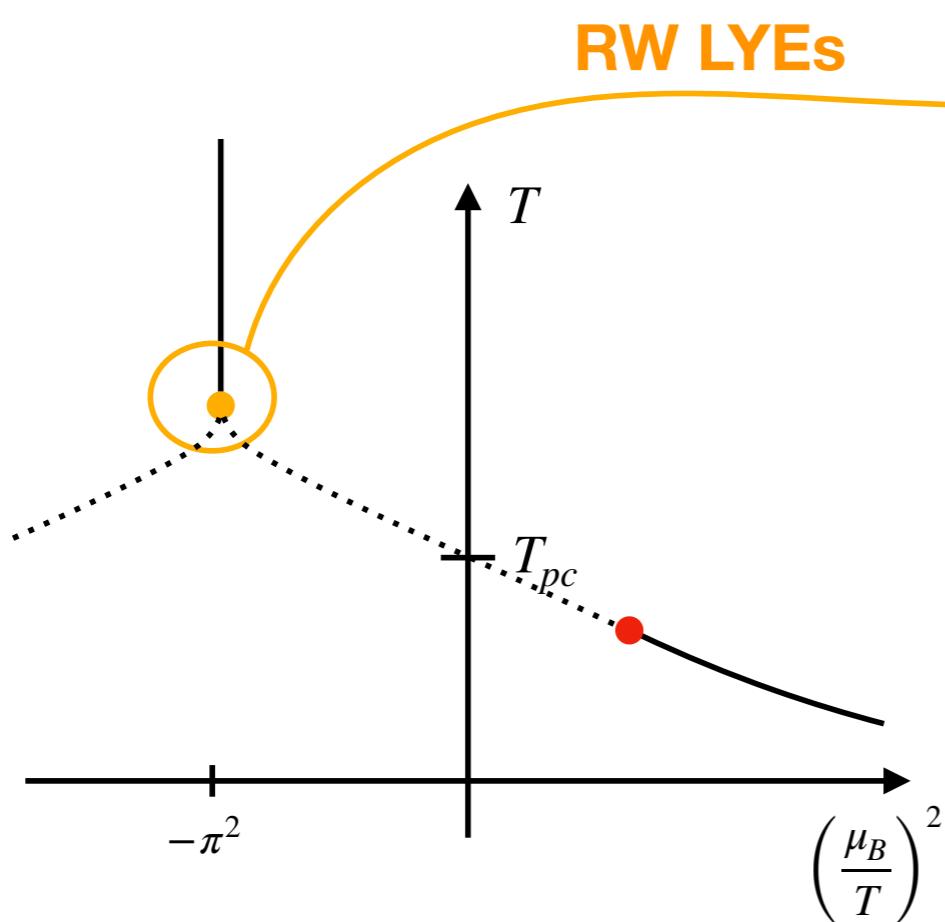
Singularity searches by studying LYES

In (2+1)-flavor QCD one could have three critical points.

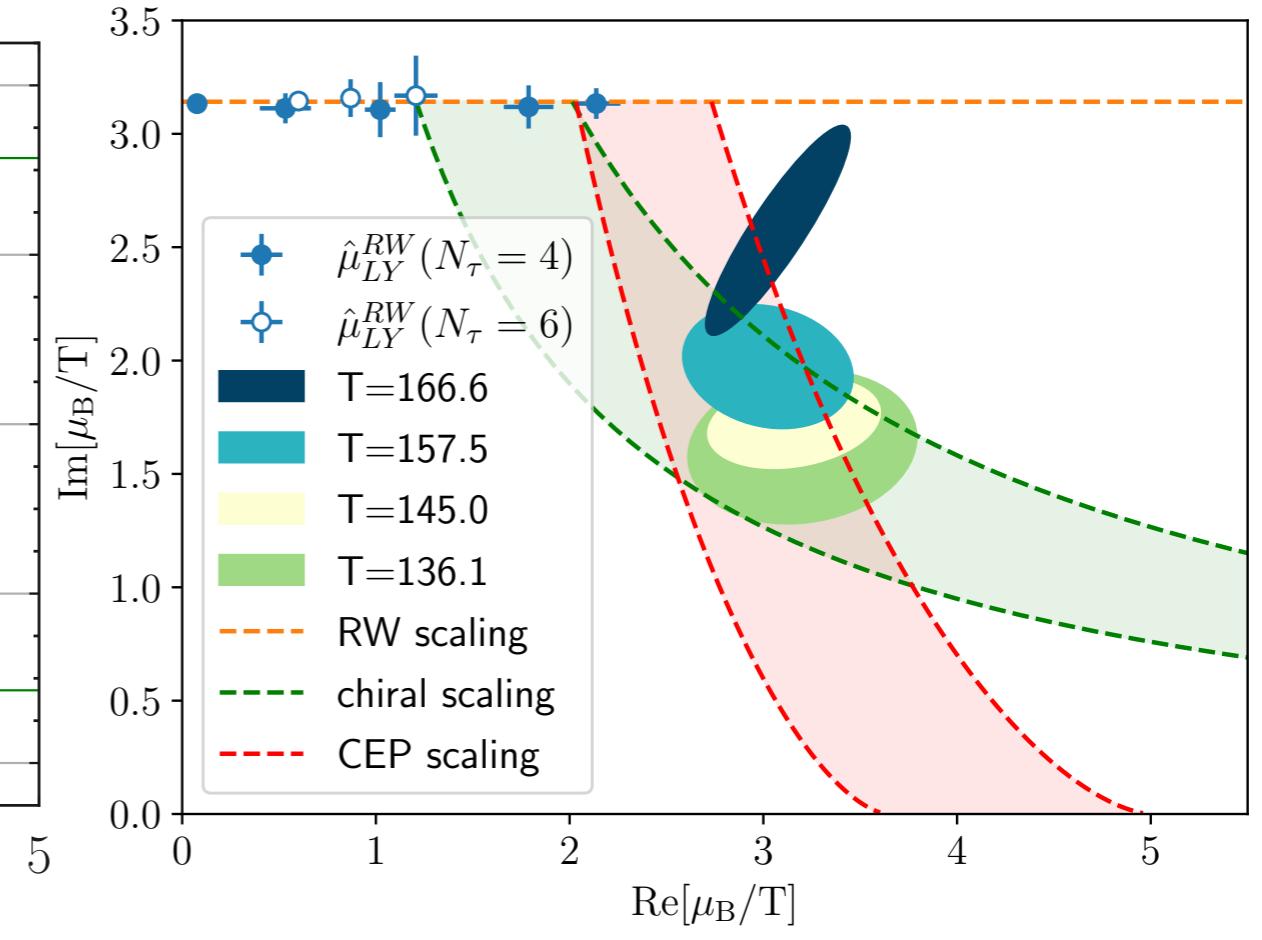
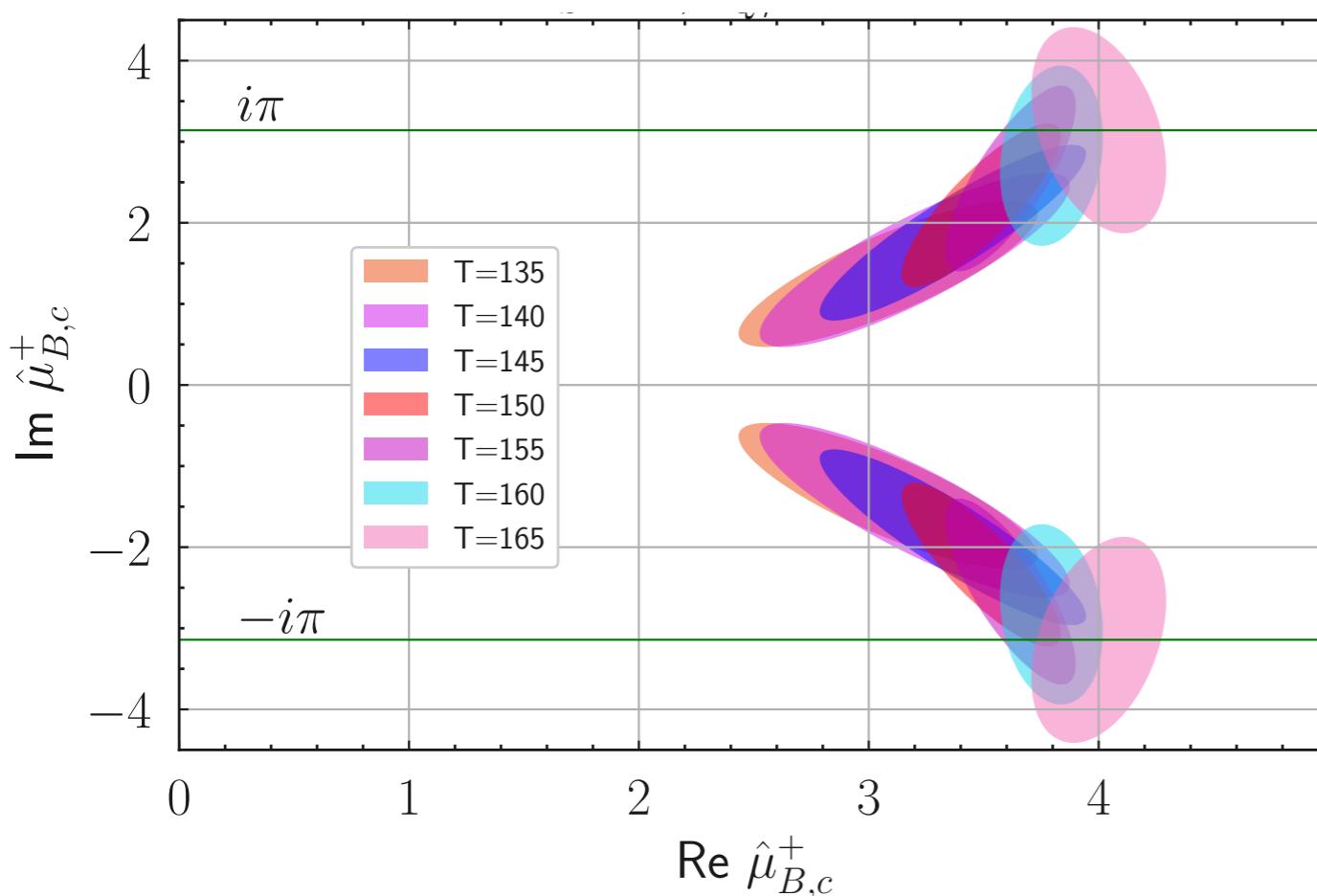
$T_{RW}, i\mu_B/T|_{RW} = \pi$, RW critical point.

$T_c(\mu_B), m = 0$, chiral critical point.

T_{CEP}, μ_{CEP} , QCD critical point ??



LYEs related to CEP ??



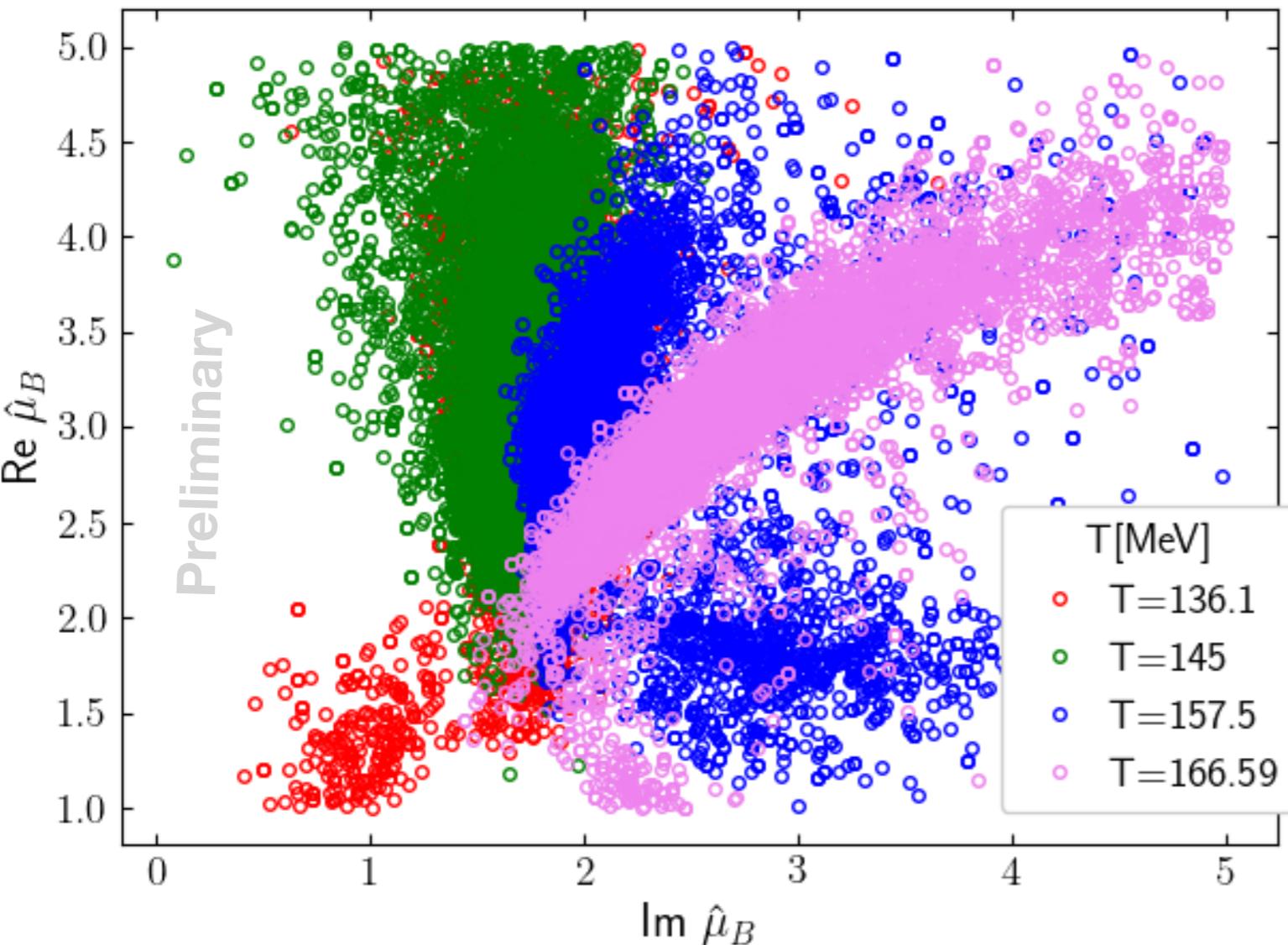
$$N_\sigma^3 \times N_\tau = 24^3 \times 4, 36^3 \times 6$$

Poles of the [4,4]-Padè based on 8-th
order Taylor expansion

Poles of Multi point Padè

Poles show hint for a movement towards real axis.

Machine learning model for the LYE_s



The distribution of the closest singularity (LYEs) obtained by bootstrapping over the data

MADE : masked auto encoder for density estimation.

MADE is a modified autoencoder architecture designed for distribution estimation in machine learning, enabling the modeling of complex, dependent distributions.

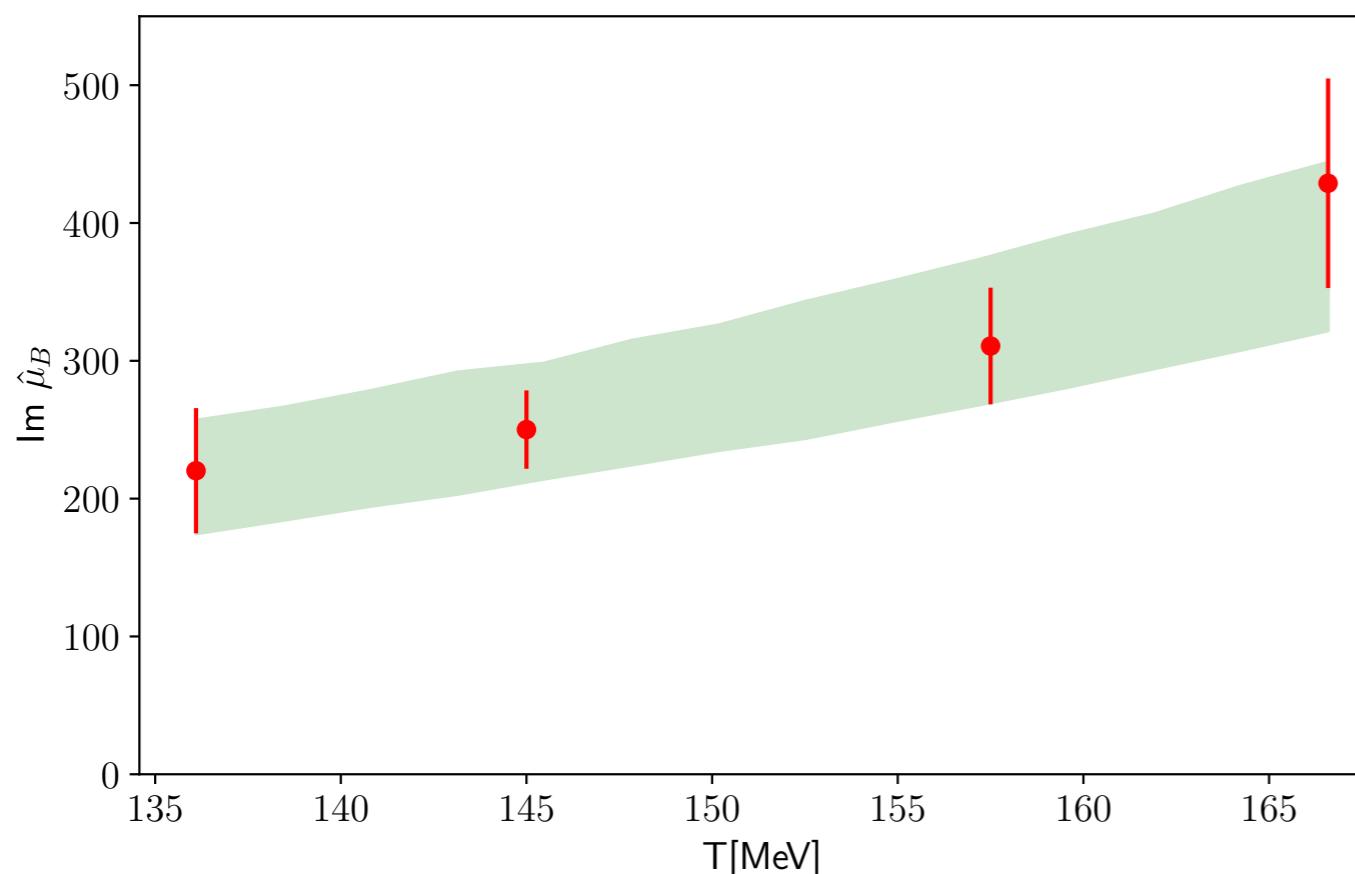
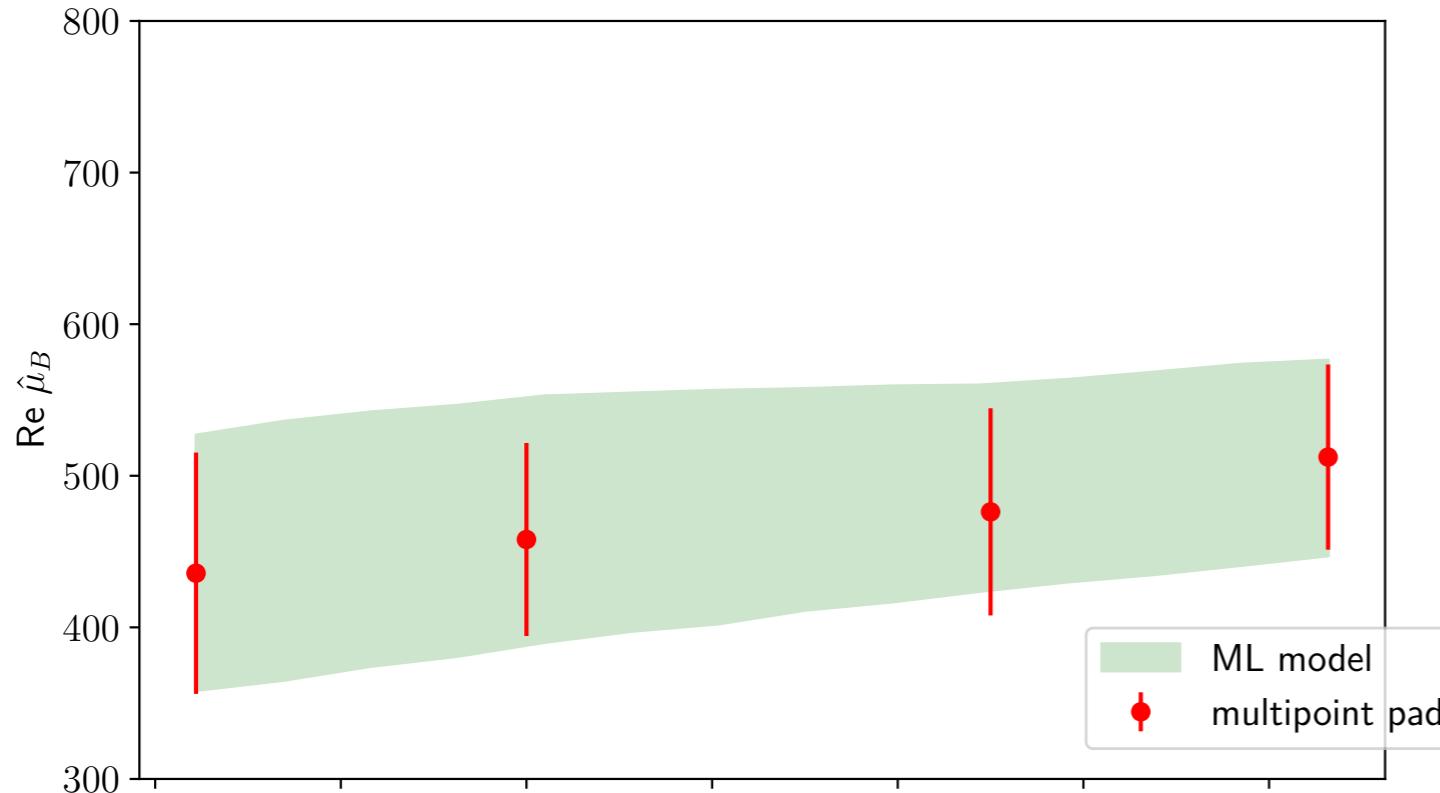
We want to learn the probability distribution of the LYE_s using machine learning modelling.

$$p(\text{Re } \hat{\mu}_B, \text{Im } \hat{\mu}_B | T)$$

$$N_\sigma^3 \times N_\tau = 36^3 \times 6$$

For a control interpolation of the real and imaginary part of μ_B between temperatures.

Machine learning model for the LYE_s



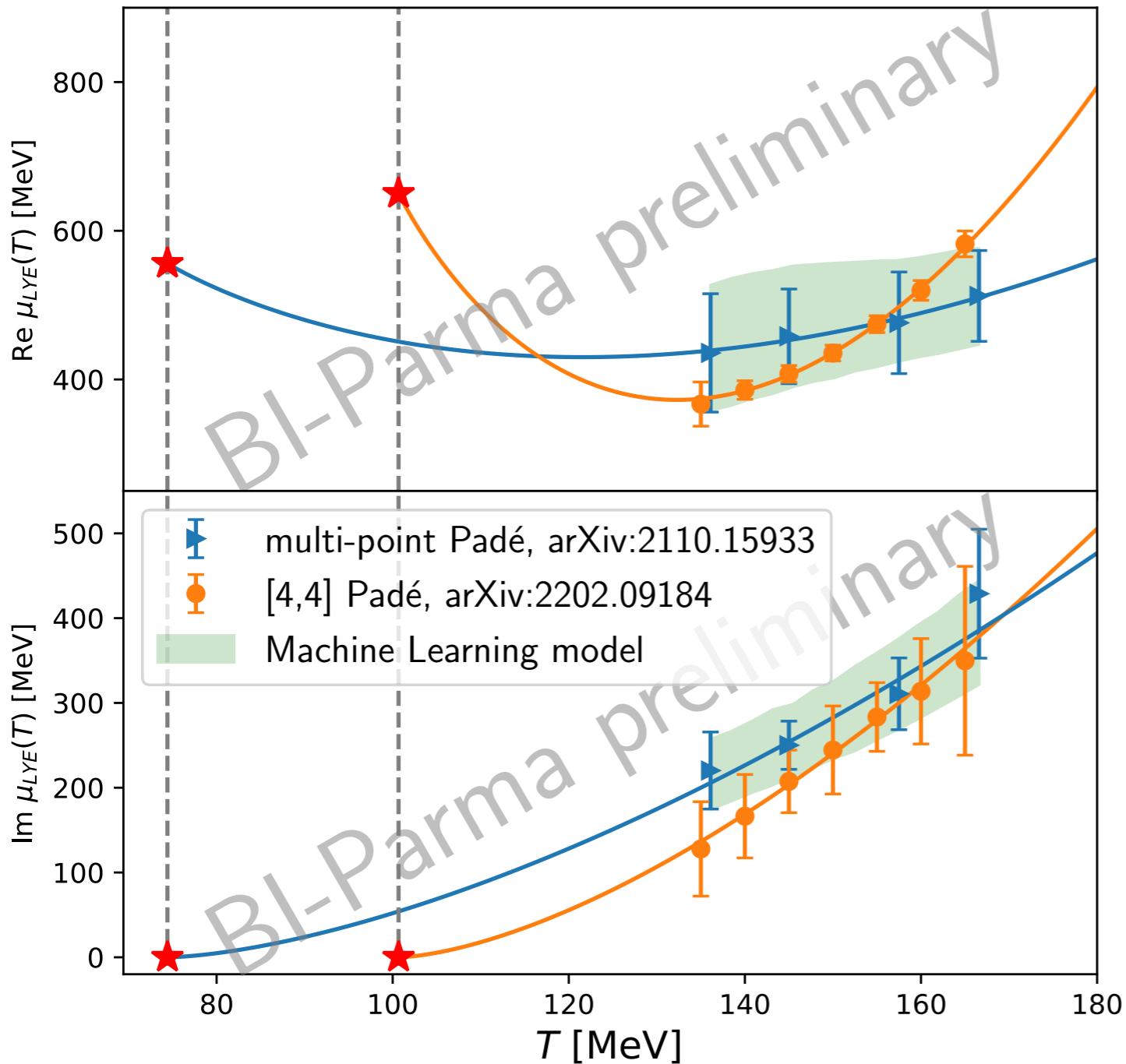
MADE : masked auto encoder for density estimation.

In future Work : We want to use MADE to classify LYE_s related to chiral phase transition ($m_l \rightarrow 0$) and LYE_s related to CEP on several volumes and Quark masses.

$$p(\text{Re } \hat{\mu}_B, \text{Im } \hat{\mu}_B | T, m_l, N_\sigma)$$

Simulations with the smaller than physical quark masses are ongoing.

CEP extrapolation



Extrapolated estimate for the CEP from HotQCD ($N_\tau = 8$) and Multi-point Padè ($N_\tau = 6$) is,

$$T_{CEP} = 90(10) \text{ MeV} \text{ and } \mu_{BCEP} \sim 600(80) \text{ MeV}$$

Consistent with FRG, Phys. Rev. D, 101.5, 054032 (2020). and Dyson-Schwinger, Phys. Rev. D, 104.7, 074035 (2021)

LYEs with many unknown parameters,

$$\mu_{LY} = \mu_{cep} - c_1(T - T_{cep}) + i c_2 |z_c|^{-\beta\delta} (T - T_{cep})^{\beta\delta}$$

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

Summary

New Method

We [Bielefeld-Parma] have developed a multipoint Padé method to extract positions of singularities from number densities in the complex μ plane. It can be seen as a combination of Taylor-expansion method and analytic continuation. Our method has been tested in the vicinity of the RW transition.

Phys.Rev.D 105 (2022) 3, 034513

LYE for chiral transition

No results yet. Smaller than physical quark mass calculations are ongoing.

LYE for CEP

With [4,4]-Padé [HotQCD] and multi-point Padé [Bielefeld-Parma] we find singularities in the complex μ_B shows an approach to the real axis for decreasing temperature. A preliminary extrapolation to the critical point was performed, but needs more control.

Calculations on smaller temperatures are ongoing.

We want to use machine learning modelling for different singularities.

More controlled interpolation between the T and m_q .

Test Case : LYE_s for RW transition

The universal scaling function for 2nd order phase transition [$t = (T - T_c)/T_c \rightarrow 0$, $h \rightarrow 0$],

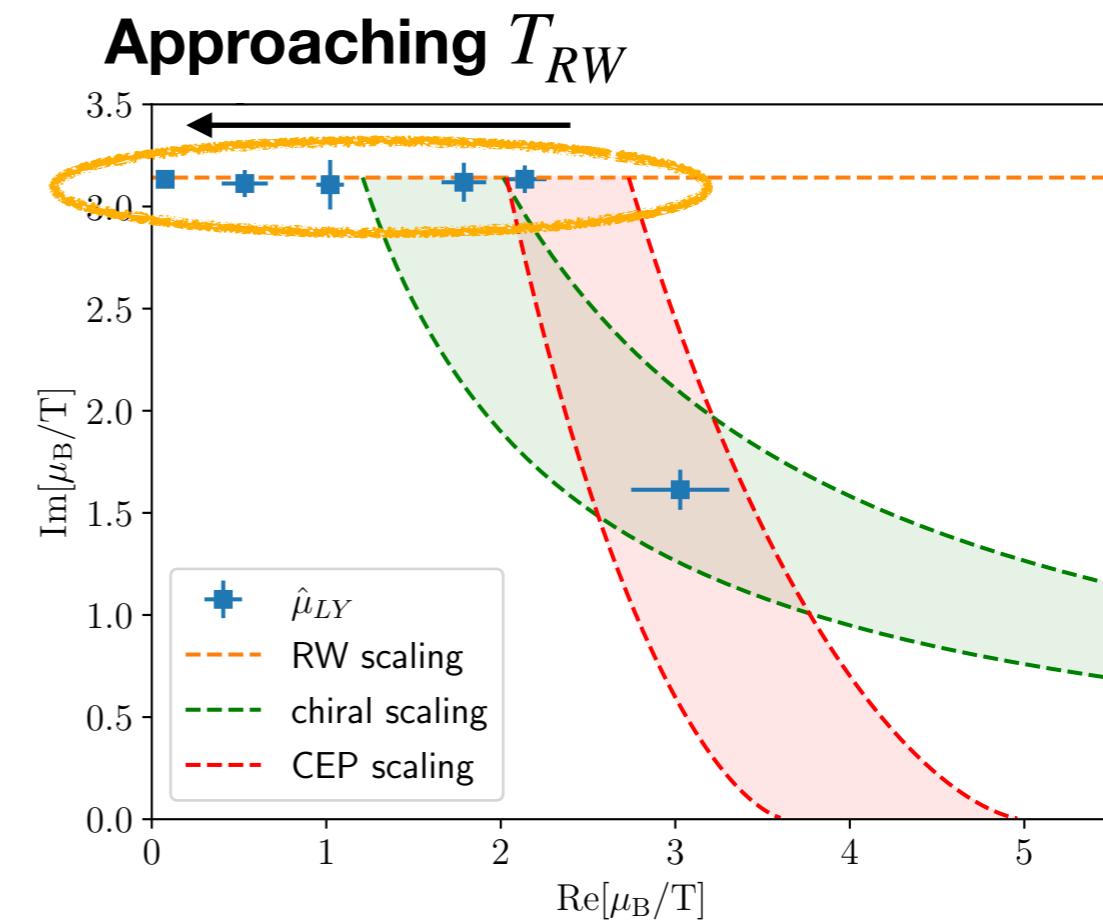
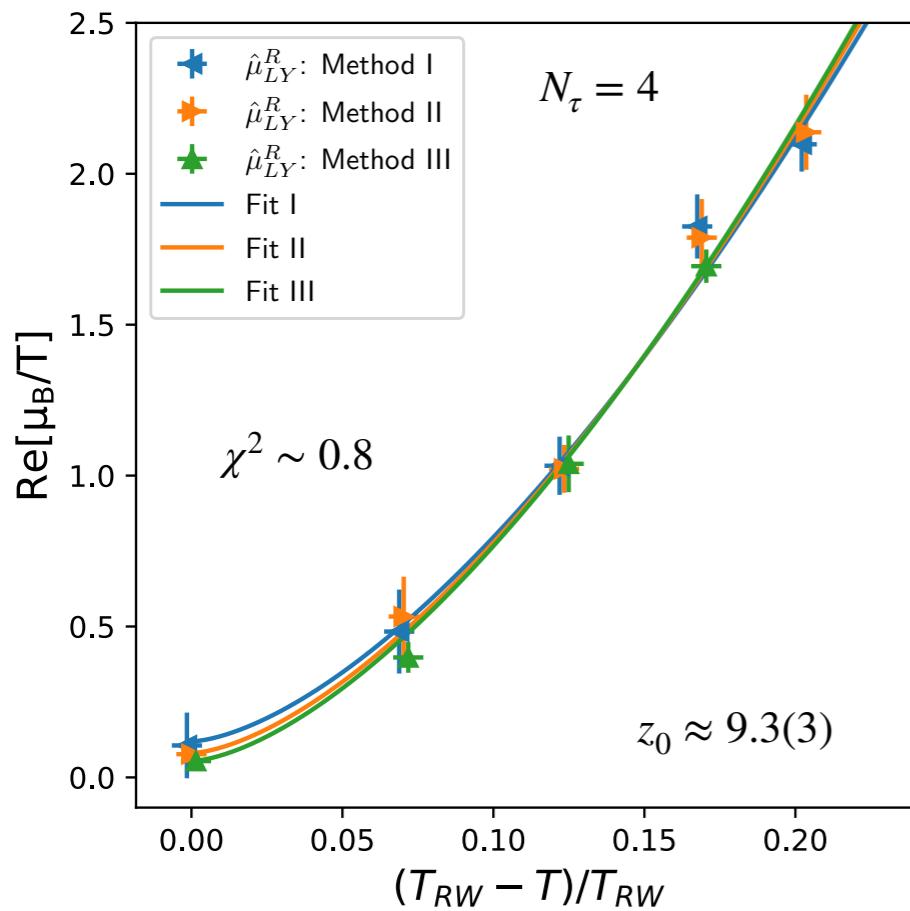
$$f = b^{-d} f_s(b^{y_t} t, b^{y_h} h) + \text{regular}, z = t/h^{1/\beta\delta} \quad f \sim h^{\frac{2-\alpha}{\beta\delta}} f_s(z)$$

Lee-Yang edge singularities are universal in the complex plane,

By solving, $z = z_c$

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

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



$N_\sigma = 24, N_\tau = 4$

Method I : Solving the linear system in μ_B plane.

Method II : Generalized χ^2 method.

Method III : Solving the system in the fugacity plane, $\exp(\mu_B/T)$, and then mapping back to μ_B plane.