Padé approximations and Lee yang zeros

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Based On

HotQCD Collaboration:
[PRD 105 (2022) 7, 074511, arXiv: 2202.09184]
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“Taylor expansion and Padé approximation of pressure at finite chemical potential”

Bielefeld Parma Collaboration:
[PRD 105 (2022) 3, 034513, arXiv: 2110.15933]
Authors :
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- Guido Nicotra
- Christian Schmidt
- Simran Singh **Previous talk!!**
- Kevin Zambello

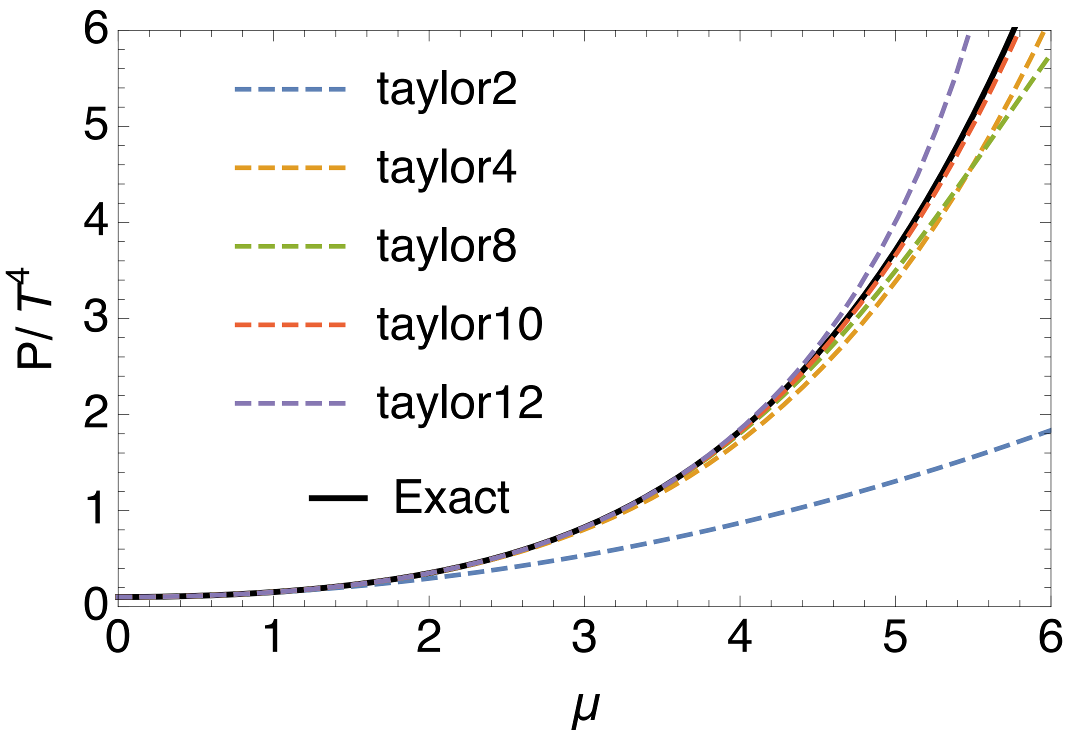
“Multi point Padé approximation of number density at multiple non-zero imaginary chemical potential”

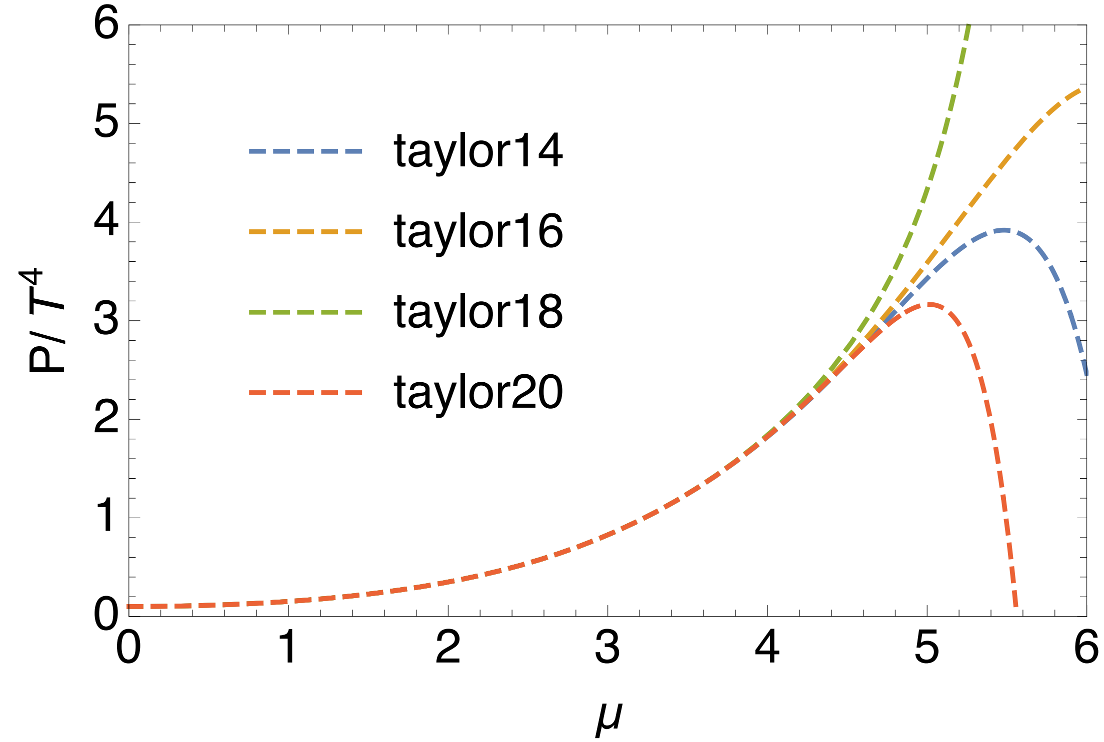
Analytic structure of Fermi gas pressure

CRC-TR 211

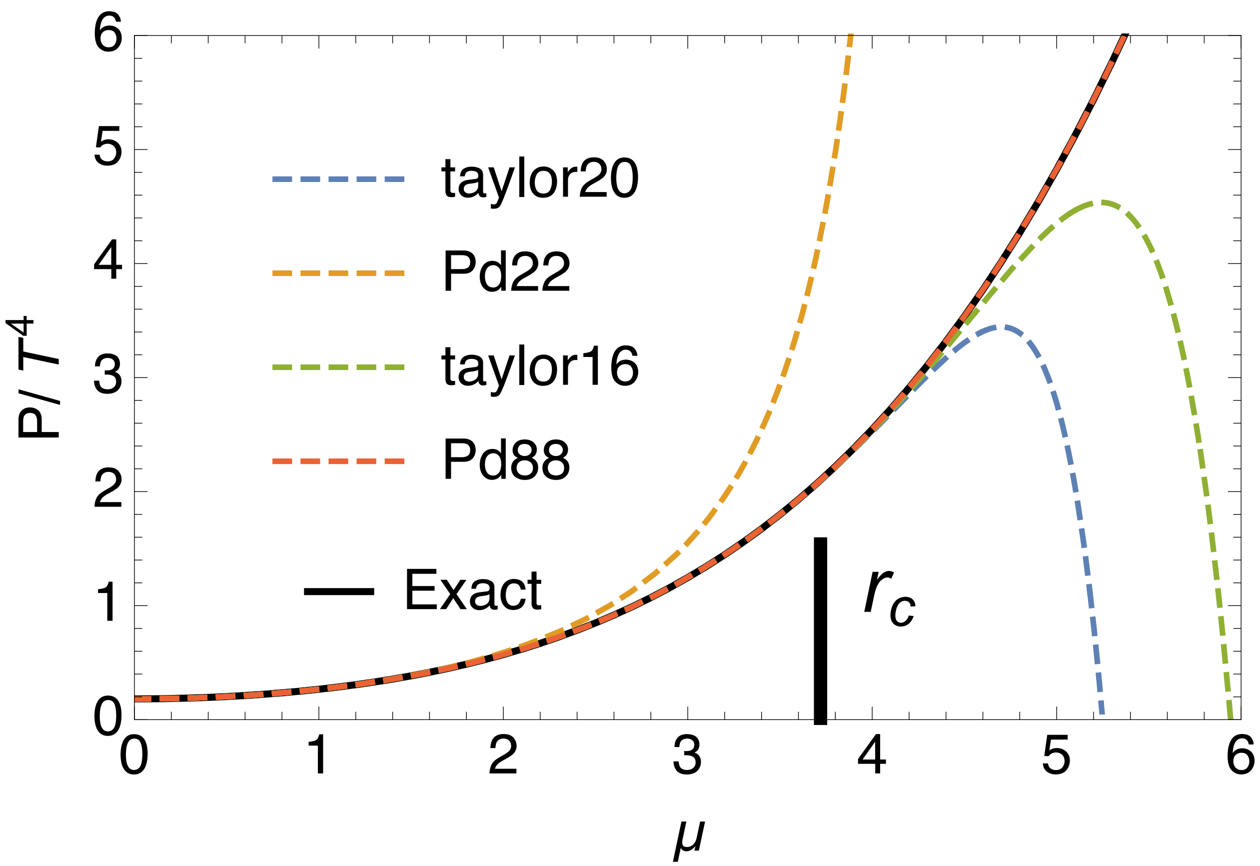
- Pressure of the massive fermi gas looks like,
- $$p(T,\mu) = \frac{g}{6\pi^2}\int_0^\infty dp\, \frac{p^4}{\sqrt{p^2+m^2}}\left[\frac{1}{e^{(\sqrt{p^2+m^2}-\mu)/T}+1}+\frac{1}{e^{(\sqrt{p^2+m^2}+\mu)/T}+1}\right].$$
  The **closest** branch points to the origin occur at the,
  $$\frac{\mu}{T} = \pm\frac{m}{T} \pm i\pi\,.$$
- These singularities in the complex plane set the **radius of convergence** of Taylor series at $\mu = 0$,
  $$R = \sqrt{\left(\frac{m}{T}\right)^2 + \pi^2}\,.$$

Taylor series of fermi gas

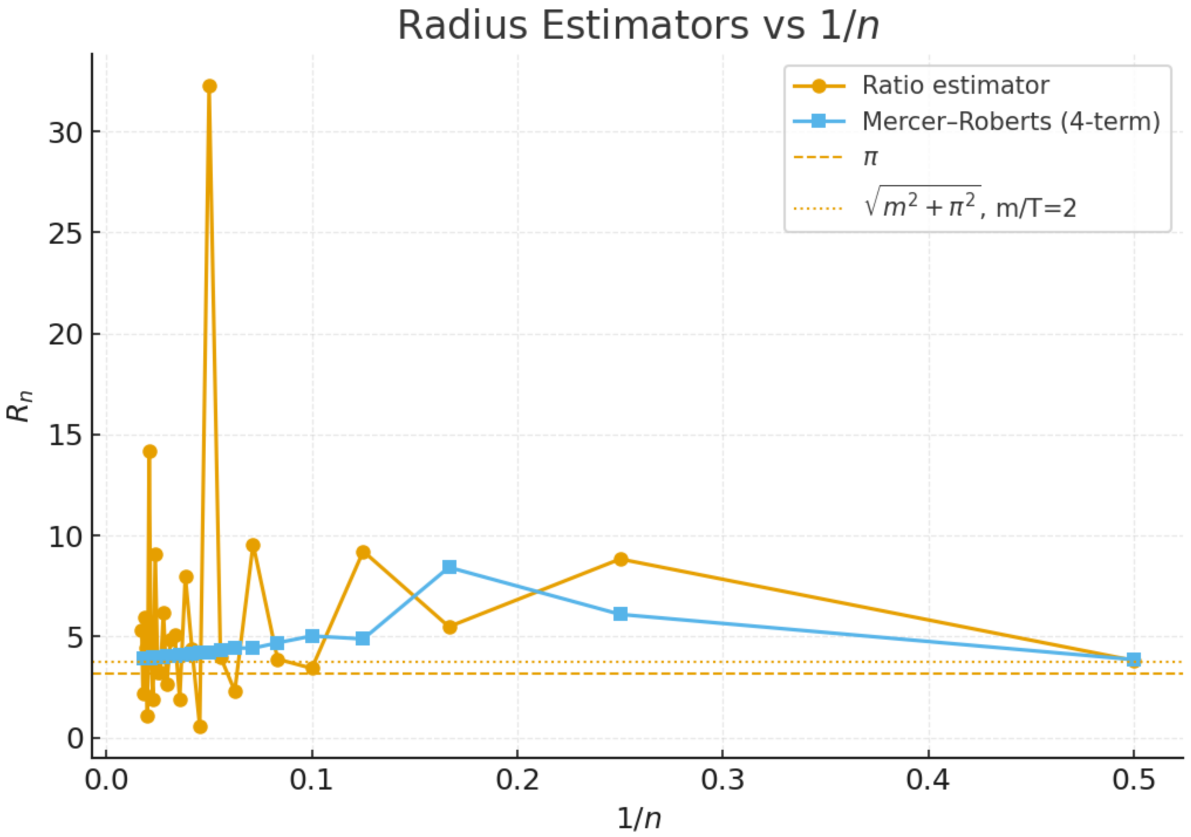


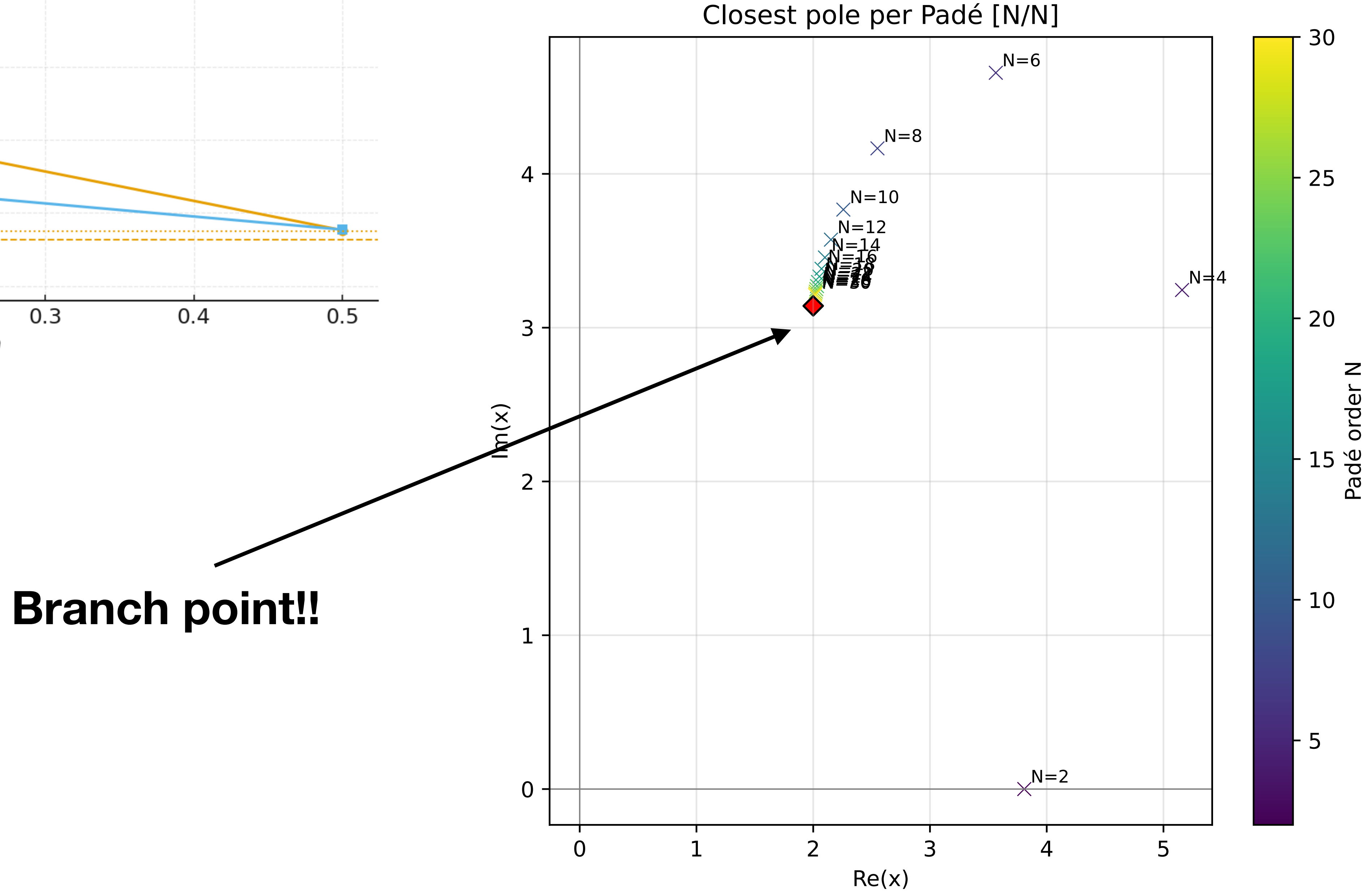


Lower order Taylor expansion approximate the original function very well.
Larger order co-efficient show oscillatory behaviour indicating that the limiting singularity are in complex plane.



Radius of convergence estimator





Thermodynamics using Lattice QCD

The partition function of QCD: **HISQ, $N_f = 2 + 1$-flavor**

$$\mathcal{Z}_{QCD} = \int \mathcal{D}U \, \det[M(m_u, \mu_u)]^{1/4} \det[M(m_d, \mu_d)]^{1/4} \det[M(m_s, \mu_s)]^{1/4} \, e^{-S_G(U)}$$

Real chemical potential makes the determinant complex,

- The Taylor series of the QCD pressure at finite temperature and density:

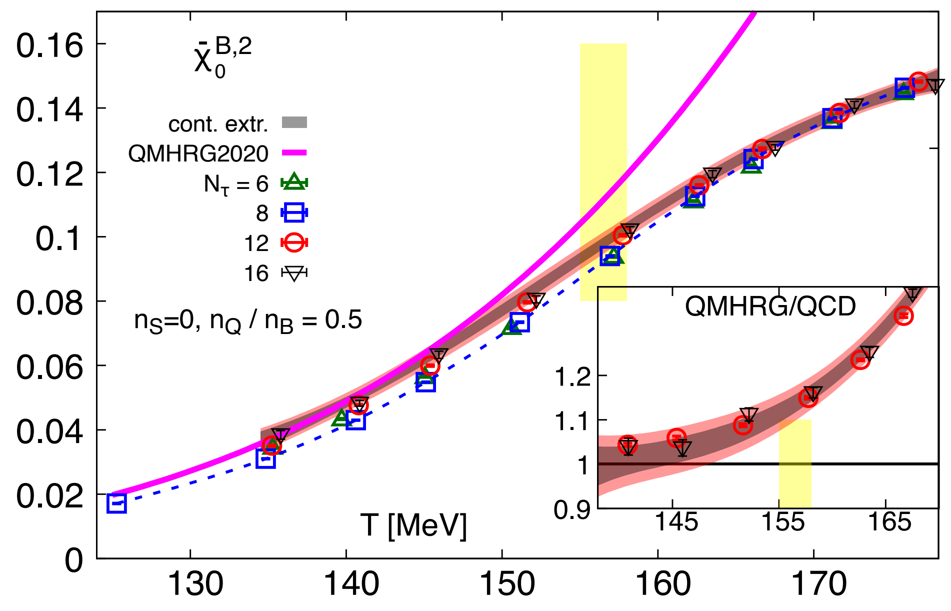
$$\frac{P(T, \vec{\mu})}{T^4} = \frac{1}{VT^3} ln \mathcal{Z}_{QCD} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk}^{BQS} \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k \ , \ \hat{\mu} = \mu/T$$

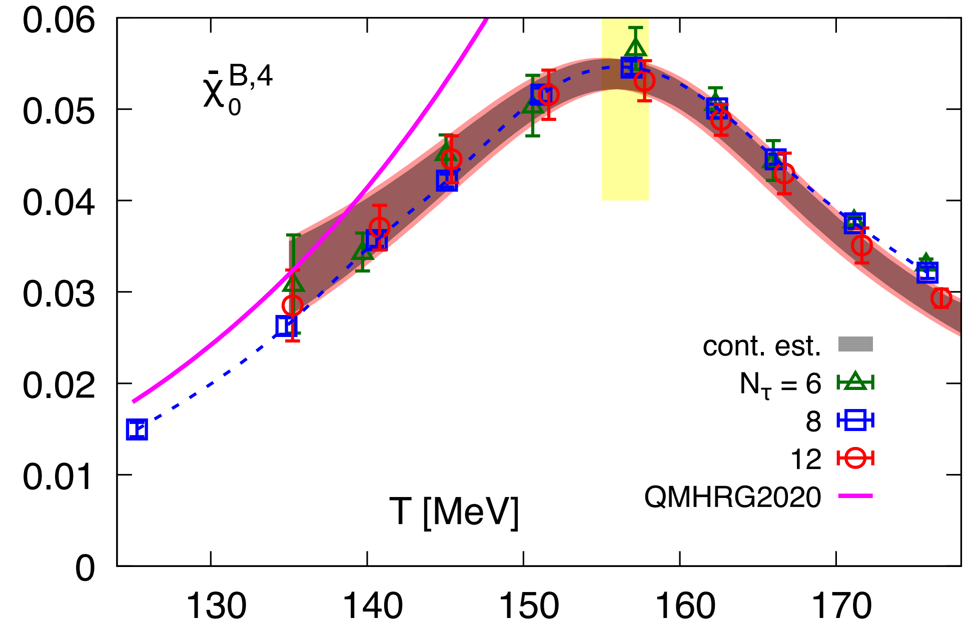
- Cumulants at vanishing chemical potential,

$$\chi_{ijk}^{BQS}(T,0) = \left. \frac{\partial^{i+j+k} P/T^4}{\partial \hat{\mu}_X^{i,j,k}} \right|_{\mu_X=0} , \ X = B, Q, S$$

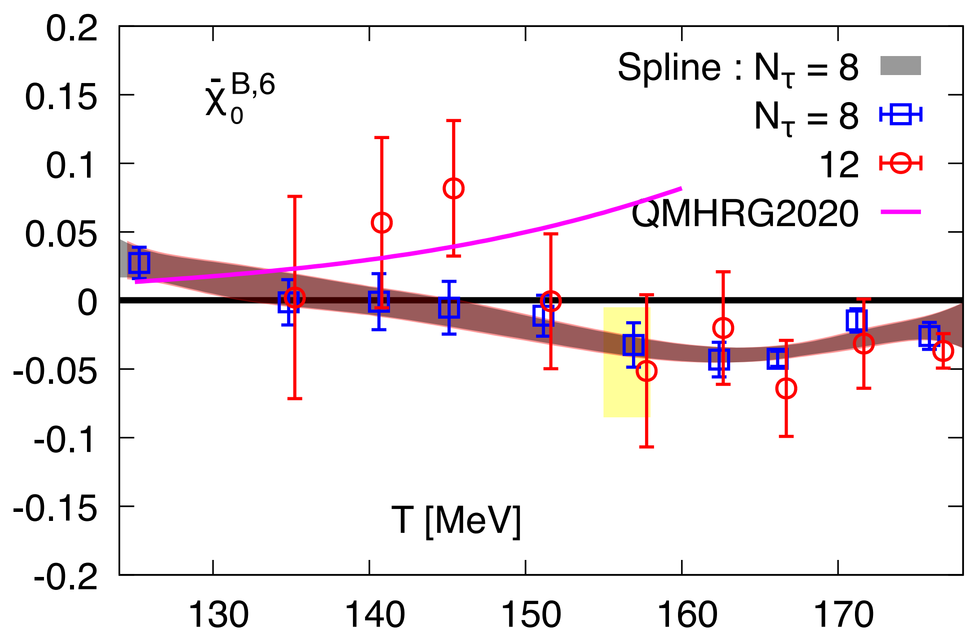
$$\mu_u = \frac{1}{3}\mu_B + \frac{2}{3}\mu_Q \ ,$$
$$\mu_d = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q \ ,$$
$$\mu_s = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q - \mu_S \ .$$

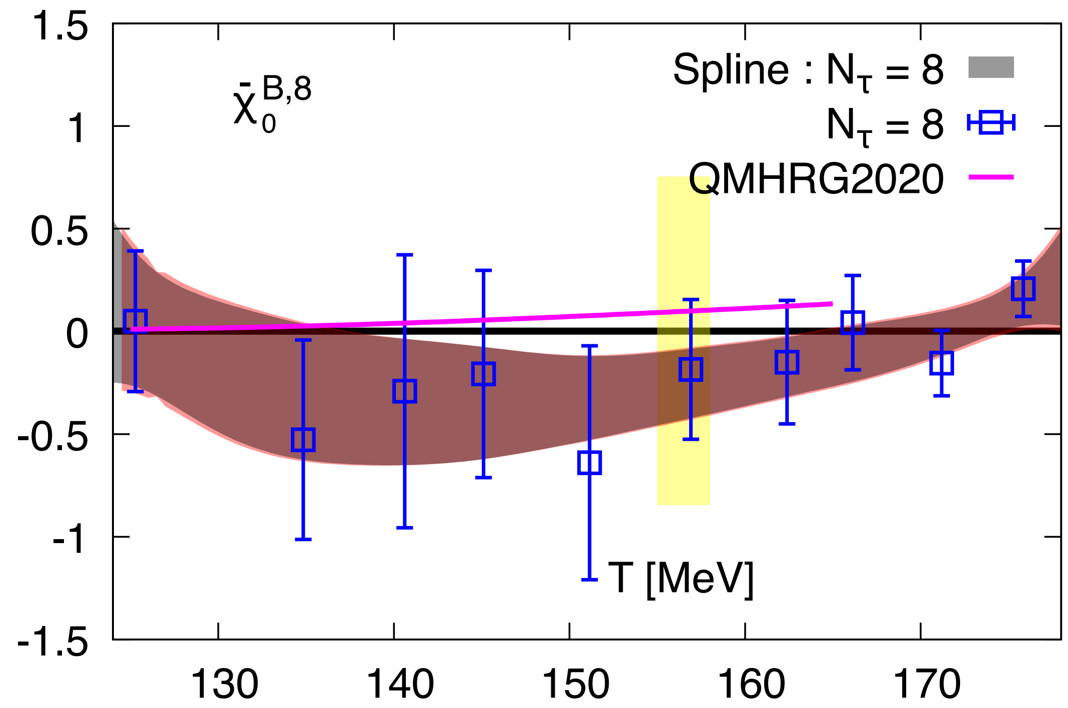
Expansion coefficients of the Taylor series





- For the $N_\tau = 8$ dataset, we have generated ~ 1.5 million gauge configurations per T.





Lee yang zeros from Padé approximants

- **Lee Yang** : Phase transitions are related to singularities of the Taylor series on the real axis.

- If all the expansion coefficients are of same sign, could be an indication that the singularity of the series is on the real axis and hence is an indication of a critical point.

- Alternatively, one could construct Padé approximants which are rational functions of the form, $f(x) = \frac{\sum_{i=0}^{a} c_i x^i}{1 + \sum_{j=0}^{b} d_j x^j}$, and evaluate its singularities.

Useful Formulas

CRC-TR 211

$$\Delta P/T^4 = \sum_{k=1}^{4} P_{2k}(T)\hat{\mu}_B^{2k} = (\bar{x}^2 + \bar{x}^4 + c_{6,2}\bar{x}^6 + c_{8,2}\bar{x}^8)P^2/P_4,\ \bar{x} = \sqrt{\frac{P_4}{P_2}}\ \hat{\mu}_B$$

Reminder : P_2 and P_4 are strictly positive for all temperatures.

- One can construct various $[m,2]$ and $[n,4]$ Padé's from the above series.[$m \in \{2,4,6\}$ and $n \in \{2,4\}$]
- The convergence of Padé approximants will be unaffected by a singularity in the complex plane contrary to the Taylor series.
- The poles of the Padé approximants closest to the origin determine the radius of convergence.
- The poles of a general $[m,2]$ and $[n,4]$ Padé's are the usual ratio estimator (r_c^n) and Mercer Roberts estimator (r_c^{MR})[*For two pair of complex poles] of radius of convergence of the Taylor series.

$$r_c^{MR} = \left| \frac{c_{n+2}\, c_{n-2} - c_n^2}{c_{n+4}\, c_n - c_{n+2}^2} \right|^{1/4},\ n \text{ even}$$

G. N. Mercer and A. J. Roberts, SIAM J. Appl. Math. 50, 1547 (1990)

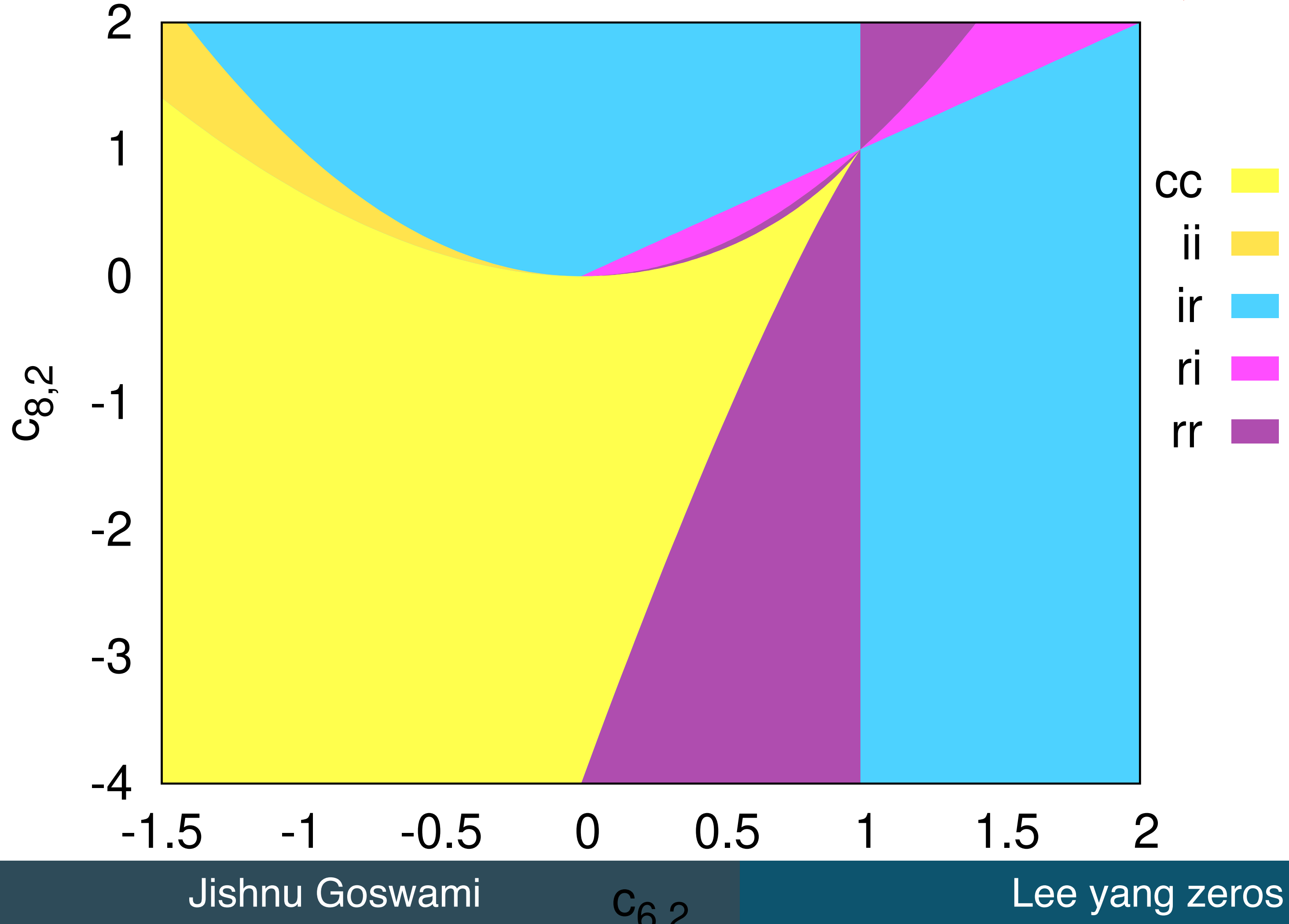
Constraints for a real pole of [4,4] Padé

Reminder : Critical points are related to the singularities on the real axis.
All expansion coefficients have to be positive for a singularity in the real axis.
$\chi_0^{B,6}, \chi_0^{B,8}$ are negative for temperature range, $T \in [135:165]$ MeV.

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

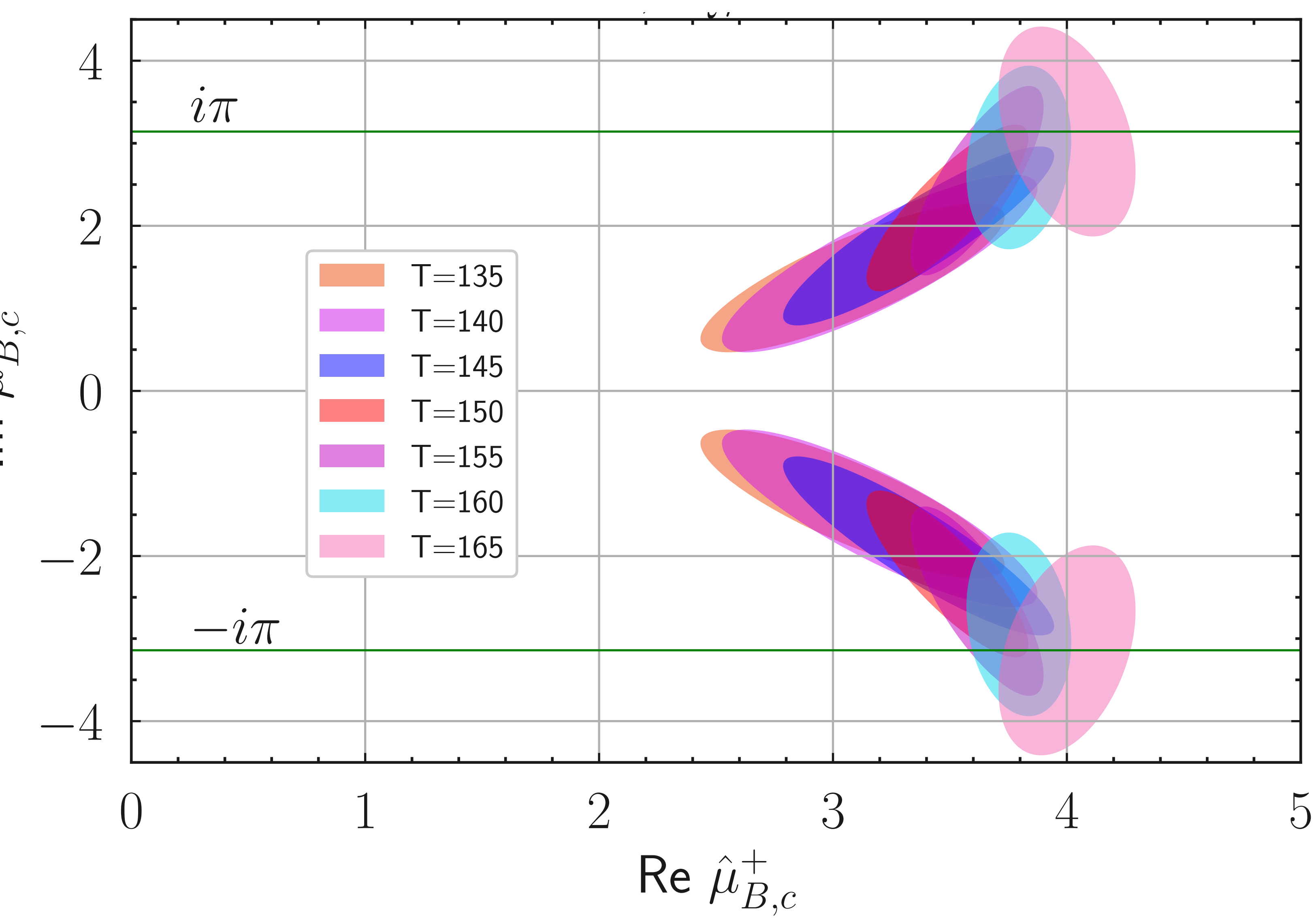
Poles can be written as,

$$z \equiv \bar{x} \qquad z^{\pm} = \frac{c_{8,2} - c_{6,2} \pm \sqrt{(c_{8,2}-c_{8,2}^{+})(c_{8,2}-c_{8,2}^{-})}}{2(c_{8,2}-c_{6,2}^2)}; \; c_{8,2}^{\pm} = -2 + 3c_{6,2} \pm 2(1-c_{6,2})^{3/2}$$



Values(including sign) of $c_{6,2}$ and $c_{8,2}$ which are related to χ_6^B and χ_8^B are crucial to have a pole in the real axis.

Padé approximations



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

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

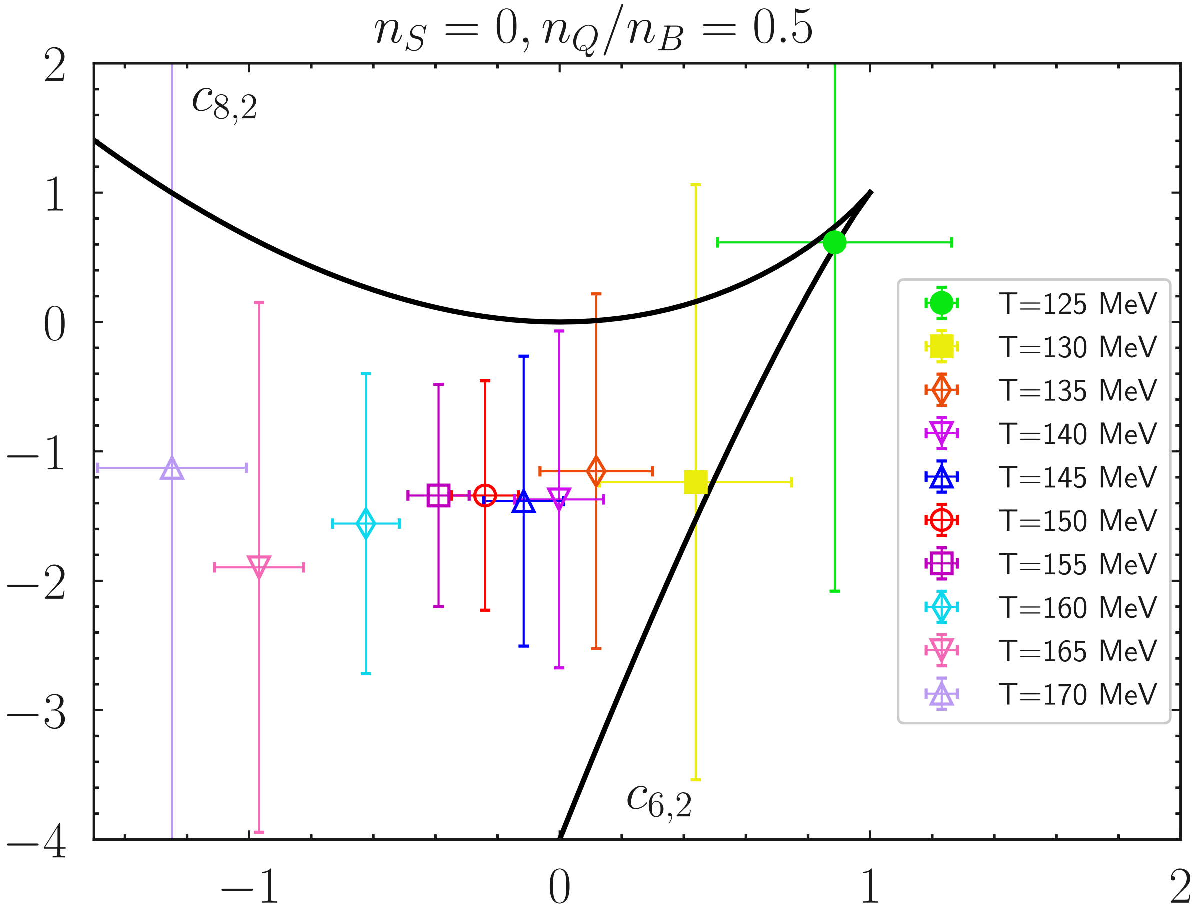
Bound for CEP :

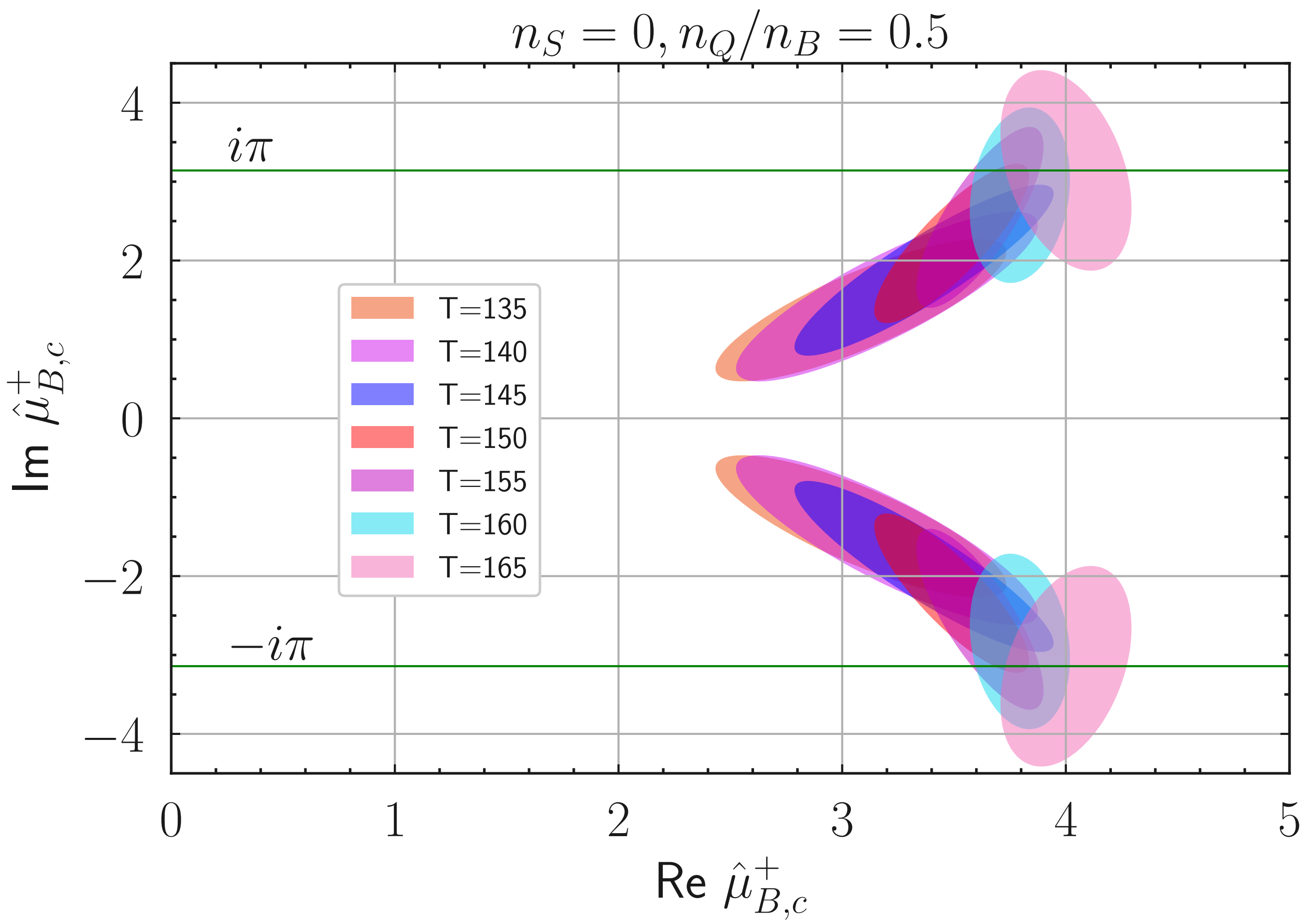
$T^{CEP} < 132$ MeV, $\hat{\mu}_B/T > 2.5$

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

- Lee-yang theorem: Singularity in the real axis is a hint for a critical point.

Location of the poles from [4,4] Padé approximants for QCD





Poles are complex for the temperature range, $T \in [135 : 165]$ MeV.
The possibility of occurrence of a real pole cannot be ruled out for $T < 135$ MeV

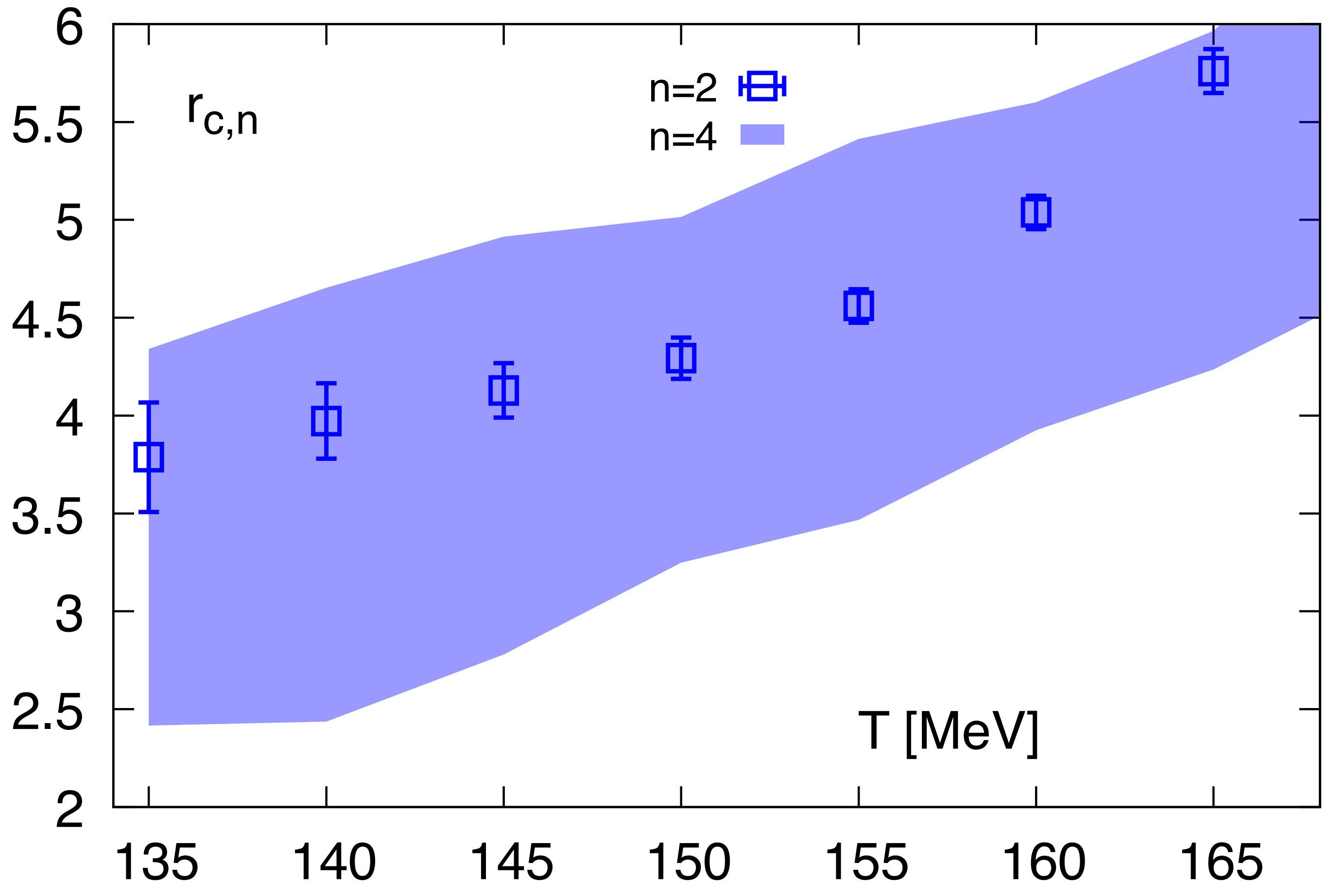
Only complex poles having a positive real part are shown.
The poles show a tendency to move to real axis for $T < 135$ MeV

Bound for CEP is,
T^{CEP} < 135 MeV.
Consistent with $T^{CEP} < T_c^{chiral}$ (~ 130 MeV) [arXiv:1903.04801]

Radius of convergence from diagonal Padé approximants

$$r_{c,2} = \sqrt{12\bar{\chi}_2^B / \bar{\chi}_4^B}$$

$$r_{c,4} = r_{c,2}\,|z^+ z^-|^{1/4} = \sqrt{\frac{12\bar{\chi}_0^{B,2}}{\bar{\chi}_0^{B,4}}}\left|\frac{1-c_{6,2}}{c_{6,2}^2 - c_{8,2}}\right|^{1/4}$$



The radius of convergence of $[2,2]$ and $[4,4]$ Padé in the temperature range $T \in [135 : 165]$ MeV obtained as, $\left|\hat{\mu}_B^c\right| \sim [2.5 : 5.5]$.

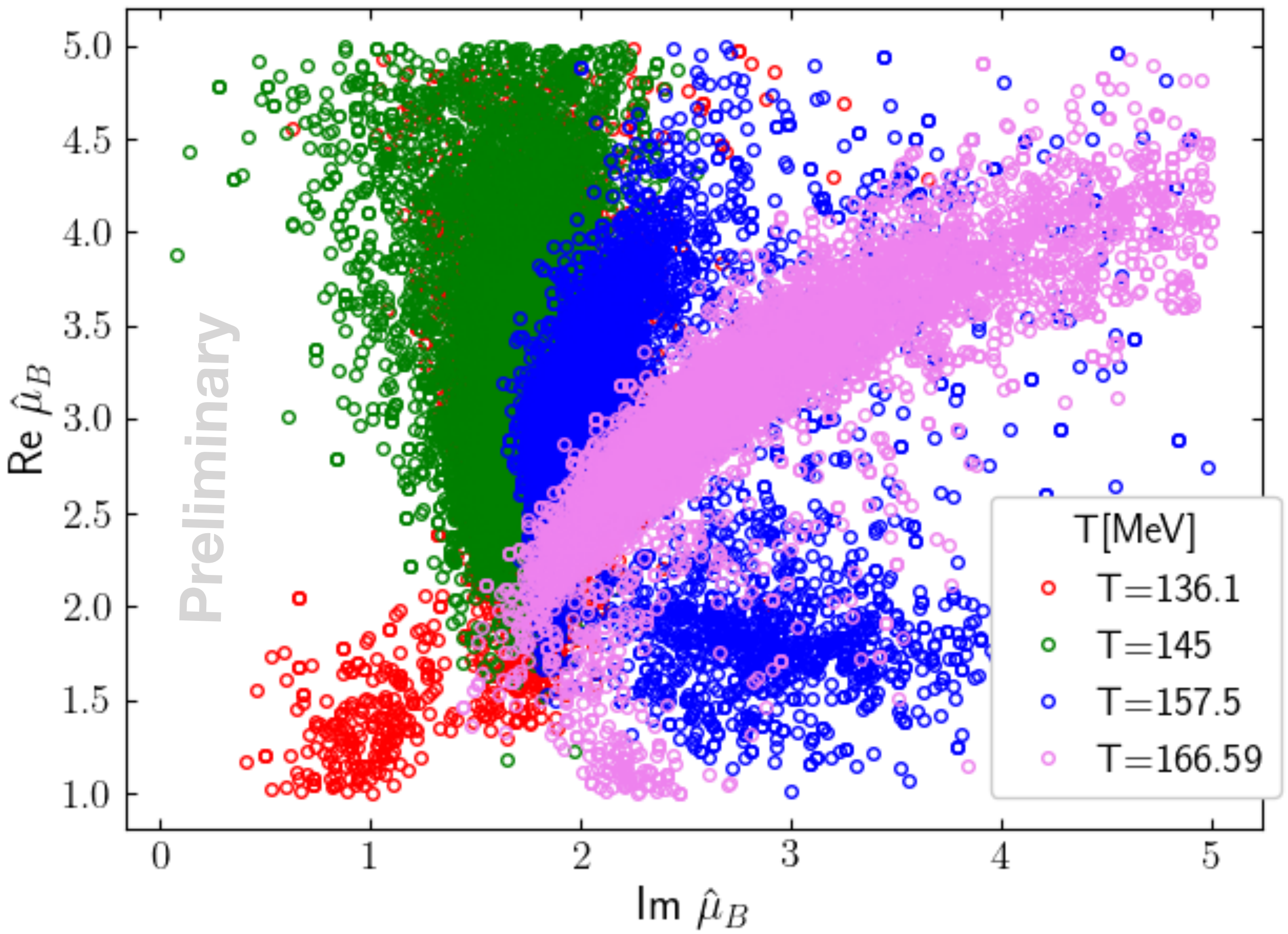
This is also the current updated estimate for the radius of convergence (r_c) from a $\hat{\mu}_B^8$ Taylor series.

Bound for CEP is,

$$\hat{\mu}_B^{CEP} > 2.5.$$

Distribution of the poles from bootstrap sampling

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



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

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

Learning Temperature-Conditioned Pole Distributions with Conditional MAF

- **Goal:** model the conditional distribution of complex poles as a function of temperature,
  $$p(y \mid x = T), \quad y = \begin{bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{bmatrix} \in \mathbb{R}^2, x \in \mathbb{R}\,.$$

Motivation:

- Smooth interpolation in T; sample plausible pole clouds at arbitrary temperature.
- Exact likelihood for calibration and quantitative diagnostics.

Preprocessing:

- Z-score standardization per dimension (train-set stats).
- Train/val split on triples $(\mathrm{Re}, \mathrm{Im}, T)$.

Conditional Probability & Chain Rule

- **Conditional probability:** For random variables A, B with $p(B) > 0$,

$$p(A \mid B) = \frac{p(A, B)}{p(B)}, \qquad p(A, B) = p(A \mid B)\, p(B) = p(B \mid A)\, p(A)\,.$$

- *Analogy*: A = “carry an umbrella”, B = “it is raining.” Then $p(A \mid B)$ is the probability I carry an umbrella “given” that it’s raining. Clearly $p(A \mid B) \gg p(A)$, because the context (rain) changes the likelihood.
- **Chain rule (autoregressive factorization).**
- For a vector $y = (y_1, \ldots, y_D)$ and context x,

$$p(y \mid x) = \prod_{i=1}^{D} p\big(y_i \mid y_{<i}, x\big), \qquad y_{<i} = (y_1, \ldots, y_{i-1})\,.$$

- In our case$D = 2 \quad (Re, Im)$, so, $p(y \mid x) = p(y_1 \mid x)\, p(y_2 \mid y_1, x)\,.$

From Joint to Autoregressive Factorization

- For a 2D variable $\mathbf{y} = (y_1, y_2)$ conditioned on $\mathbf{x}$ (temperature): $p(\mathbf{y} \mid x) = p(y_1, y_2 \mid x)$
- Chain rule : $p(y_1, y_2 \mid x) = p(y_1 \mid x)\, p(y_2 \mid y_1, x)$
- Key idea: instead of modeling one complicated D-dimensional density, we reduce it to a sequence of D one-dimensional conditionals.
- This factorization motivates MADE/MAF: masks enforce the dependence on $y_{<i}$, while x(temperature) is injected unmasked, yielding a tractable Jacobian and exact log-likelihood.

Conditional Normalizing Flow

- A *normalizing flow* is just an invertible change of variables: $z = f_\theta(y; x)$, where z is mapped into a **simple Gaussian.**
- So instead of modeling p(y|x) directly, we model the transformation that maps it to Gaussian space.
- $\log p_\theta(y \mid x) = \log p(z) - \log |\det J_{f_\theta}(y; x)|$
- $\log p(z) = -\frac{1}{2}||z||^2 - \frac{D}{2}\log(2\pi), \quad D = 2.$
- **Conditioning:**(temperature) is injected unmasked into all MADE layers so f_θ varies smoothly with T.

We learn an invertible map that sends the pole distribution to a Gaussian. The log-likelihood splits into the Gaussian prior term and a Jacobian correction. Temperature enters unmasked in every MADE layer, so the learned transformation depends smoothly on T.

MADE and MAF Implementation

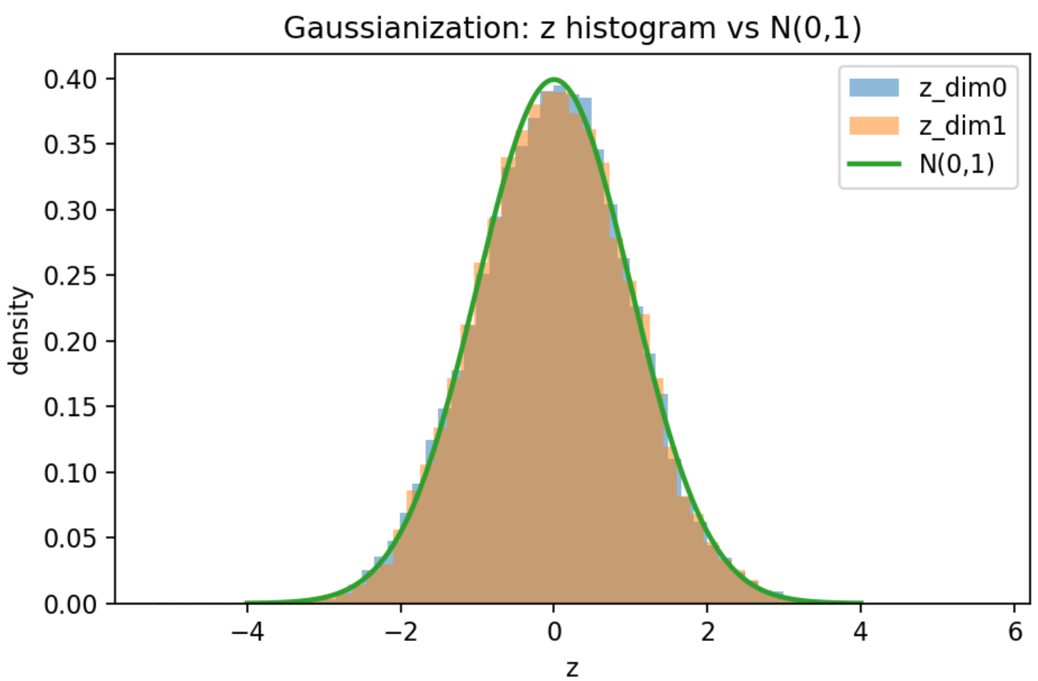
- How do we actually build such an invertible map?
- Each conditional factor is modelled as a Gaussian with autoregressive parameters: $p(y_i \mid y_{<i}, x) = \mathcal{N}\left(y_i \;\middle|\; \mu_i(y_{<i}, x),\, \sigma_i^2(y_{<i}, x)\right)$, predicted by a neural network.
- MADE (Masked Autoencoder):
  - Neural network with binary masks on connections.
  - Ensures μ_1, σ_1depend only on x, not on y_2.
  - Ensures μ_2, σ_2 can depend on (y_1, x).
- MAF (Masked Autoregressive Flow):

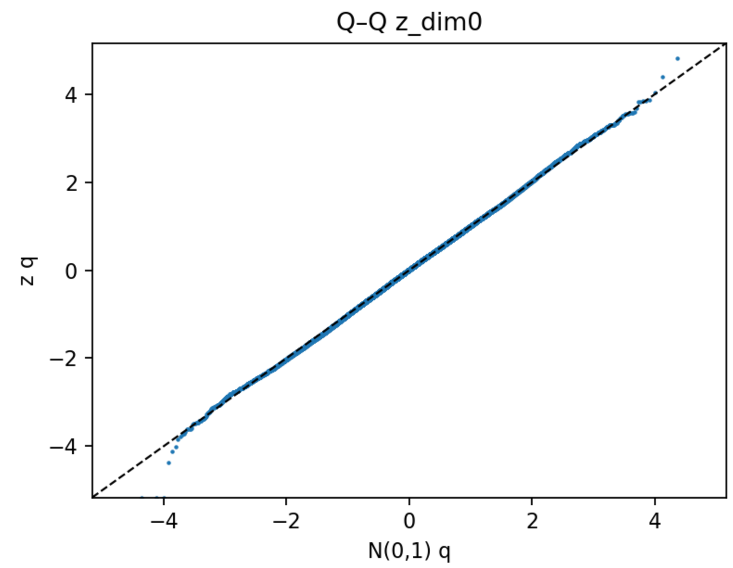
$$z_i = \frac{y_i - \mu_i(y_{<i}, x)}{\sigma_i(y_{<i}, x)}, \log \left|\det J\right| = -\sum_i \log \sigma_i$$

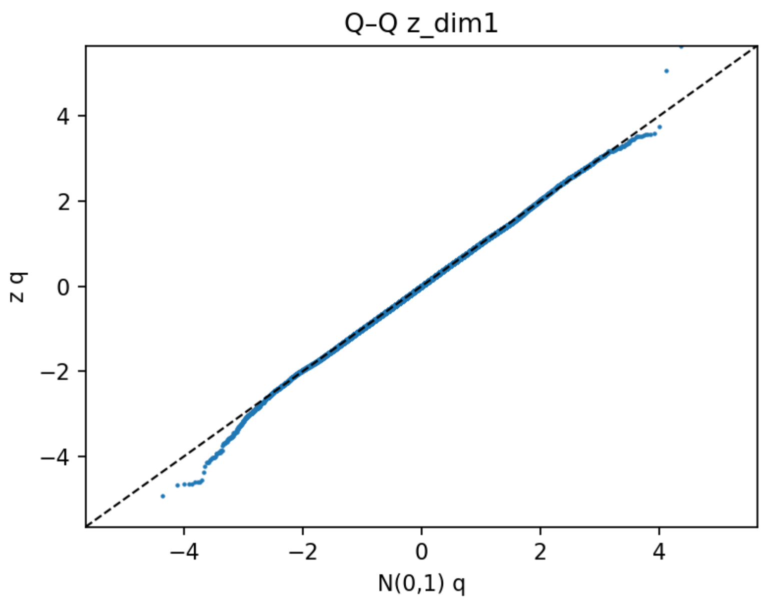
Stacking K MADE layers with permutations increases flexibility.

Validation of the flow transformation (Gaussianization + Q-Q plots)

- First we check that the normalizing flow correctly maps the input distribution into an isotropic Gaussian.
- The histograms of the latent dimensions align very well with $N(0,1)$, and the $Q-Q$, plots confirm near-perfect Gaussianity.
- This ensures the flow transformation is behaving as expected.

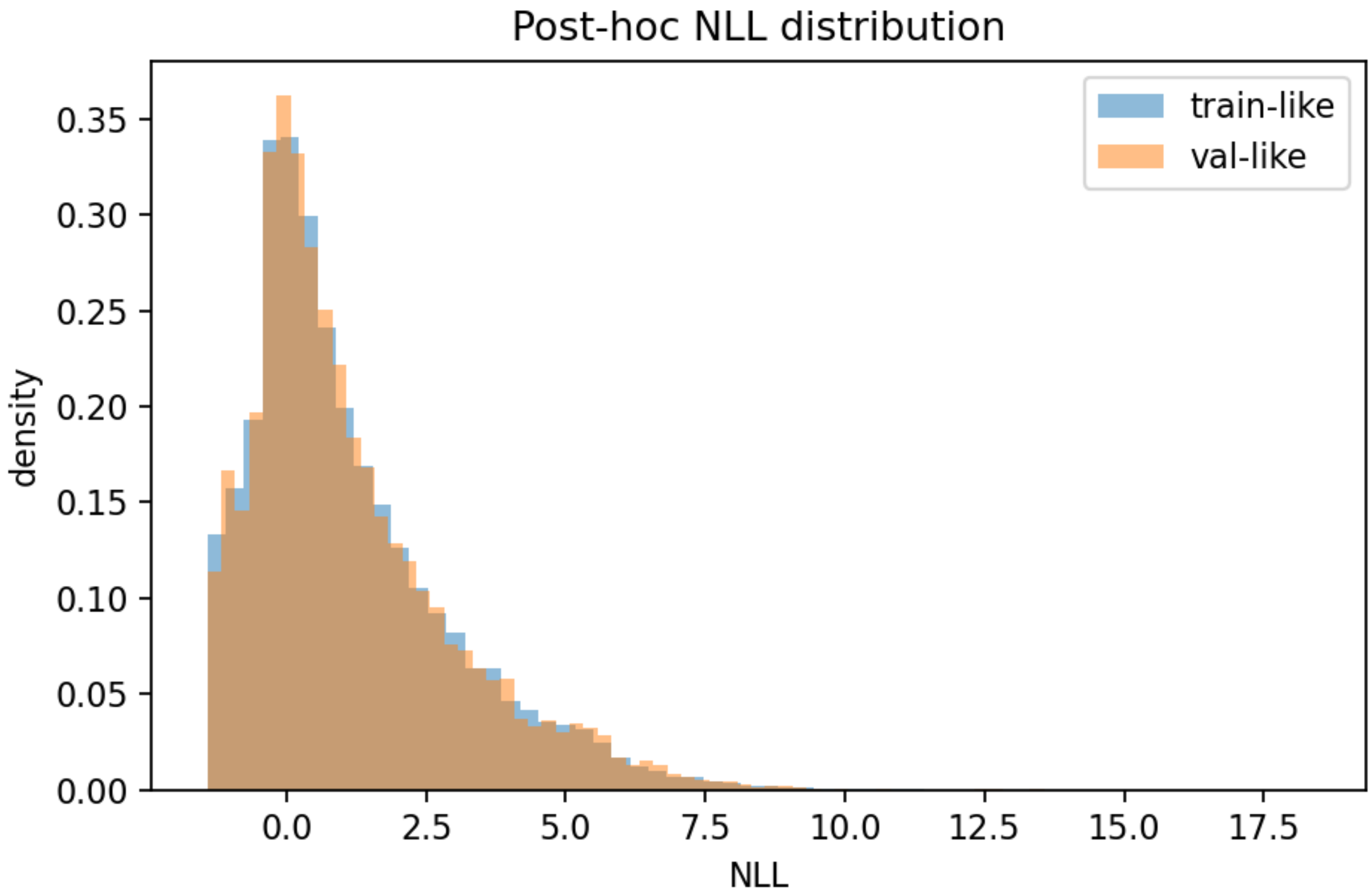






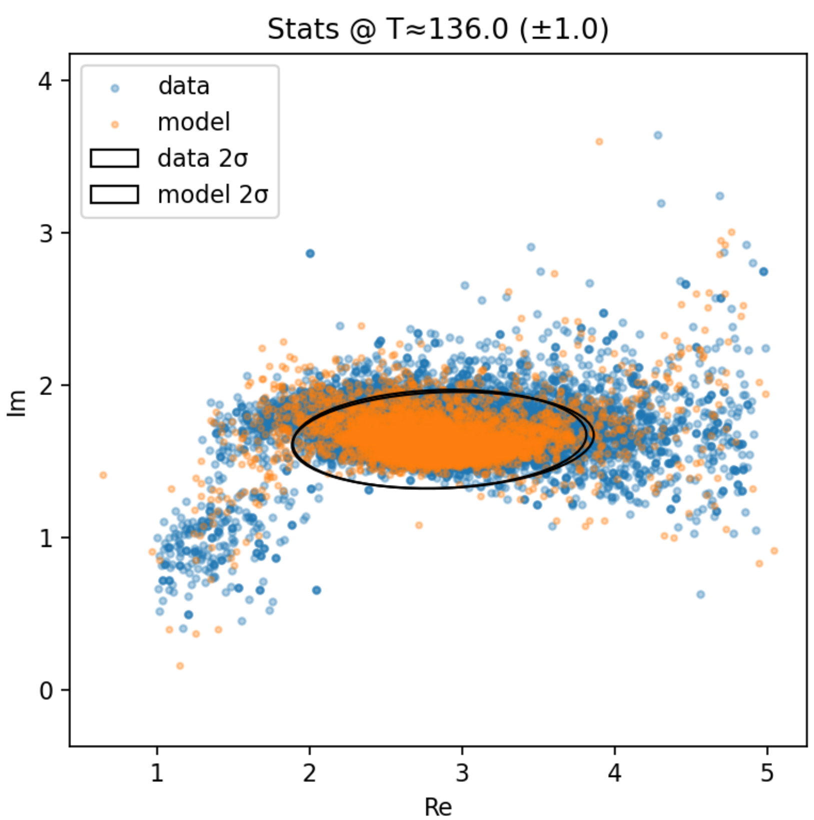
Likelihood Calibration

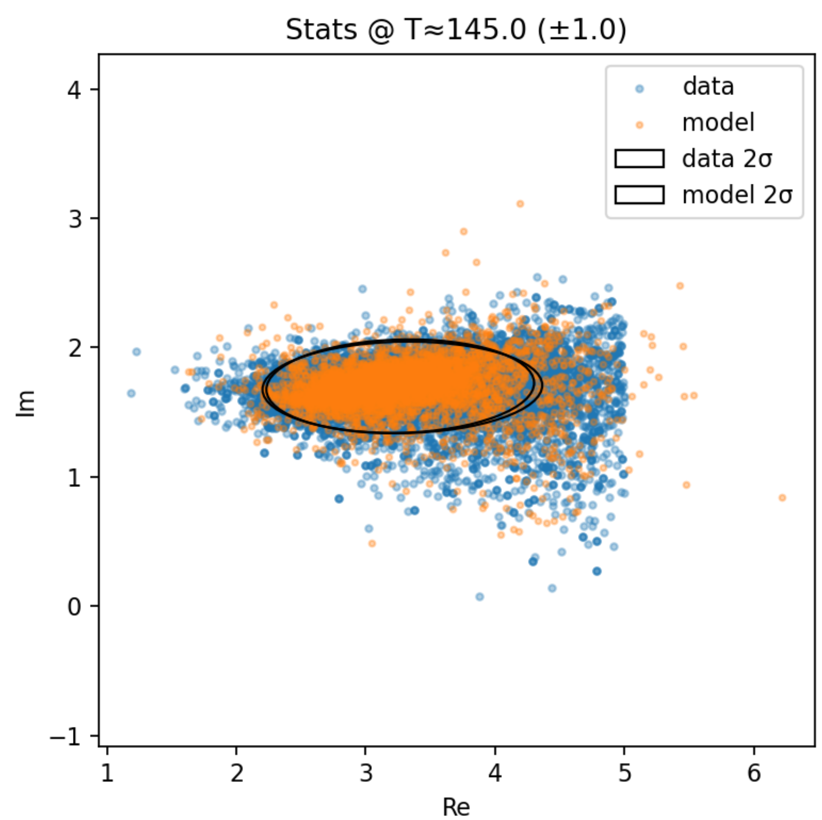
- Next, we look at the post-hoc negative log-likelihood distribution for both training-like and validation-like samples.
- The excellent overlap demonstrates that the model is not overfitting, and the likelihood calibration is robust.

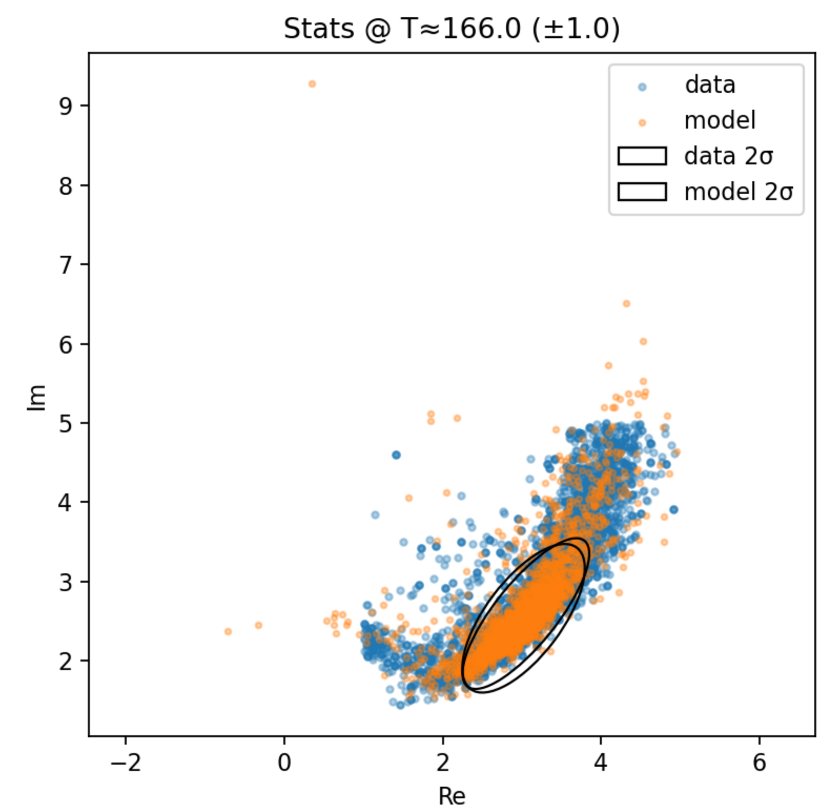


Model vs Data: Pole Distributions

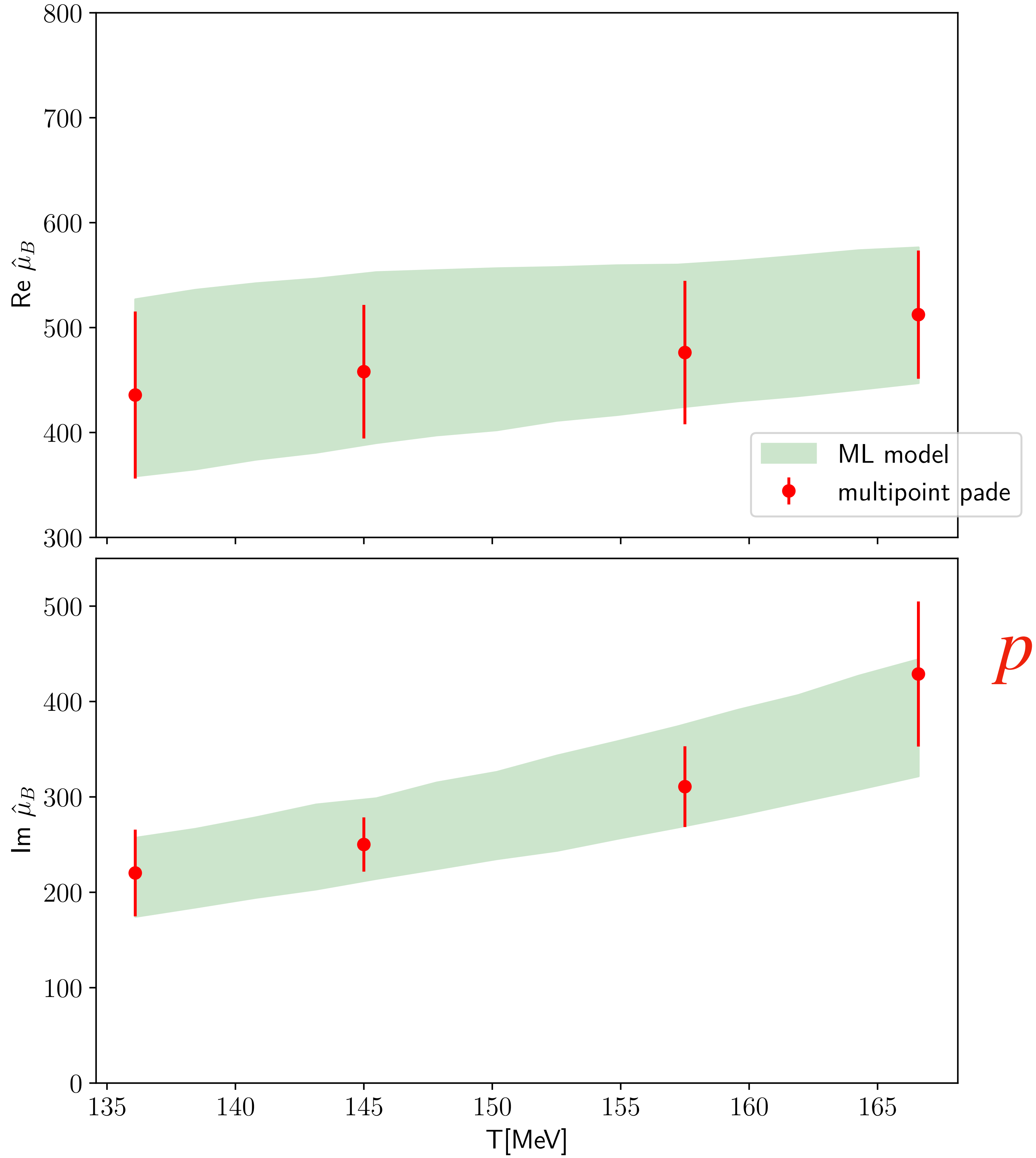
- Now we compare the pole distributions learned by the model (orange) with the original bootstrap data (blue) at different temperatures.
- The ellipses represent the 2σ contours.
- We see that across a wide range of T, the model reproduces both the shape and spread of the pole clouds.
- At lower T, the distribution tends to broaden and shift, and the model captures this smoothly.







Machine learning model for the LYEs



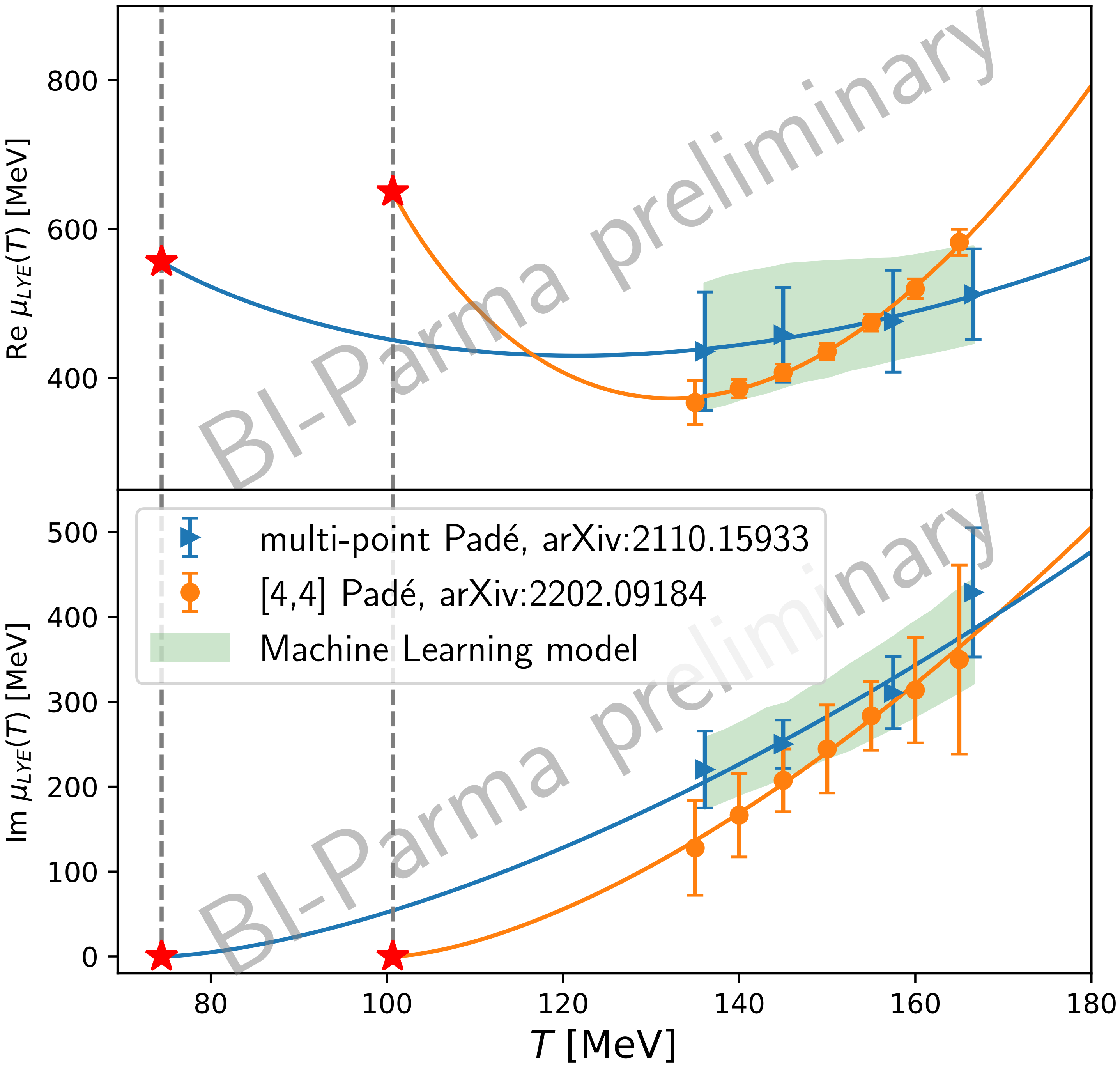
MADE : masked auto encoder for density estimation.

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

$$p(\mathrm{Re}\ \hat{\mu}_\mathrm{B}, \mathrm{Im}\ \ \hat{\mu}_\mathrm{B} \,|\, \mathrm{T}, \mathrm{m_l}, \mathrm{N}_\sigma)$$

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,

LYEs with many unknown parameters,

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

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

Summary and Outlook

- We discuss the analytic structure of fermi gas and QCD at finite temperature and chemical potentials with Taylor expansions and Pade approximations.
- We also show how [4,4] pade constructed from a eight order Taylor expansion shows a trend for the poles to go to the real axis at low temperatures.
- Furthermore we show that these singularities obtained from [4,4] pade is consistent with expected Lee yang edge singularities and fall on the similar scaling as obtained from the multi point pade poles.
- We also explain how to learn density estimation of real and imaginary distribution of poles using a neural network.

Thank you for your attention!!

Useful Formulas

$$\Delta P/T^4 = \sum_{k=1}^{4} P_{2k}(T)\hat{\mu}_B^{2k} = (\bar{x}^2 + \bar{x}^4 + c_{6,2}\bar{x}^6 + c_{8,2}\bar{x}^8)P^2/P_4,\ \bar{x} = \sqrt{\frac{P_4}{P_2}}\ \hat{\mu}_B$$

Reminder : P_2 and P_4 are strictly positive for all temperatures.

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