Exploring the QCD phase diagram with Taylor expansion and analytic continuation

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Faculty of Physics

CRC-TR 211
Strong-interaction matter under extreme conditions

DFG

EuroPLEx
H2020

HotQCD Collaboration, Phys.Rev.D 101 (2020) 7, 074502 and work in progress

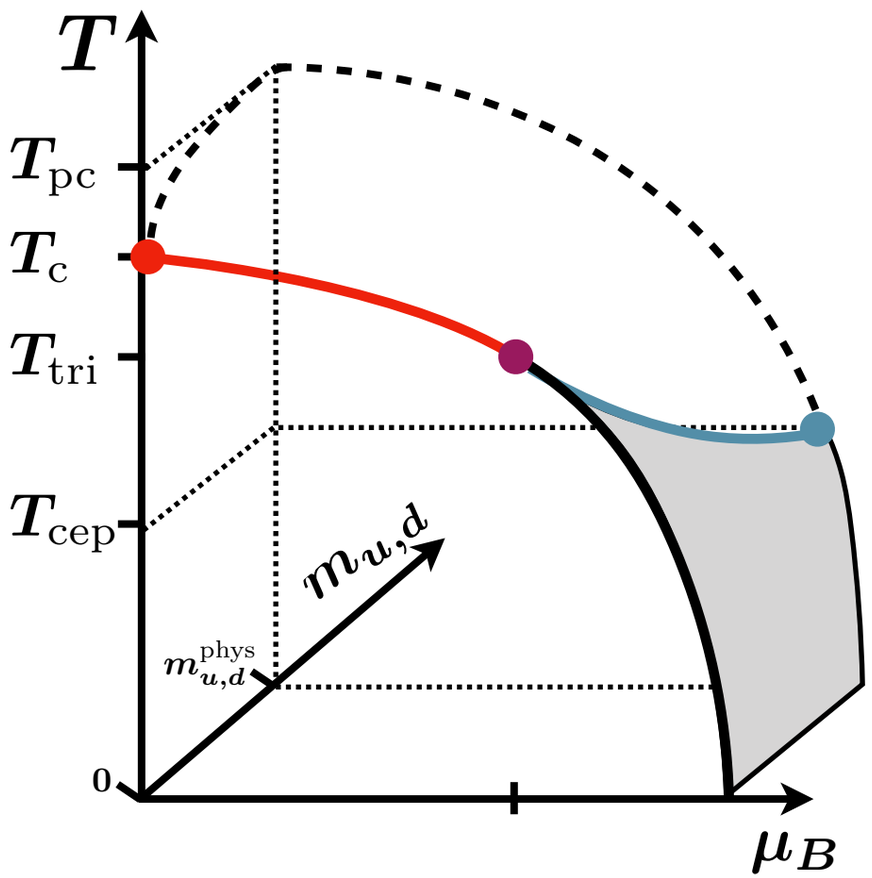
A. Bazavov, D. Bollweg, H.-T. Ding, P. Enns, J. Goswami, P. Hegde, O. Kaczmarek, F. Karsch, A. Lahiri, R. Larsen, S.-T. Li, Swagato Mukherjee, H. Ohno, P. Petreczky, C. Schmidt, S. Sharma, P. Steinbrecher

Bielefeld-Parma Collaboration, arXiv: 2101.02254 and work in Progress

P. Dimopoulos, F. Di Renzo, J. Goswami, G. Nicotra, C. Schmidt, S. Singh, K. Zambello, F. Ziesché

Exploring High-μ_B Probes with rare Probes, ECT*, Oct 11-15, 2021

Motivation: The QCD Phase diagram



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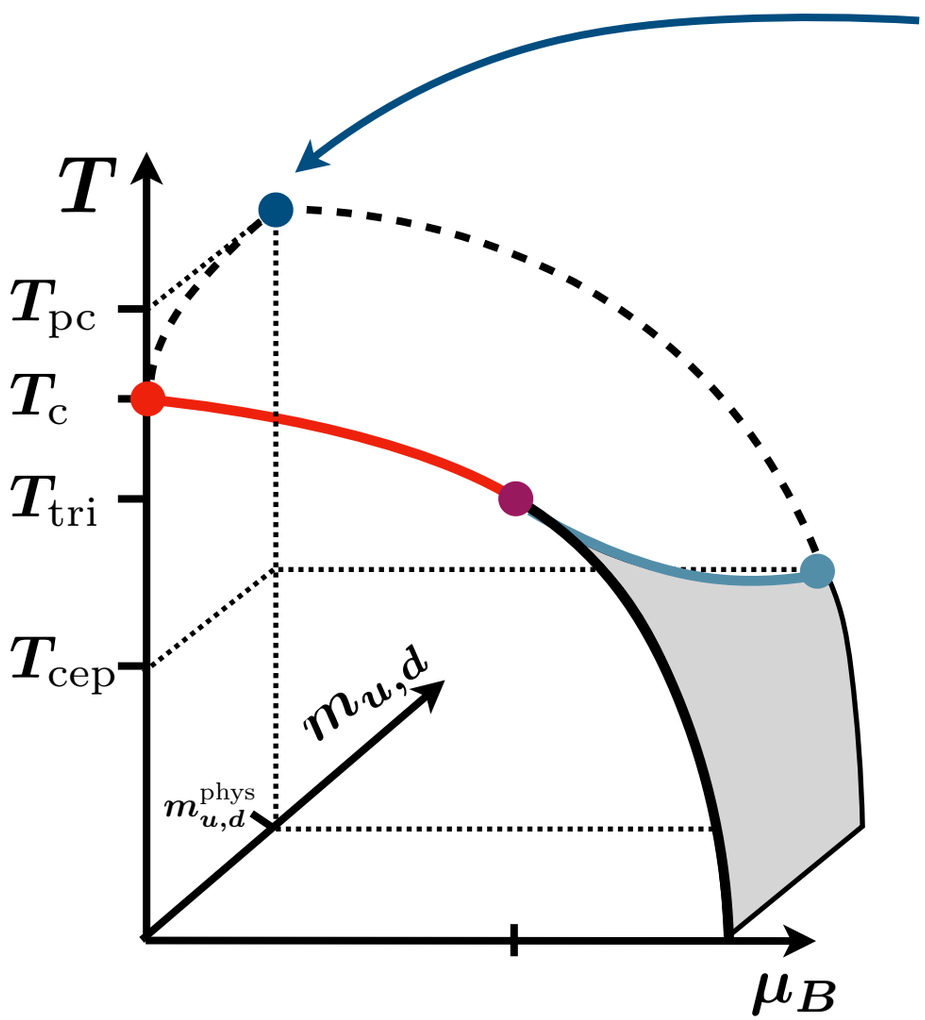

- Precise determination of the QCD transition temperature $T_{\rm pc} = 156.5 \pm 1.5$ MeV

HotQCD: PLB 795 (2019) 15

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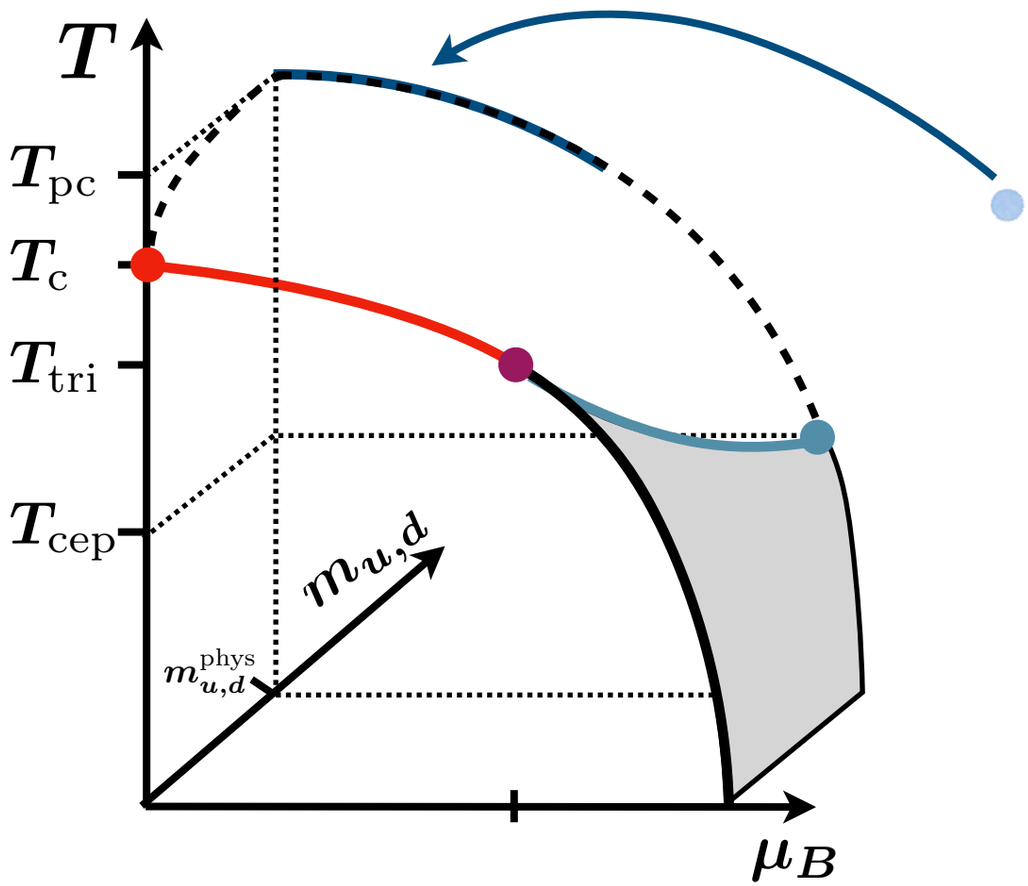

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HotQCD: PLB 795 (2019) 15

- The chiral crossover line with respect to μ_B

$$T_{\rm pc}(\mu_B) = T_{\rm pc}^0 \left(1 - \kappa_2^{B,f} \left(\frac{\mu_B}{T_{\rm pc}^0} \right)^2 - \kappa_4^{B,f} \left(\frac{\mu_B}{T_{\rm pc}^0} \right)^4 \right)$$

$$\kappa_2^{B,f} = 0.012(4), \quad \kappa_4^{B,f} = 0.00(4)$$

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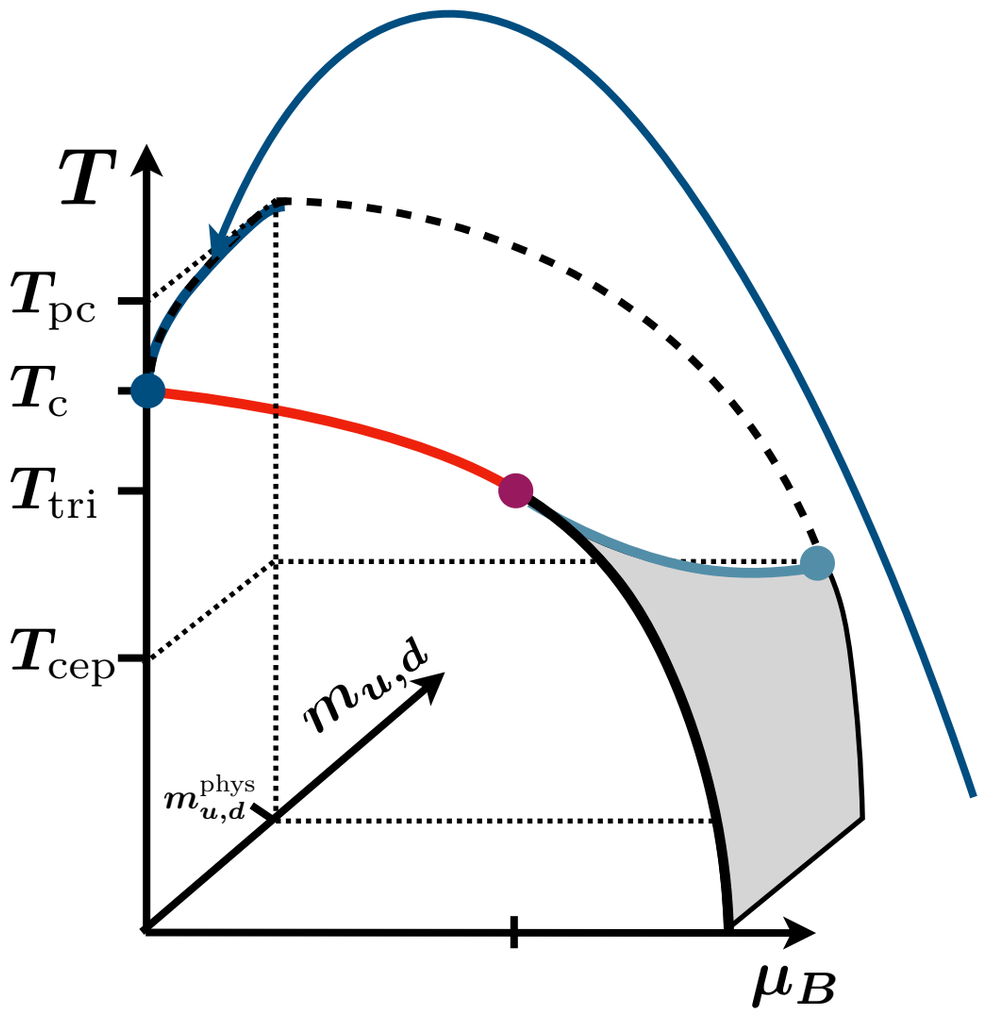

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HotQCD: PLB 795 (2019) 15

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HotQCD: PRL 123 (2019) 062002

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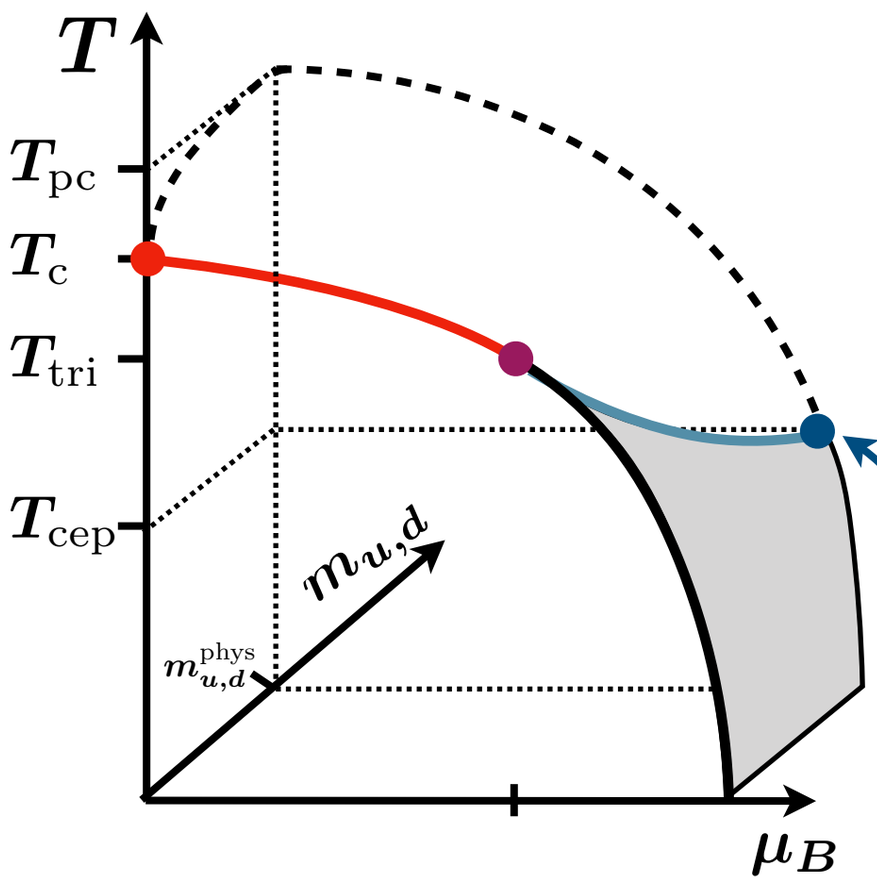

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- Expected bounds on the QCD critical end-point

$$T_{\rm cep} < T_{\rm c} = 132^{+3}_{-6} \text{ MeV}$$

$$\mu_B^{\rm cep} \gtrsim 3\, T_c$$

Universal behaviour

- Universal critical behaviour guides our thinking on the QCD phase diagram. Often considered in the vicinity of the chiral critical point.

$$\frac{p}{T^4} = \frac{1}{VT^3} \ln Z(V,T,\vec{\mu}) = -h^{(2-\alpha)/\beta\delta} f_f(z) - f_r(V,T,\vec{\mu})$$

Universal scaling function

Effective model O(4)/O(2)/Z(2):

- 3 relevant scaling fields
  - t reduced temperature
  - h reduced symmetry breaking field
  - L^{-1} inverse system size

map QCD to the effective model

controlled by non-universal parameter:

t_0, h_0, l_0
T_c, H_c, κ_2^B

(2+1)-flavor QCD:

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

$$h = \frac{1}{h_0}(H - H_c), \quad H = \frac{m_l}{m_s}$$

$$l = l_0 L^{-1}$$

κ_2^B

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Universal scaling function

- We can calculate derivatives of $\ln Z$. Singular behaviour is characteristic to the universality class. E.g. here: O(4)

O(4)-critical exponents:

$$\alpha = -0.21$$
$$\beta = -0.38$$
$$\delta = 4.82$$

	Magnetic	Mixed	Thermal
	$\frac{\partial^2 \ln Z}{\partial h^2}$	$\frac{\partial^2 \ln Z}{\partial h\, \partial t}$	$\frac{\partial^2 \ln Z}{\partial t^2}$
	$\sim \left(\frac{m_l}{m_s}\right)^{1/\delta - 1}$	$\sim \left(\frac{m_l}{m_s}\right)^{(\beta-1)/\beta\delta}$	$\sim \left(\frac{m_l}{m_s}\right)^{-\alpha/\beta\delta}$
	$\sim \left(\frac{m_l}{m_s}\right)^{-0.79}$	$\sim \left(\frac{m_l}{m_s}\right)^{-0.34}$	$\sim \left(\frac{m_l}{m_s}\right)^{+0.11}$
Divergence:	**strong**	**moderate**	**none**

Pseudocritical Temperature

- **The order parameter:** RG invariant combination of light and strange chiral condensate

$$M \sim \frac{\partial f}{\partial H}$$

$$M = 2\left(m_s \langle\bar{\psi}\psi\rangle_l - m_l \langle\bar{\psi}\psi\rangle_s\right)/f_K^4$$

with $\langle\bar{\psi}\psi\rangle_l = \left(\langle\bar{\psi}\psi\rangle_u + \langle\bar{\psi}\psi\rangle_d\right)/2$

$\Rightarrow$ use $f_K = 156.1(9)/\sqrt{2}\ \mathrm{MeV}$

- **The susceptibility:** RG-invariant chiral susceptibility

$$\chi_M \sim \frac{\partial^2 f}{\partial H^2}$$

$$\chi_M = m_s(\partial m_u + \partial m_d)M|_{m_u=m_d}$$
$$= m_s\left(m_s\chi_l - 2\langle\bar{\psi}\psi\rangle_s - 4m_l\chi_{su}\right)/f_K^4$$

with $\chi_{fg} = \partial_{m_f}\langle\bar{\psi}\psi\rangle_g$

and $\chi_l = 2\left(\chi_{uu} + \chi_{ud}\right)$

- **Scaling functions and scaling variables:** Critical point at $(z, z_L) = (0, 0)$

$$M = h^{1/\delta} f_G(z, z_L) + f_{\mathrm{sub}}(T, H, L)$$

$$\chi_M = h_0^{-1} h^{1/\delta - 1} f_\chi(z, z_L) + \tilde{f}_{\mathrm{sub}}(T, H, L)$$

$$z = t/h^{1/\beta\delta}$$

$$z_L = l_0/(L h^{\nu/\beta\delta})$$

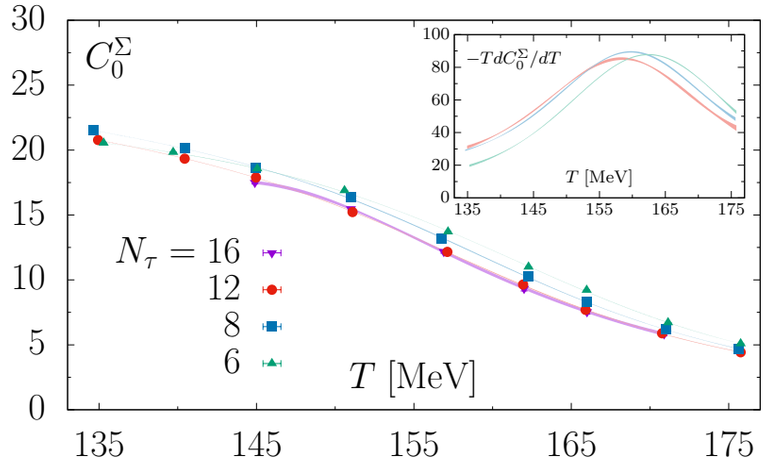
Known from the universality class

Contains corrections to scaling and regular terms

Two scaling variables

Pseudocritical Temperature

$$M \sim \frac{\partial f}{\partial H}$$



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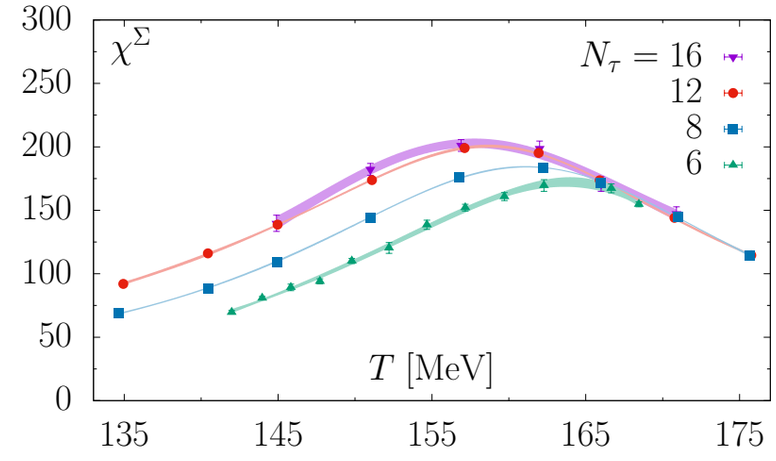
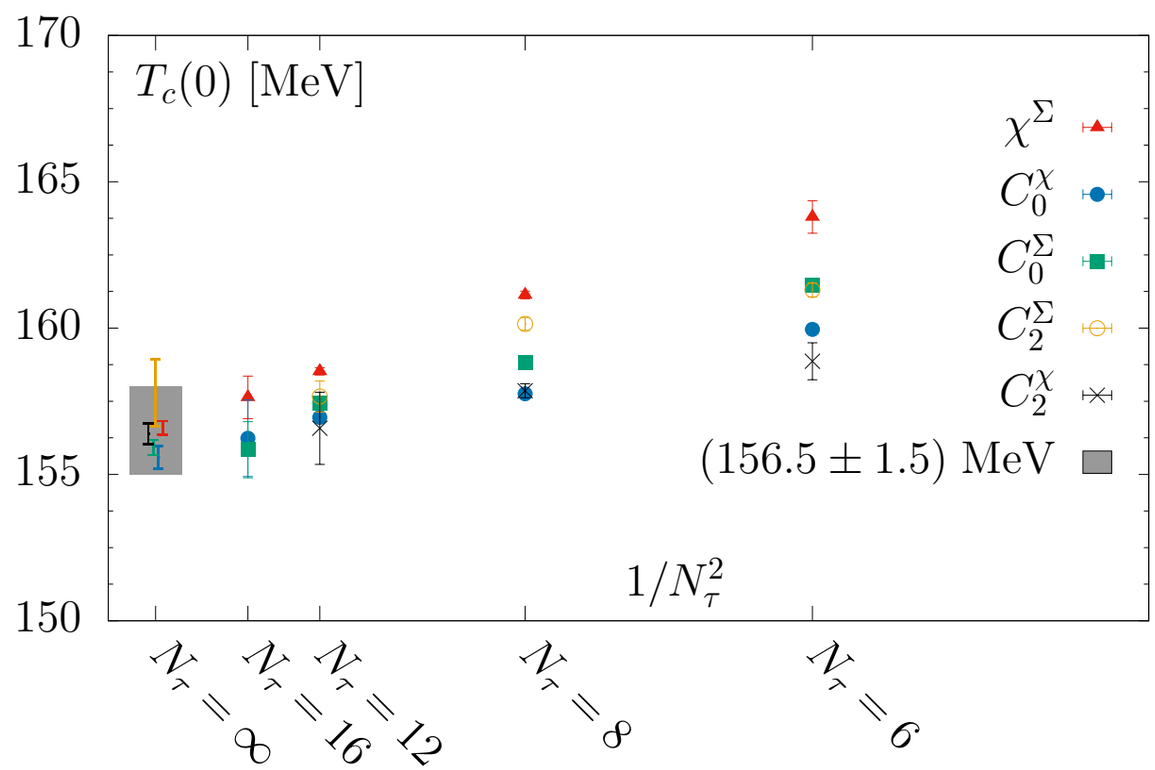
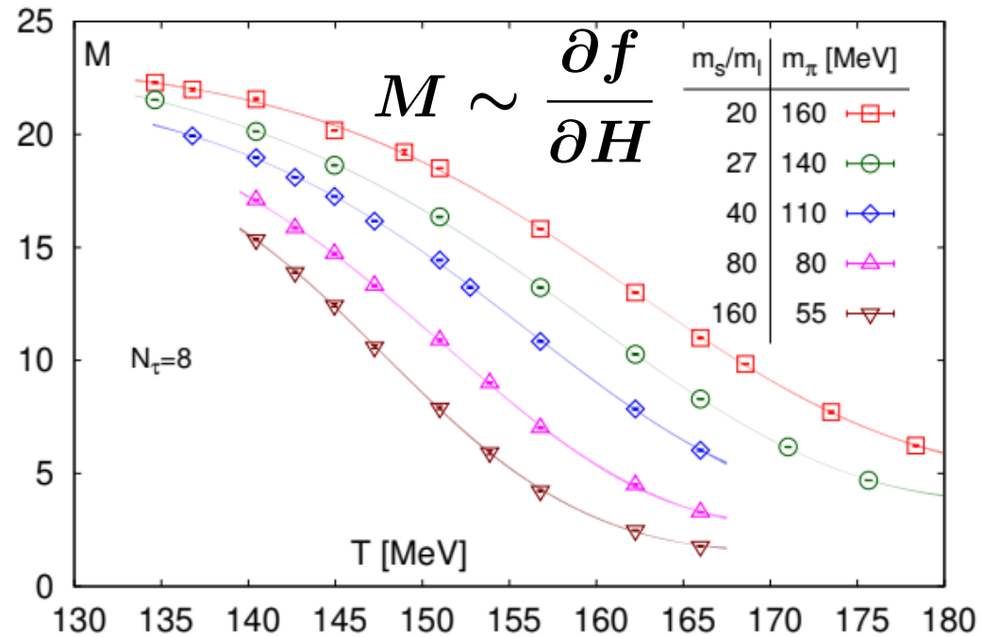




- Transition is a crossover, various definitions of T_{pc} do not need to agree
- Study 5 different definitions and perform continuum limit
- Find good agreement in the continuum limit: $T_{pc} = 156.5\ (1.5)$ MeV

A. Bazavov et al [HotQCD], Phys. Lett. B795, 15 (2019), arXiv:1812.08235

Critical Temperature (chiral limit)



Magnetic susceptibility

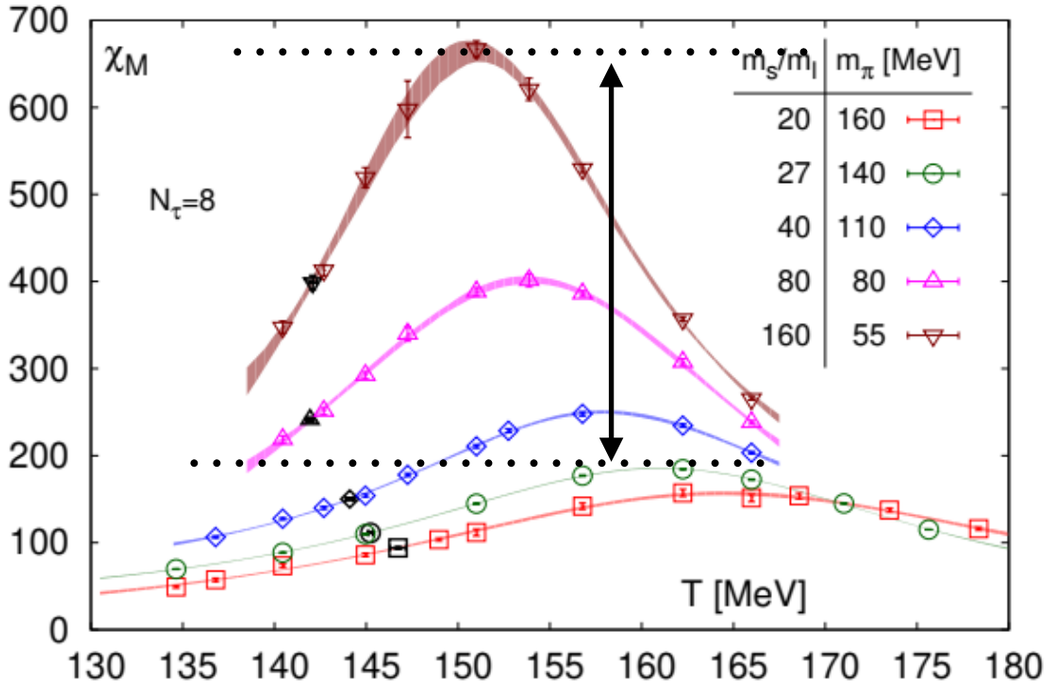
$$\sim \left(\frac{m_l}{m_s}\right)^{-0.79}$$

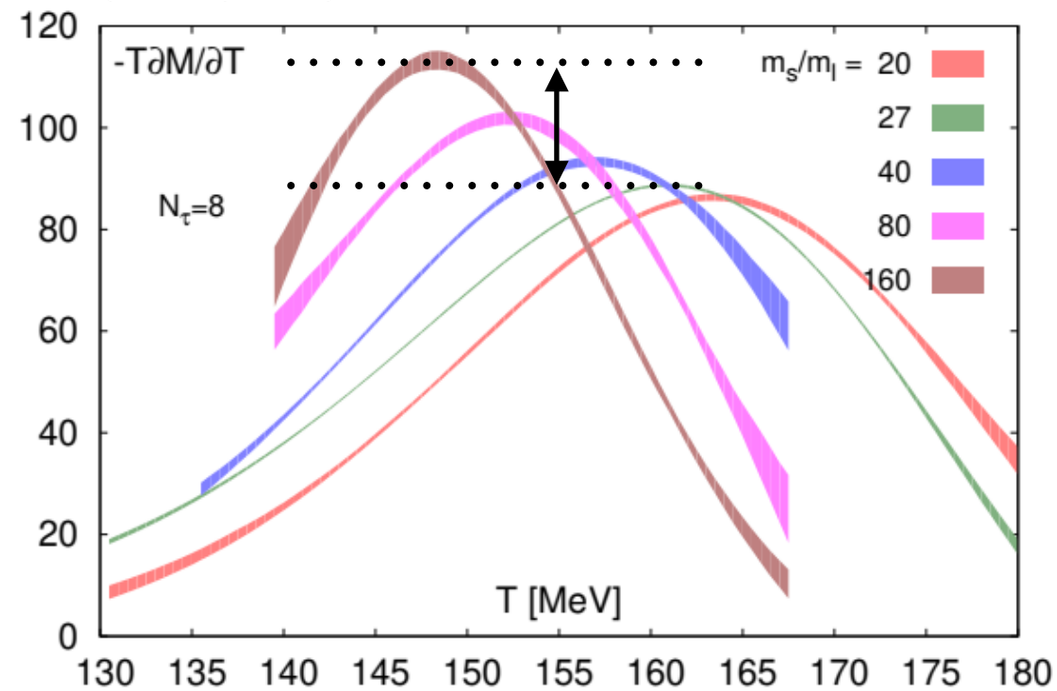
$$(160/27)^{0.79} \approx 4$$

Mixed susceptibility

$$\sim \left(\frac{m_l}{m_s}\right)^{-0.34}$$

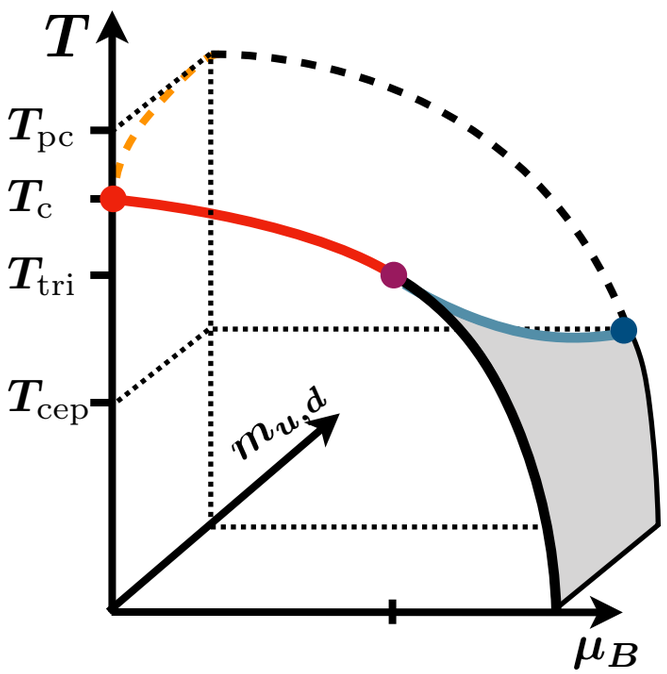
$$(160/27)^{0.34} \approx 1.8$$



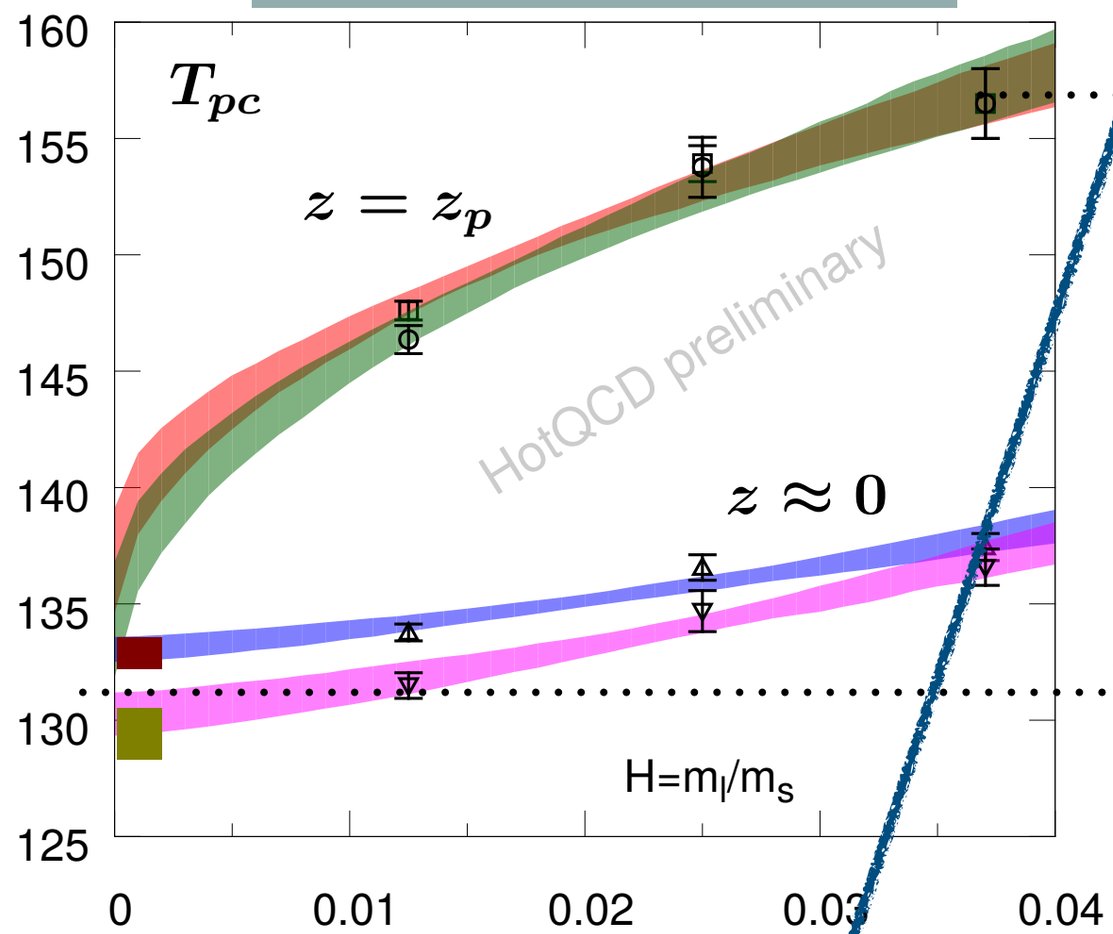


H.T. Ding et al. (HotQCD), PRL 123 (2019) 15, arXiv:1903.04801

Critical Temperature



A. Lahiri et al, arXiv:2010:1559



$\Delta T = 25$ MeV

Chiral extrapolations:

$T_c^0 = 132^{+3}_{-6}$ MeV

H.T. Ding et al. (HotQCD), PRL 123 (2019) 15, arXiv:1903.04801

Physical masses:

$T_{pc} 156.5\ (1.5)$ MeV

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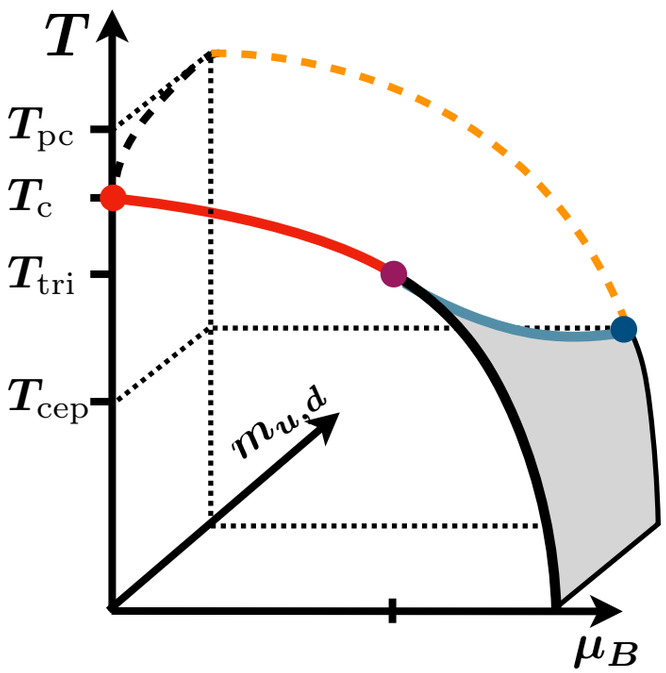
Pseudocritical Temperature at nonzero μ_B



- Consider a μ_B-dependent shift of the peak of the susceptiblities. Defining conditions are thus

$$\left.\frac{\partial^2 M(T,\mu_B)}{\partial T^2}\right|_{\mu_B} = 0 \qquad \text{or} \qquad \left.\frac{\partial \chi_M(T,\mu_B)}{\partial T}\right|_{\mu_B} = 0$$

- The condition lead to equations for κ_2, κ_4

$$T_{\rm pc}(\mu_B) = T^0_{\rm pc}\left(1 - \kappa_2^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^2 - \kappa_4^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^4\right)$$

$$\kappa_2^{B,f} = 0.012(4), \quad \kappa_4^{B,f} = 0.00(4)$$

- Universal scaling relates derivatives of M

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

$$\kappa_2 \sim \frac{T^2\partial^2 M/\partial\mu_B}{2T\partial M/\partial T}$$

Karsch et al, arXiv:1009.5211

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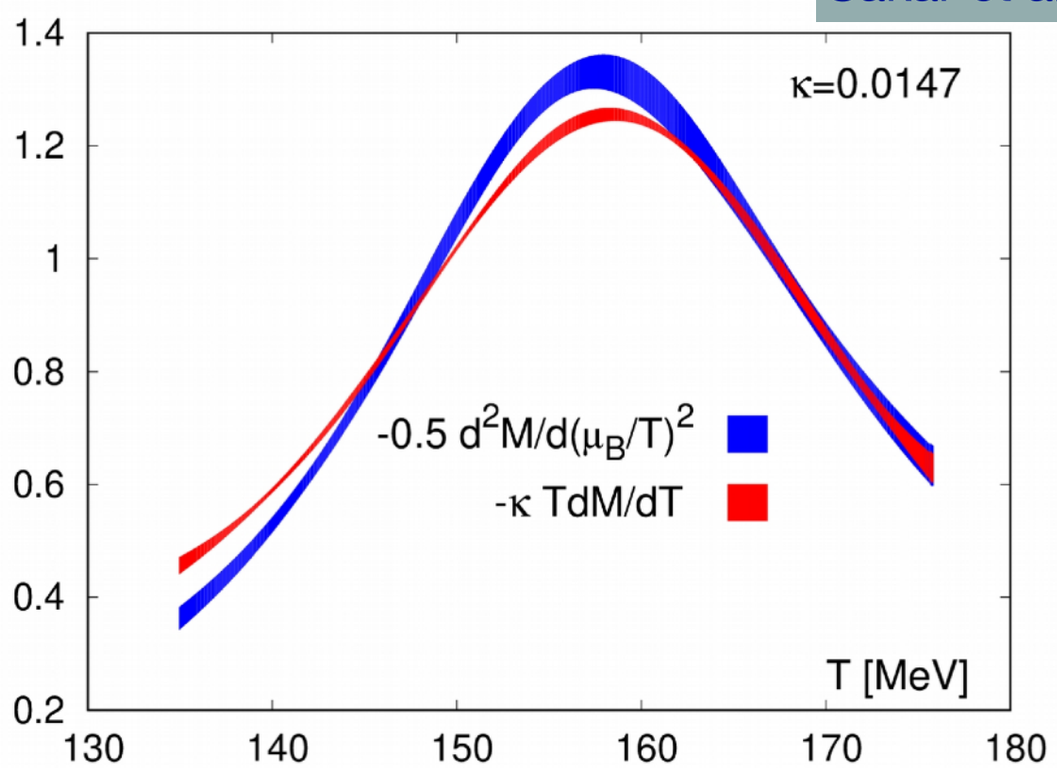
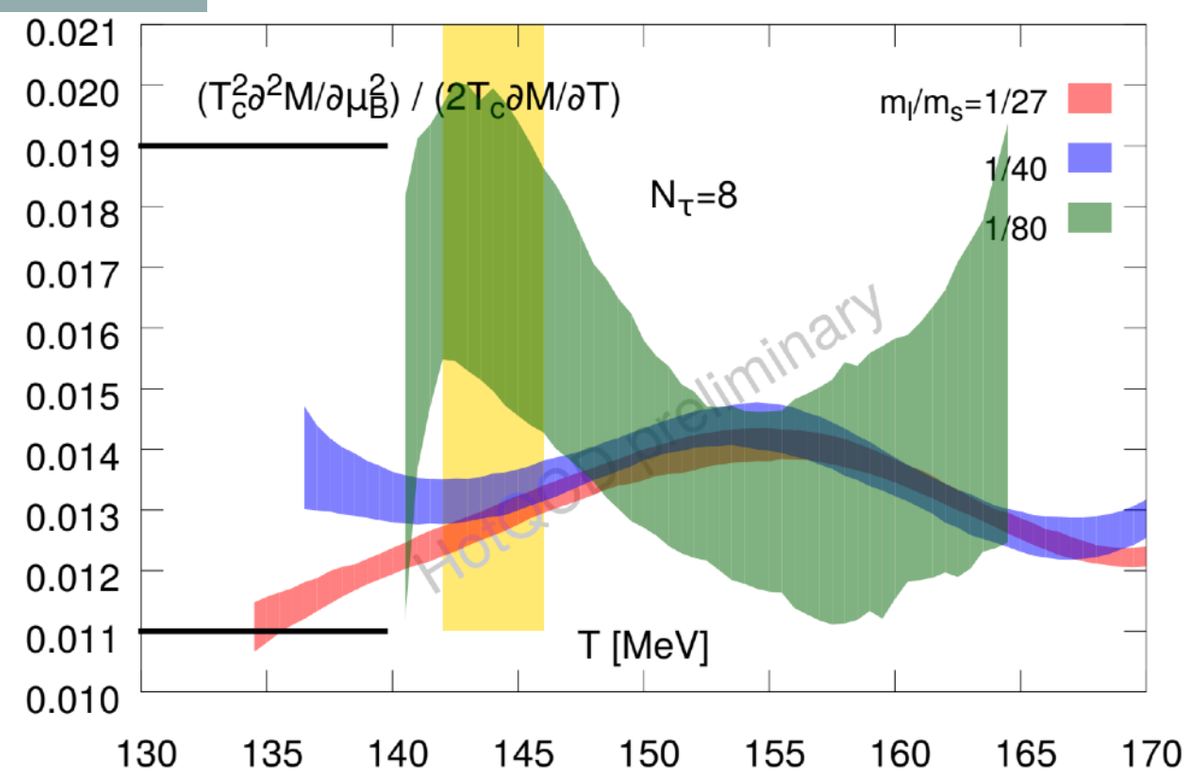
Karsch et al, arXiv:1009.5211

Sakar et al, Lattice 2021

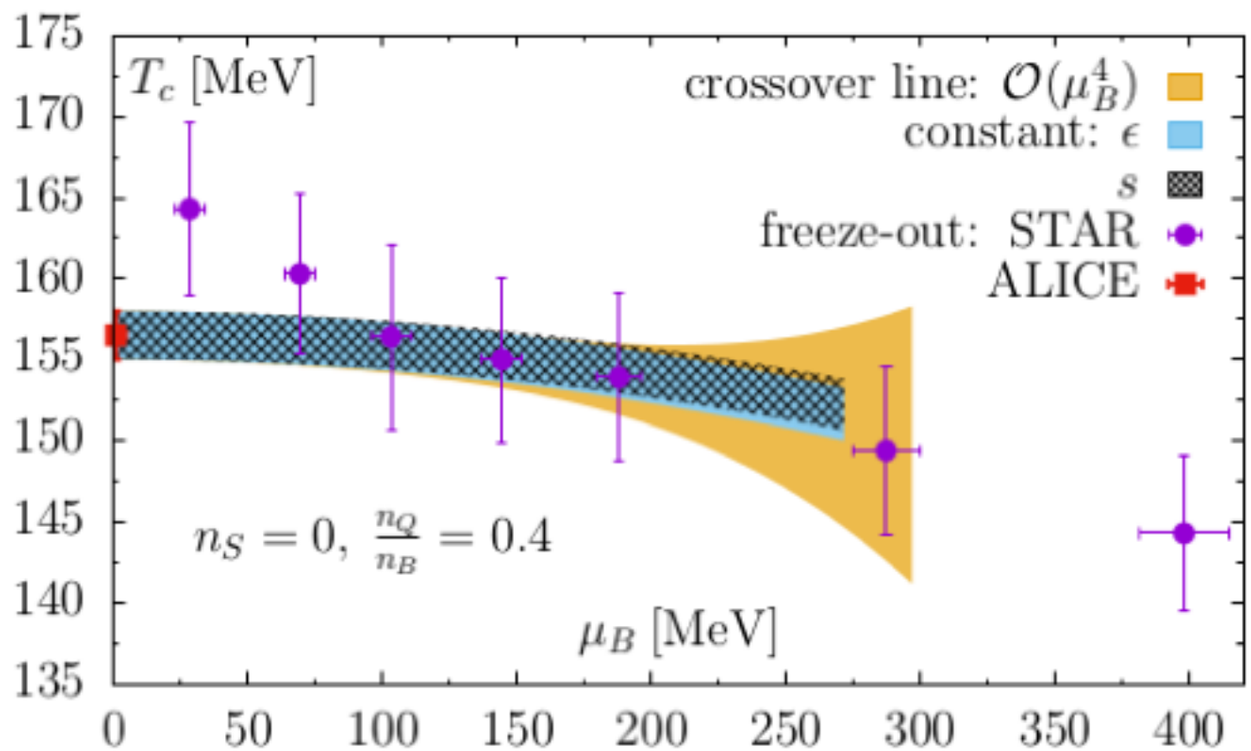




- Curvature of the pseudo critical line depends only mildly on H

Freeze-out line

$$T_{\rm pc}(\mu_B) = T^0_{\rm pc}\left(1 - \kappa_2^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^2 - \kappa_4^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^4\right)$$



STAR: arXiv:1701.07065

A. Andronic et al., Nature 561 (2018) 321

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$\kappa_2 = 0.012(4)$
$\kappa_4 = 0.00(4)$

A. Bazavov et al [HotQCD], Phys. Lett. B795, 15 (2019), arXiv:1812.08235

T_{pc} 158.0 (0.6) MeV
$\kappa_2 = 0.0153(18)$
$\kappa_4 = 0.00032(67)$

S. Borsanyi et al, arXiv: 2002.02821

The Taylor expansion method

- Compute expansion coefficients of the pressure

$$\frac{p}{T^4} = \frac{\ln Z}{T^3 V} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk,0}^{BQS} \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

Gavai, Gupta (2001)
Bielefeld-Swansea (2002)

Cumulants of conserved charge fluctuations, can also be measured as event-by-event fluctuations in heavy ion collisions

$$\chi_{ijk,0}^{BQS} = \frac{\partial^i}{\partial(\mu_B/T)} \frac{\partial^j}{\partial(\mu_Q/T)} \frac{\partial^k}{\partial(\mu_S/T)} \frac{\ln Z}{T^3 V}$$

$\Rightarrow$ A comparison with experimental data constrain freeze-out parameter

Net baryon number fluctuations diverge at the critical point

$\Rightarrow$ Search for the critical point

Cumulant ratios of conserved charge fluctuations

- Combine quark number fluctuations (χ_{ijk}^{uds}) to obtain hadronic fluctuations (χ_{ijk}^{BQS}).
- Determine strangeness (μ_S/T) and electric charge chemical (μ_Q/T) potentials by imposing strangeness neutrality $n_S = 0$ and $n_Q/n_B = 0.4$ (order by order in the expansion).
- From the pressure expansion we readily obtain the expansions for the nth-order cumulants:

$$\chi_n^B(T,\mu_B) = \sum_{k=0}^{k_{\max}} \tilde{\chi}_n^{B,k}(T)\hat{\mu}_B^k, \quad \text{with} \quad \hat{\mu}_B = \mu_B/T$$

- Define ratios to eliminate the leading order volume dependence

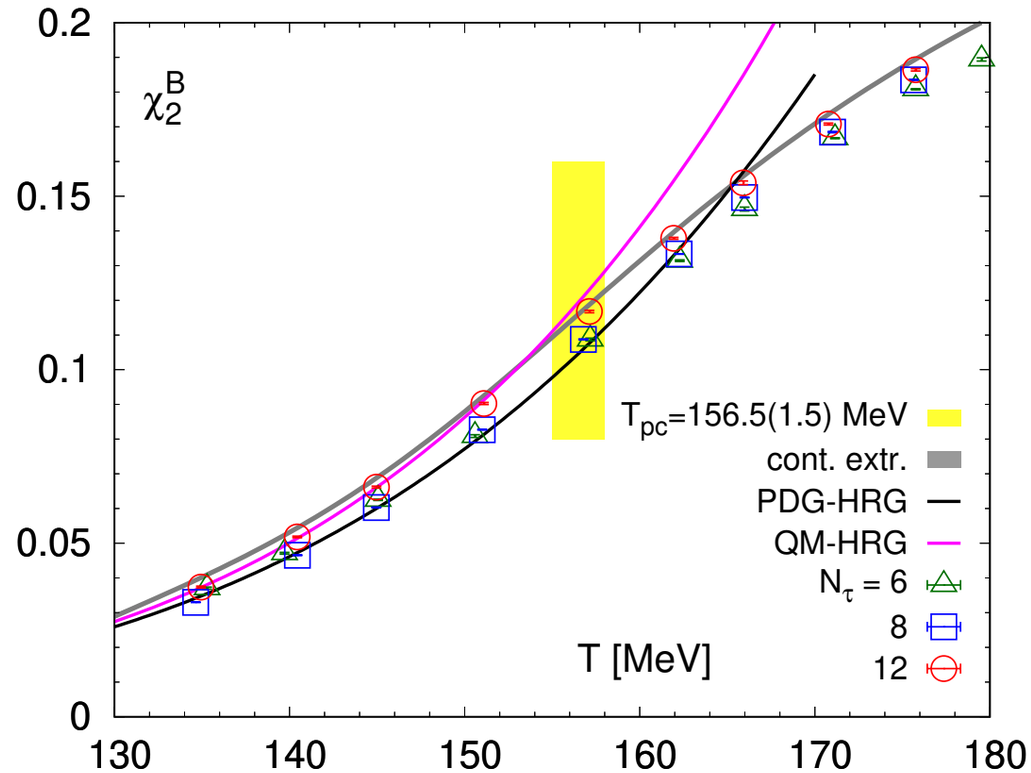
$$R_{nm}^B = \frac{\chi_n^B(T,\mu_B)}{\chi_m^B(T,\, mu_B)} = \frac{\sum_{k=0}^{k_{\max}} \tilde{\chi}_n^{B,k}(T)\hat{\mu}_B^k}{\sum_{l=0}^{l_{\max}} \tilde{\chi}_m^{B,l}(T)\hat{\mu}_B^l}$$

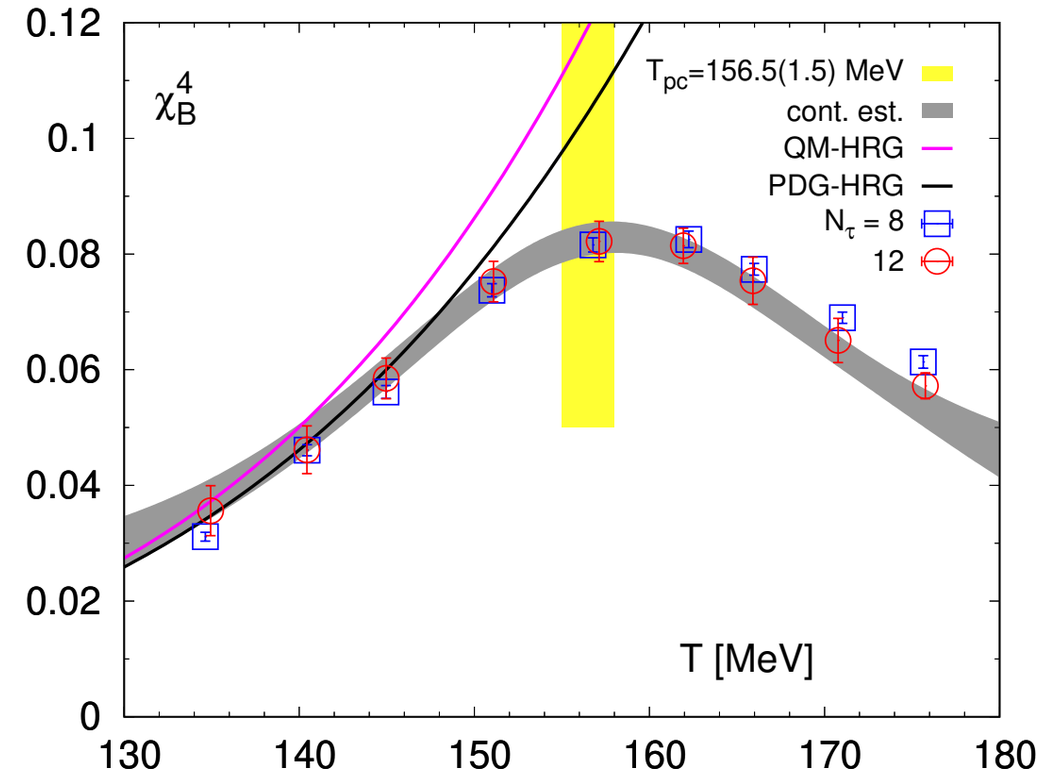
- In terms of the shape parameters of the distribution we find

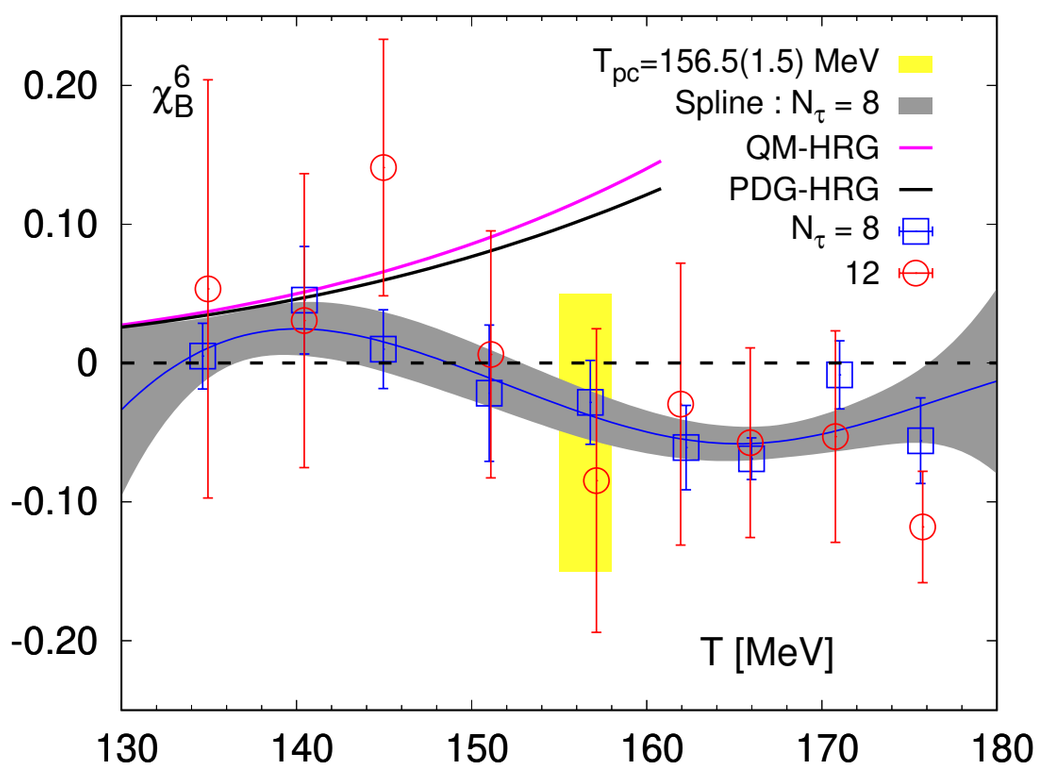
$$R_{12} = M/\sigma^2,\ R_{31} = S\sigma^3/M,\ R_{32} = S\sigma,\ R_{42} = \kappa\sigma^2,\ \ldots$$

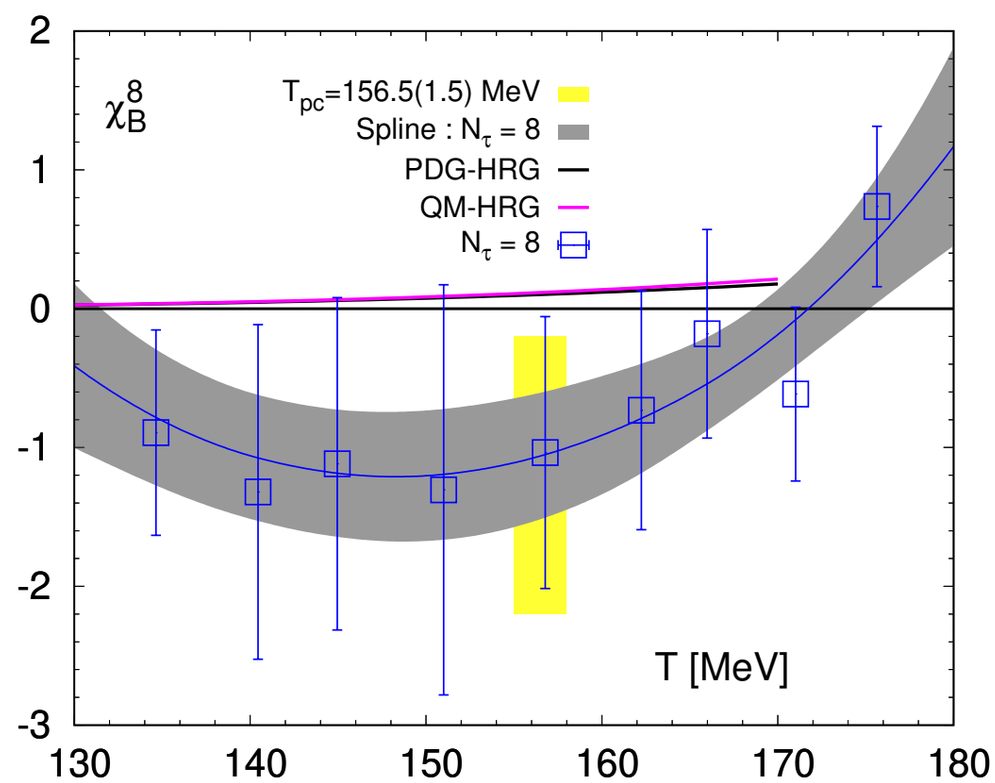
- Eventually we want calculate observables along the crossover (and freeze-out) line, we thus need spline interpolations of our data at discrete temperature values.

The expansion coefficients of the pressure

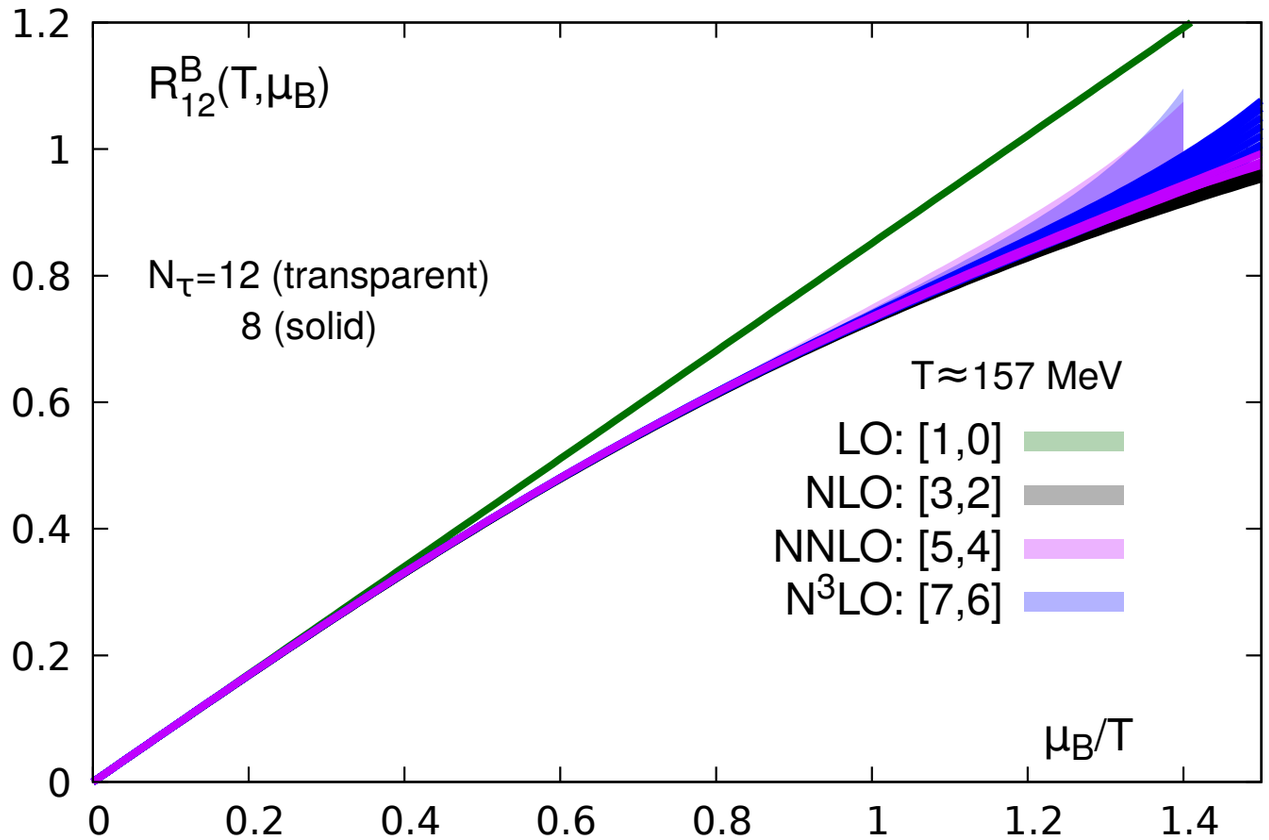








Results: The net baryon-number density R_{12}^B



- Cut-off effects are negligible for $\mu_B/T \leq 1$ and of the same order as the statistical error at $N_\tau = 12$ for $\mu_B/T \leq 1.2$.

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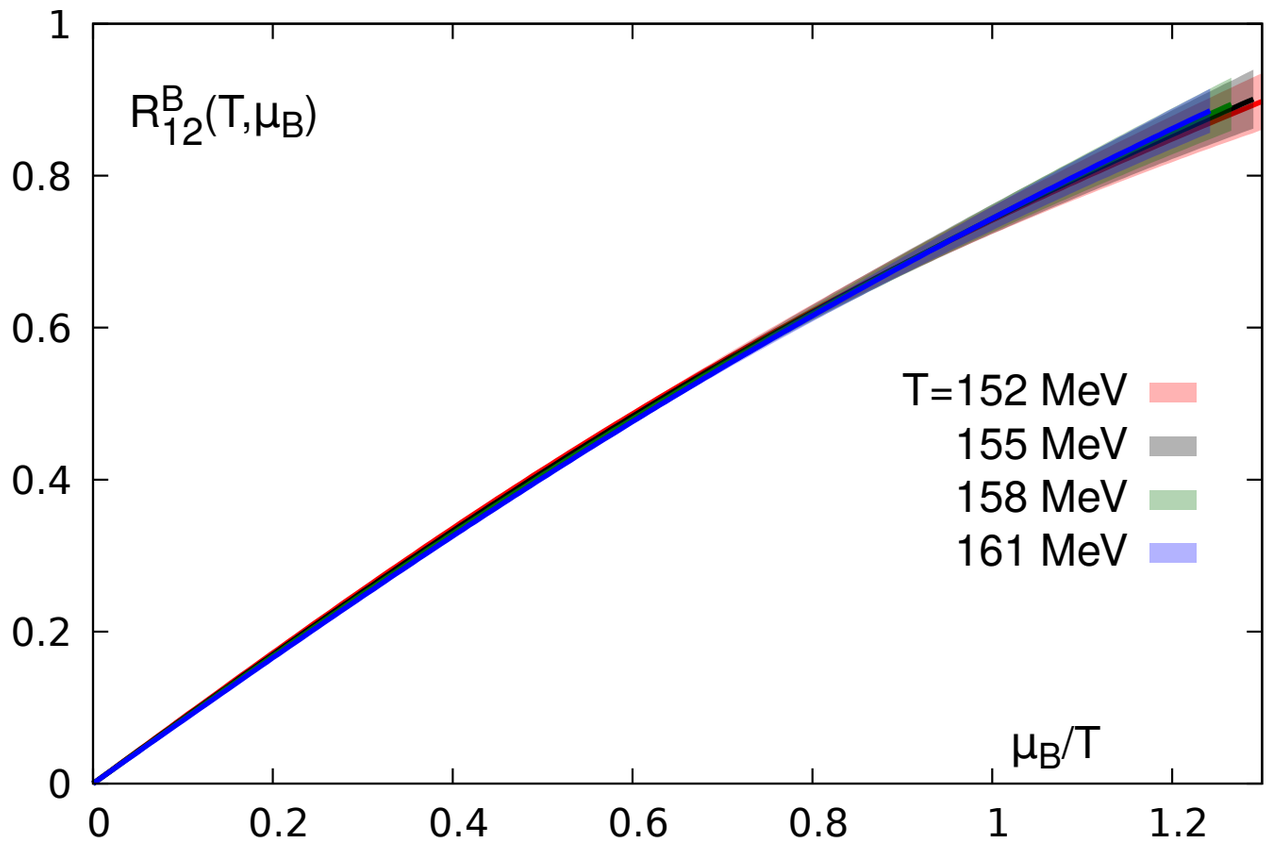

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- Temperature dependence is very mild. The curvature of the freeze-out line varies the temperature by less than 3 MeV.

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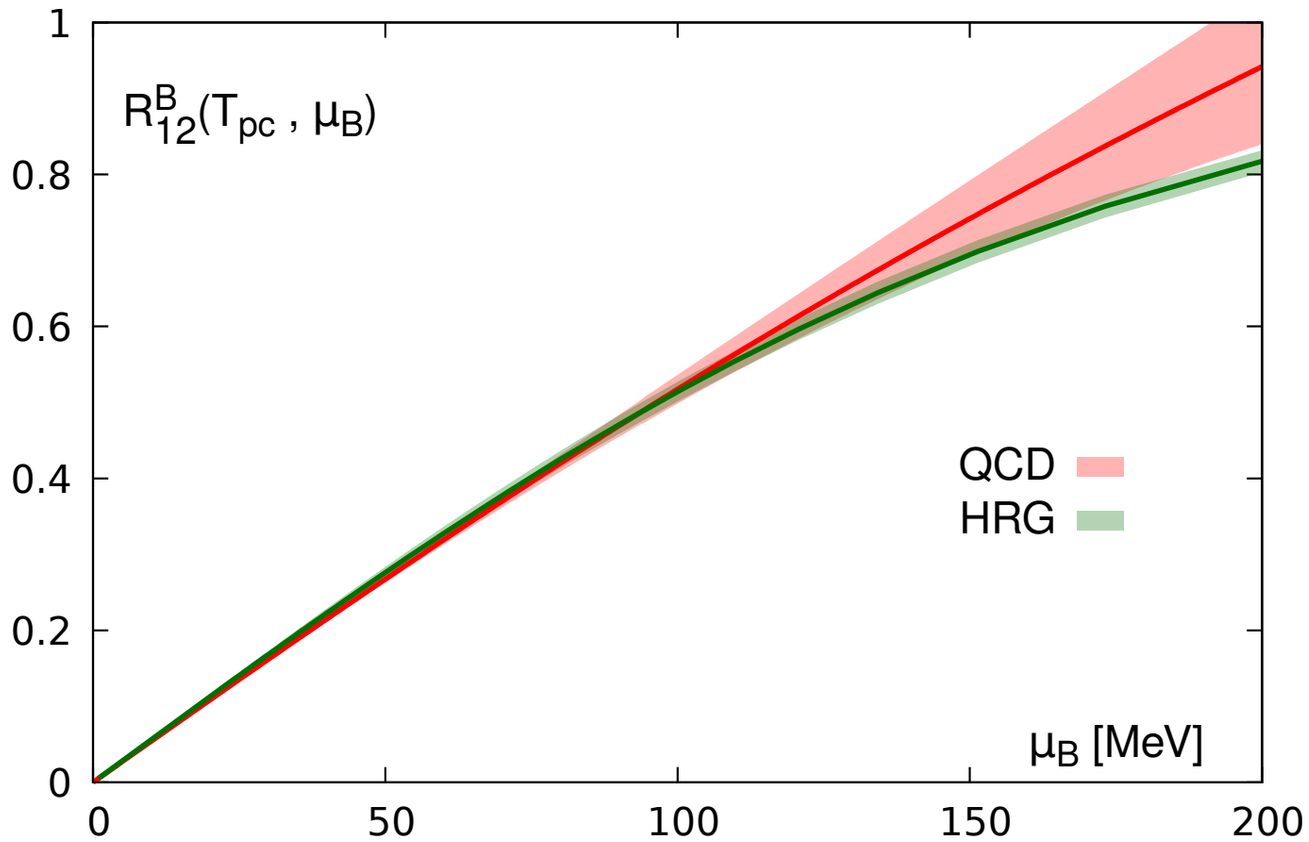

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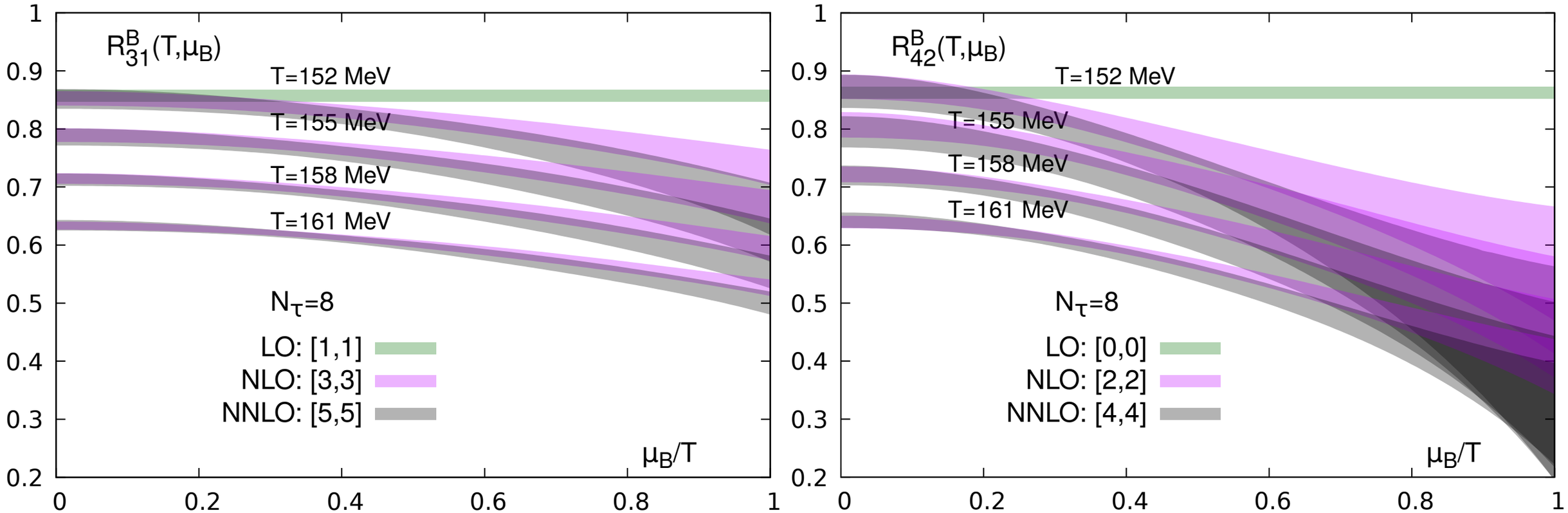
- Temperature dependence is very mild. The curvature of the freeze-out line varies the temperature by less than 3 MeV.
- Continuum extrapolation along the freeze-out line: good agreement with HRG (PDG+QM) up to $\mu_B \leq 120\ \mathrm{MeV}$

Results: Skewness and kurtosis

- Skewness and kurtosis ratios R_{31}^B and R_{42}^B on ($N_\tau = 8$)-lattices

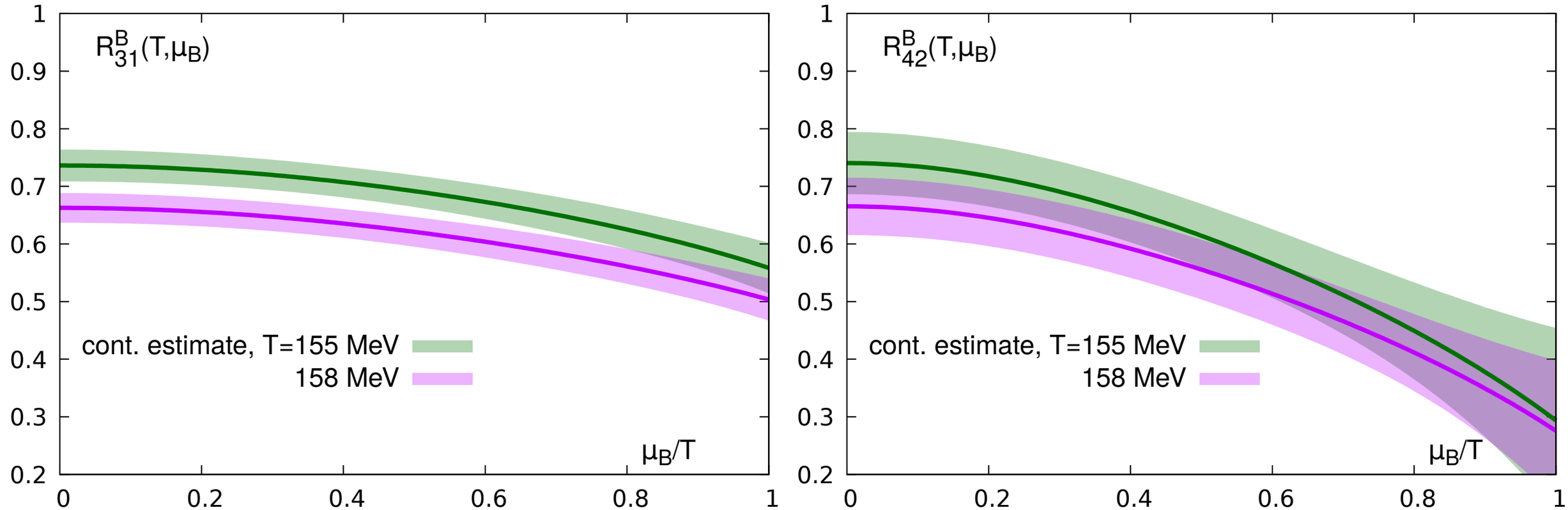


- Convergence gets worth with increasing order of the cumulant and with decreasing temperature.

- NLO and NNLO corrections are negative.

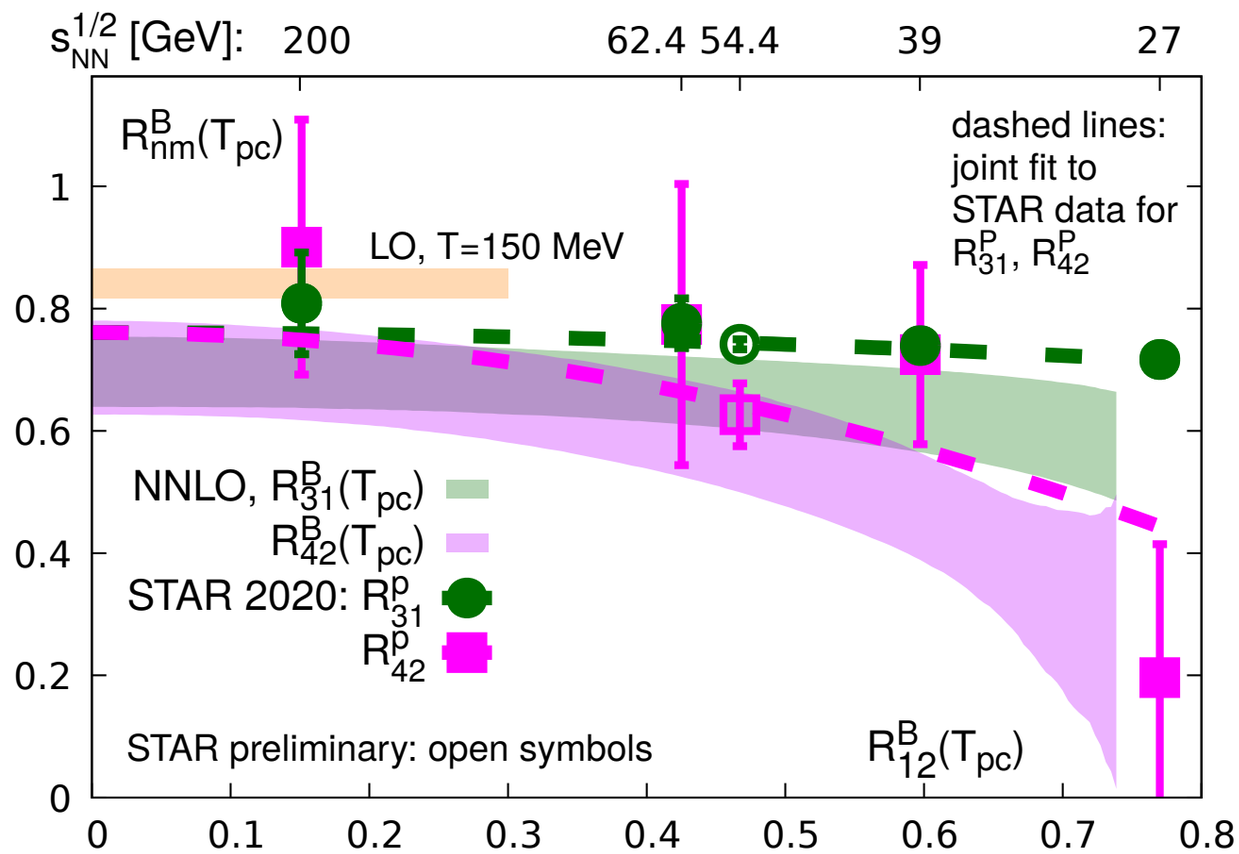
Results: Skewness and kurtosis

- Continuum estimates of R^B_{31} and R^B_{42} as function of μ_B/T for various temperatures.



- Ratios drop with increasing μ_B/T and with increasing temperature.

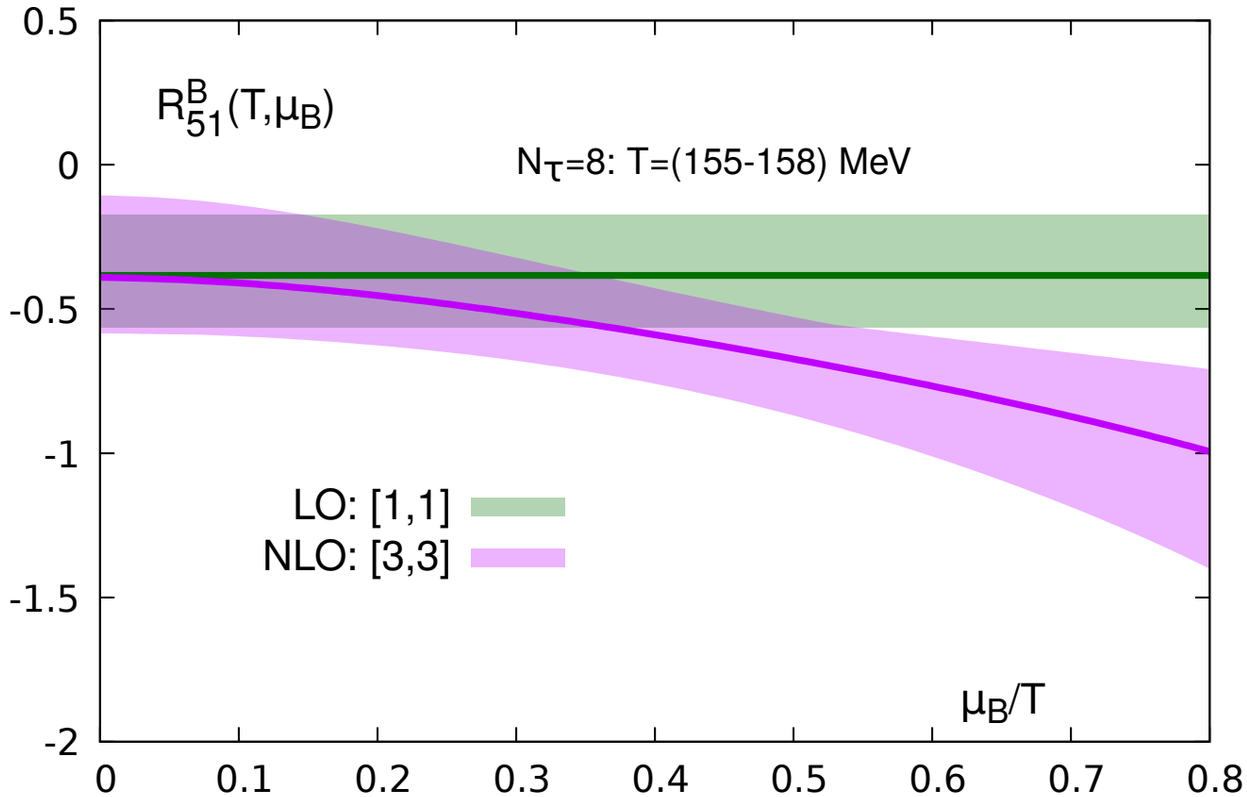
Results: Skewness and kurtosis

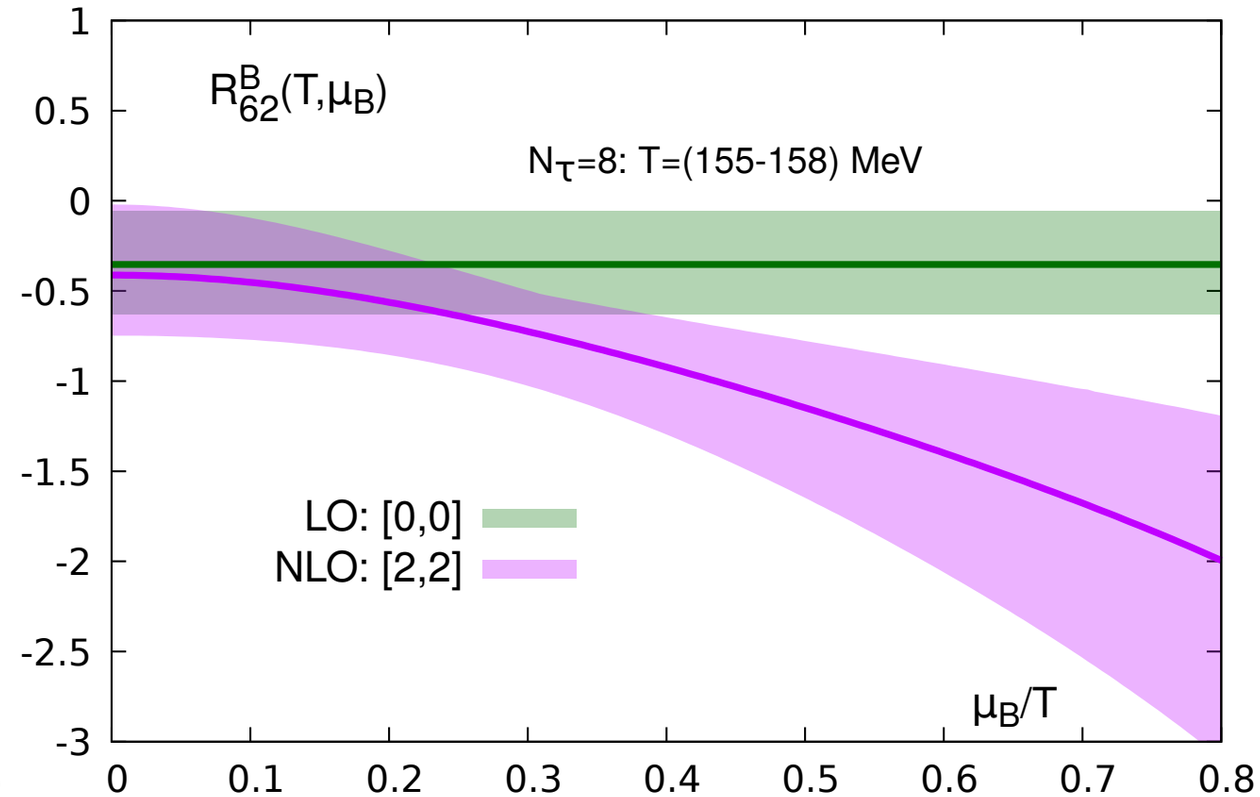


- Continuum estimates of R^B_{31} and R^B_{42} as function of R^B_{12} on the crossover line.
- Star data at $\sqrt{s_{NN}} = 54.4\ \mathrm{GeV}$ favors a freeze-out temperature slightly below the crossover.
- The estimate of the freeze-out temperature $T_\mathrm{f} = 165\ \mathrm{MeV}$ for $\sqrt{s_{NN}} = 200\ \mathrm{GeV}$ (from a statistical model analysis) is not consistent with a determination of T_f from the skewness and kurtosis data by STAR.

Results: Fifth and sixth order cumulant ratios R^B_{51} and R^B_{62}

- R^B_{51} and R^B_{62} on ($N_\tau = 8$)-lattices

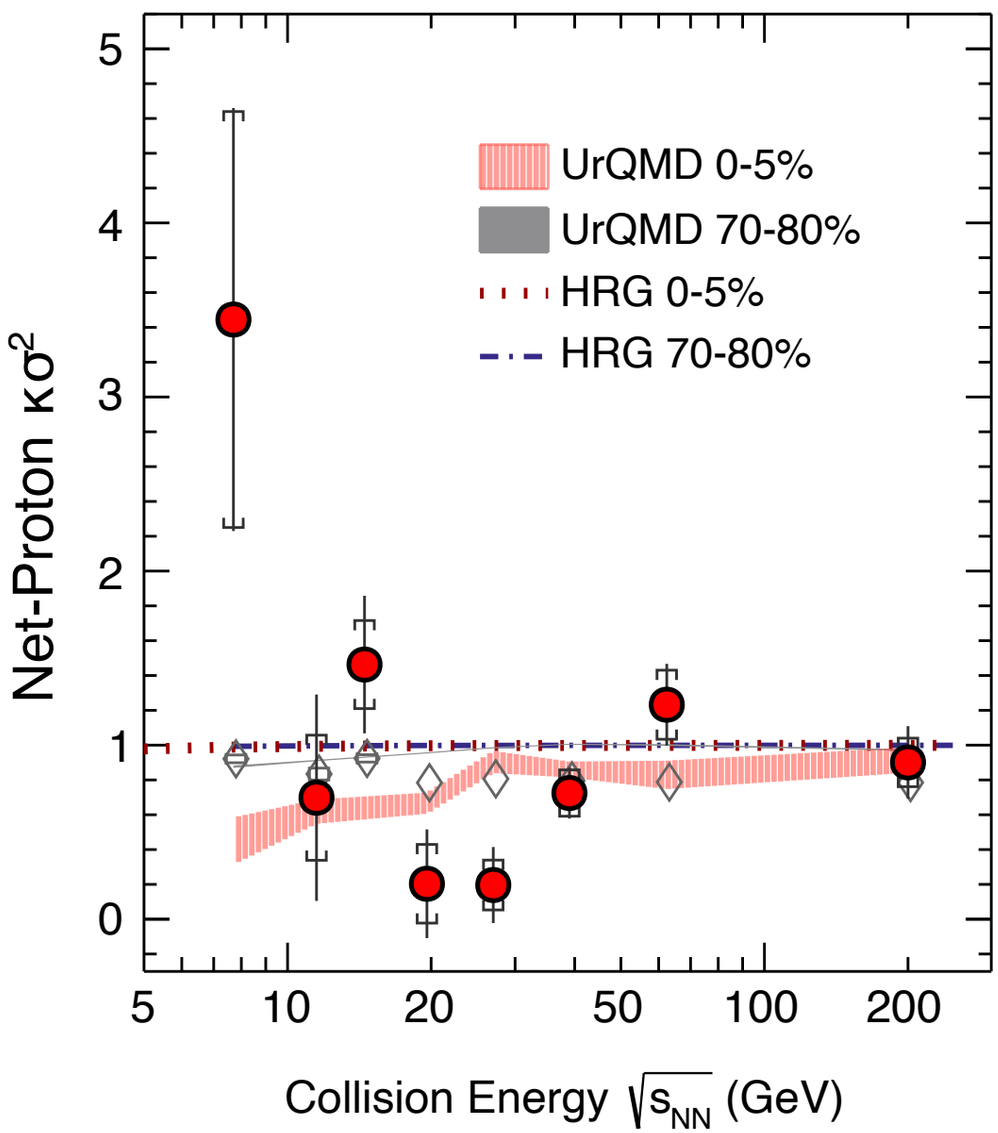




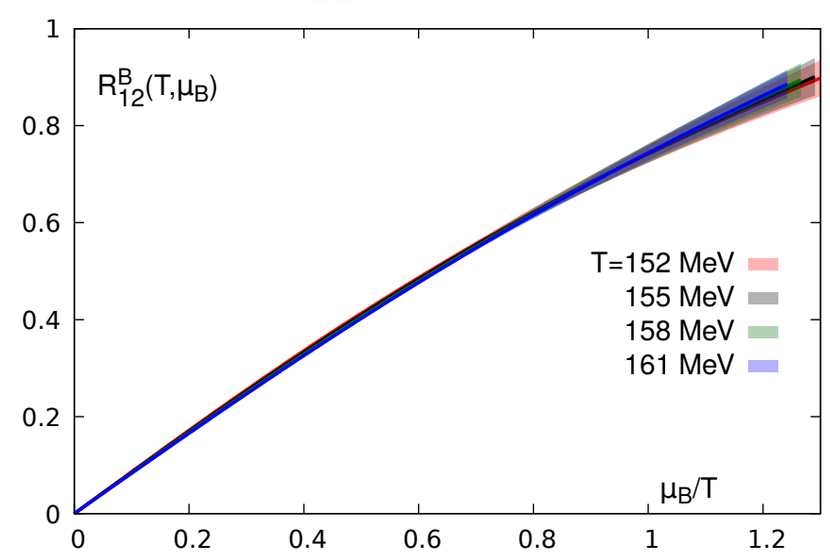
- Large statistical uncertainties
- NLO corrections are negative

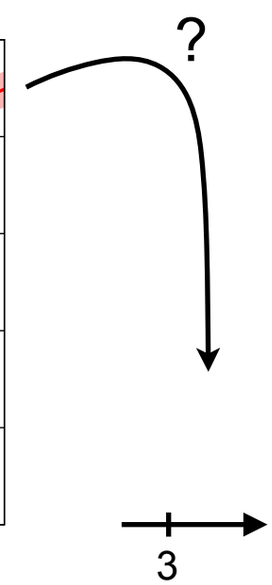
What about the critical point?

STAR, arXiv:2001.02852



- STAR: indication for non-monotonic behaviour in R^P_{42} for $s^{1/2}_{NN} < 27$ GeV with 3.0σ significance [2001.02852].
  $\Rightarrow$ Hint at the critical point?
- Lattice: would need a reliable10th-order calculation to see non-monotonic behavior in R^B_{42}.
  $\Rightarrow$ Look for a divergence of χ^B_2, a zero of R^B_{12}





$\Rightarrow$ Need smaller temperatures

$\Rightarrow$ Look for poles of χ^B_2 in the complex plane

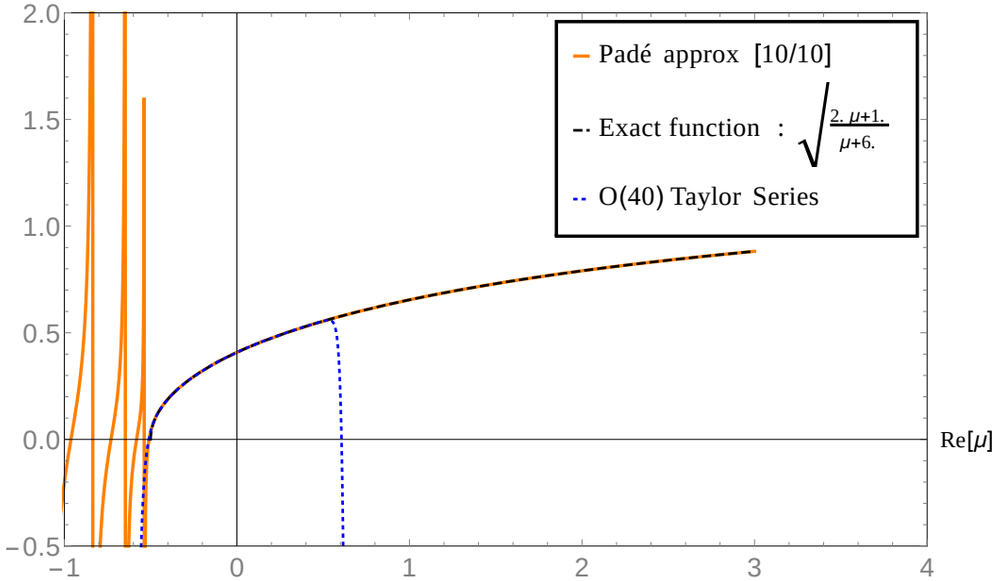
Resumming the Taylor series: single point Padé

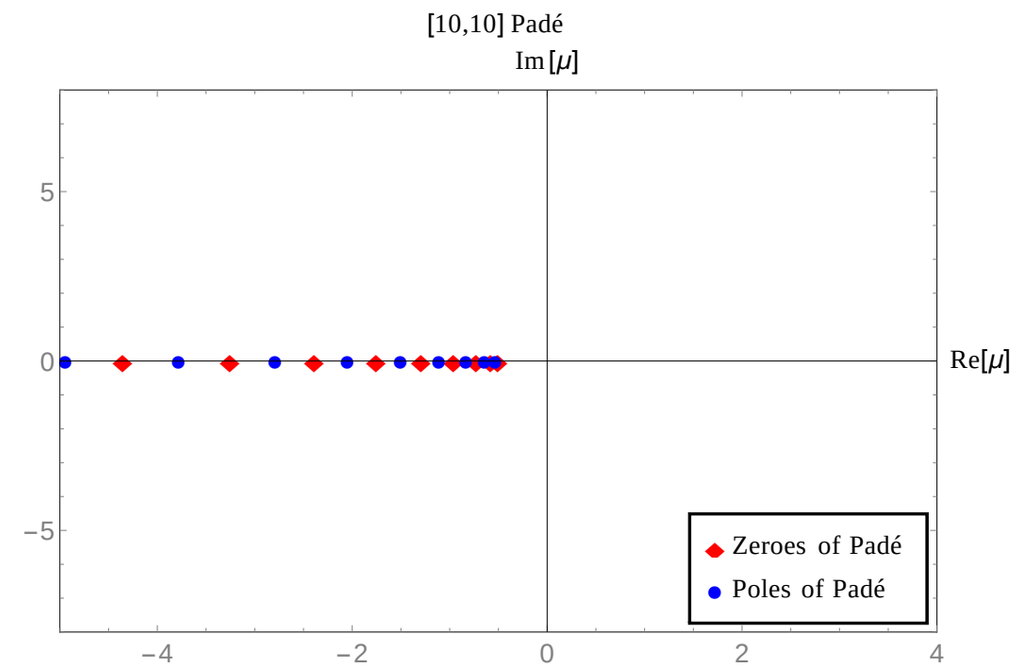
- Perform analytic continuation by a multi-point Padé

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

No surprise: rational functions can go beyond the radius of convergence, can be used to identify cuts.

S. Singh et al (Bi-Parma Collaboration), Lattice 2021





Problem: need a large number of Taylor expansion coefficients to high precision

Analytic continuation via multi-point Padé

- We can consider multiple Lattice QCD results at purely imaginary chemical potential

$$x_i = i\mu_B^I/T$$

$$P_m(x_i) - f(x)Q_n(x_i) = f(x_i)$$
$$P'_m(x_i) - f'(x)Q_n(x_i) - f(x_i)Q'_n(x_i) = f'(x_i) \qquad \forall i$$

Possible Method: solve a linear system

Example where the multi-point Padé works well: 1D-Thirring

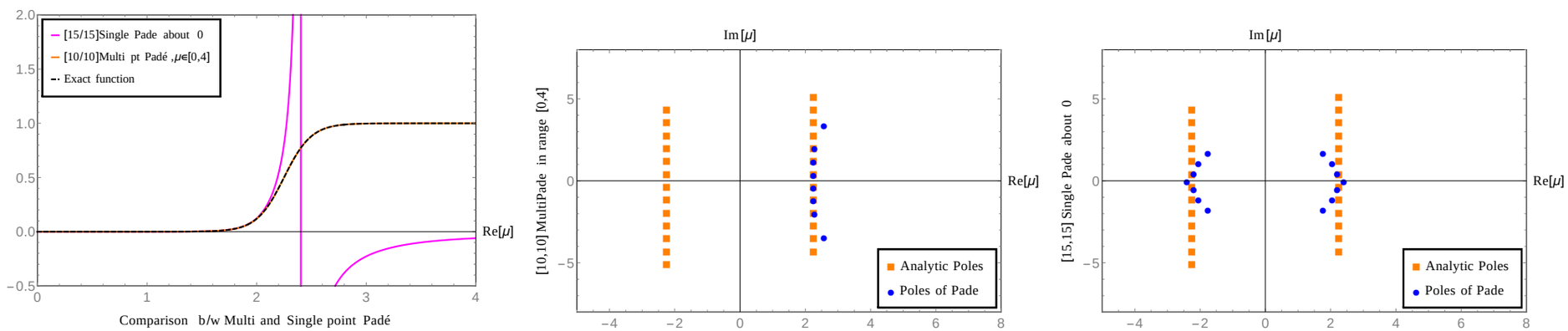


Figure: Left: multi-point vs single Padé approximating the function. (Middle) : Reconstruction of the analytic poles by the multi-point Padé and Bottom (Right) : and by the single point Padé

[FdR,KZ,SS, Phys. Rev. D 103, 034513] and [FdR,KZ : arXiv:2109.02511]

Calculations at imaginary chemical potential

- The fermion determinant stays real at imaginary chemical potential, the imaginary chemical potential is implemented as phases to the time linke link variables

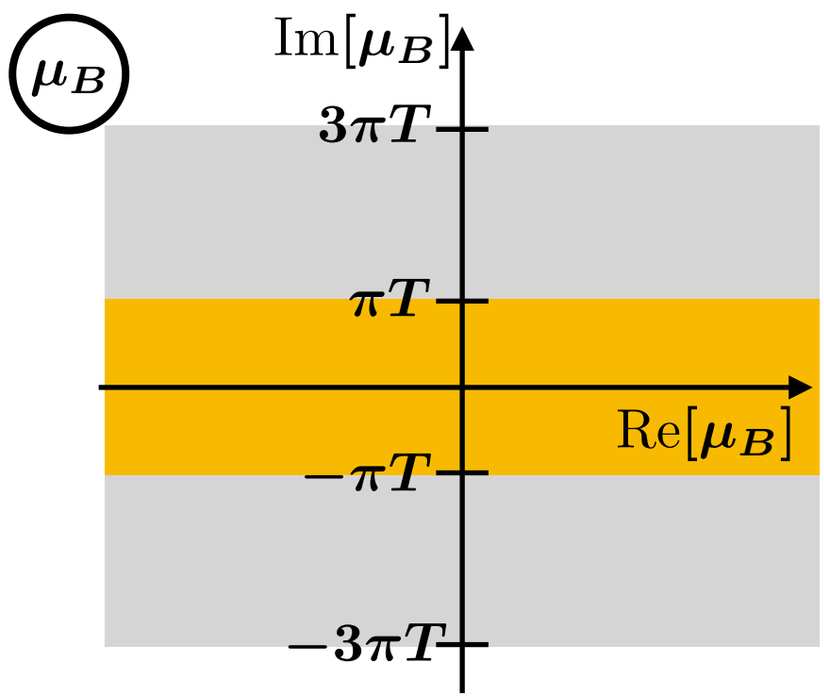
$$U_0(x) \to e^{i\hat{\mu}_I} U_0(x) \qquad U_0^\dagger(x) \to e^{-i\hat{\mu}_I} U_0^\dagger(x)$$

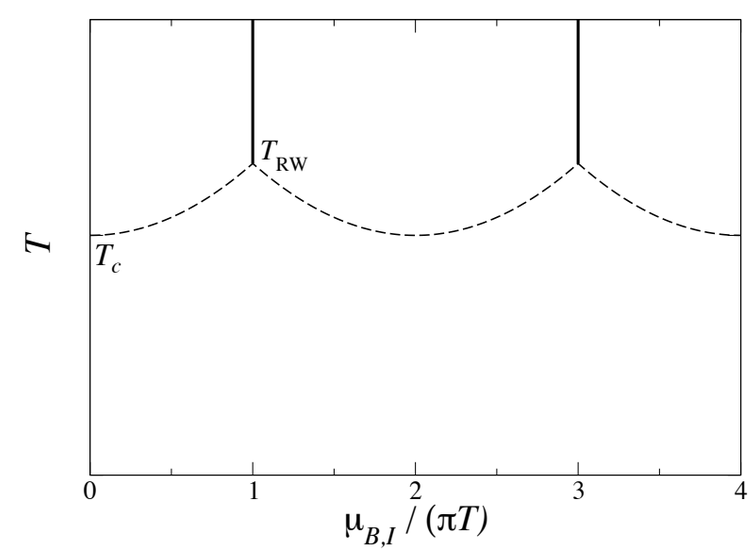
- Results can be analytically continued to real chemical potential

Taylor in $\mathrm{Im}[\mu_B]$ $\quad\to\quad$ Taylor in $\mathrm{Re}[\mu_B]$

[Borsanyi et al, JHEP 10 (2018) 205]

- The QCD partition function is periodic in $\mathrm{Im}[\mu_B]$ due to the Roberge-Weiss (RW) symmetry, with a periodicity $2\pi T$

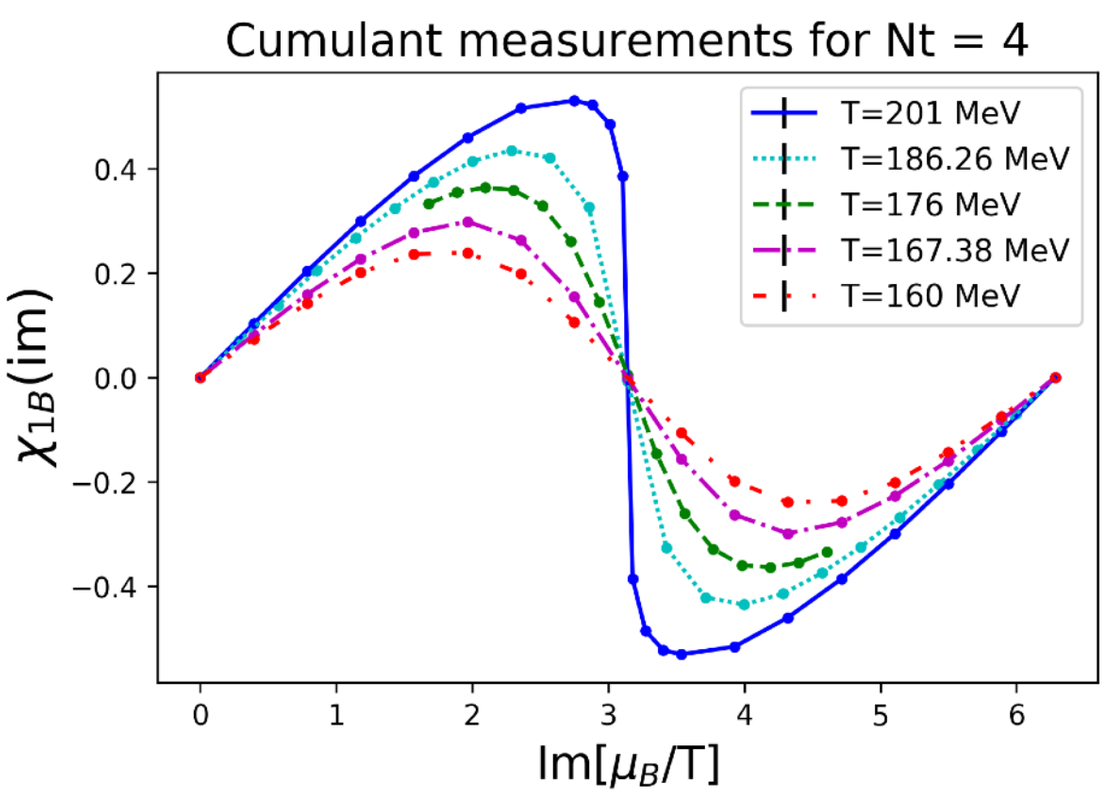


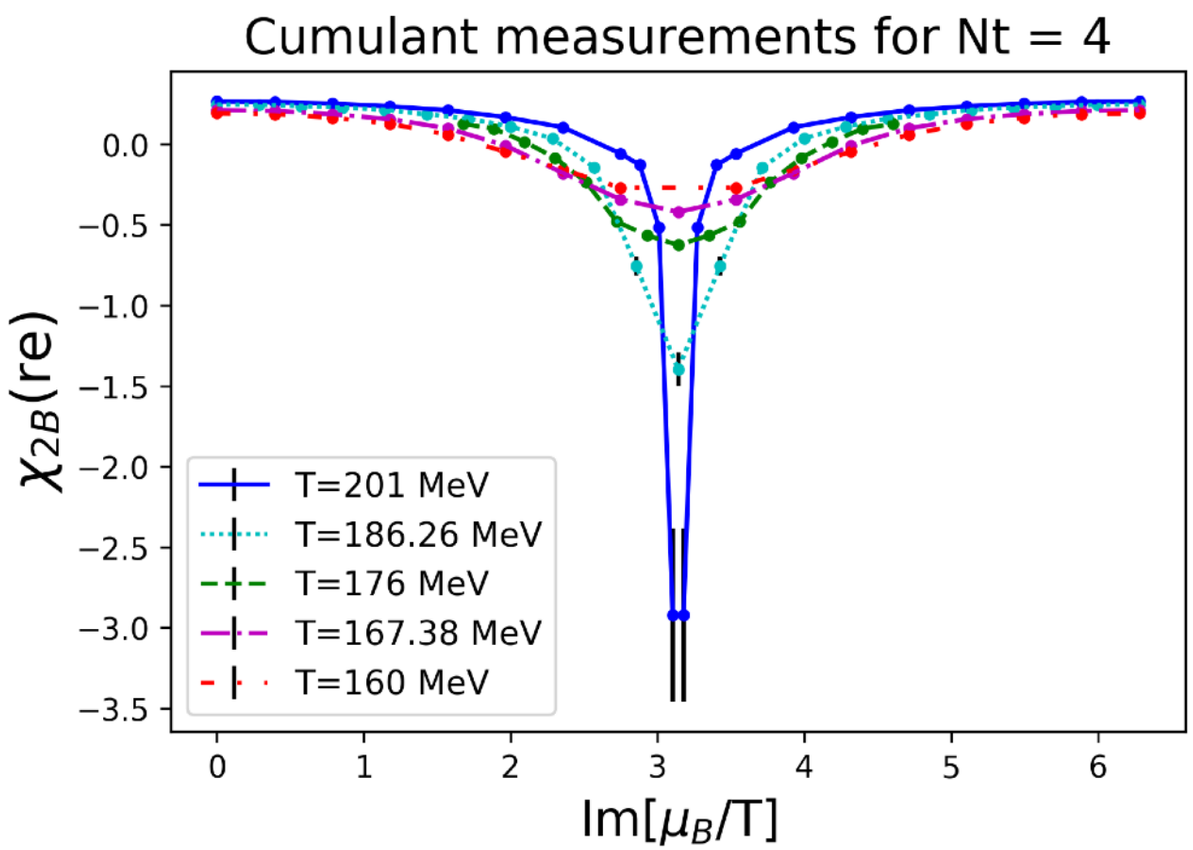


[Bonati et al, Phys. Rev. D 99, 014502 (2019)]

Calculations at imaginary chemical potential

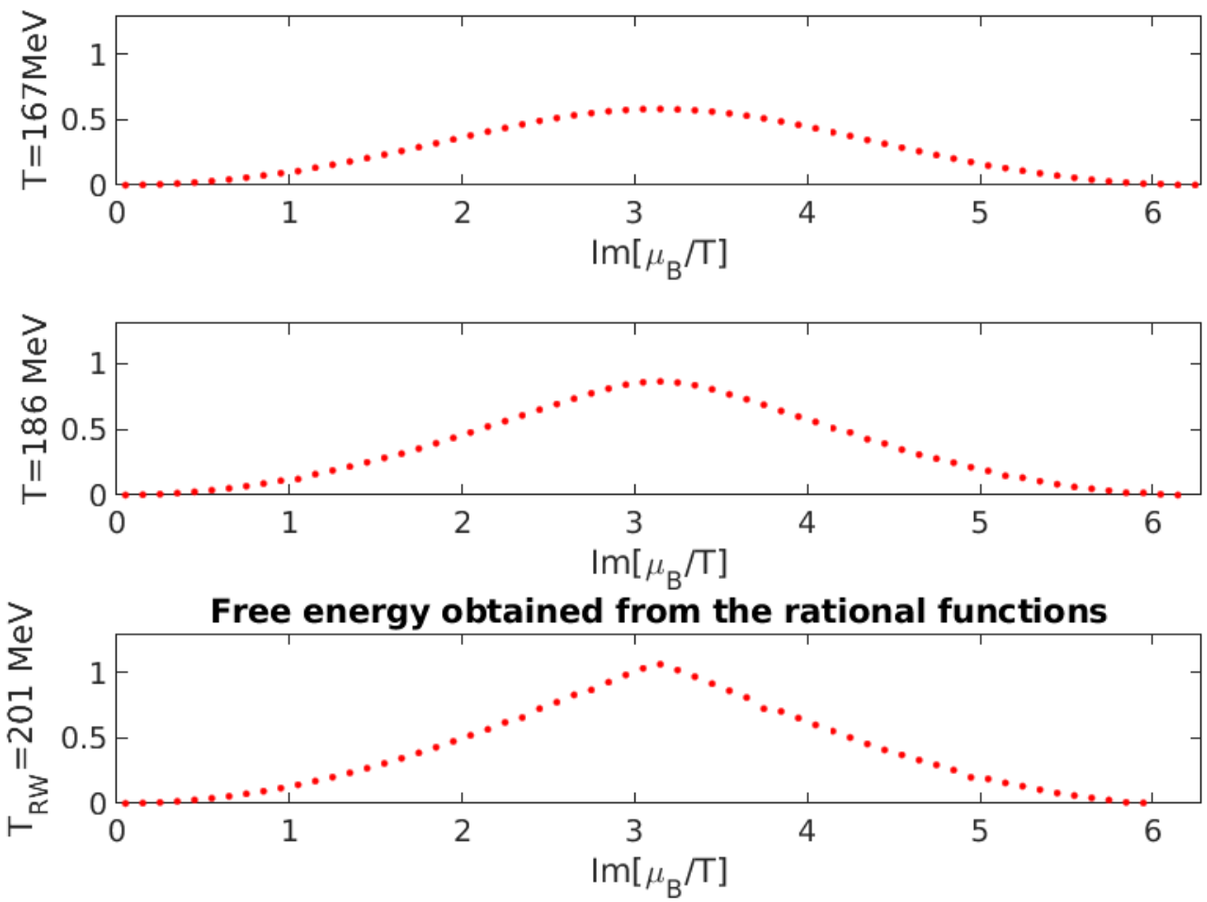
- Use again (2+1) flavour of HISQ fermions at physical masses. Lattice is still course: $N_\tau = 4{,}6$. For simplicity we chose $\mu_q = \mu_s = \mu_B/3$

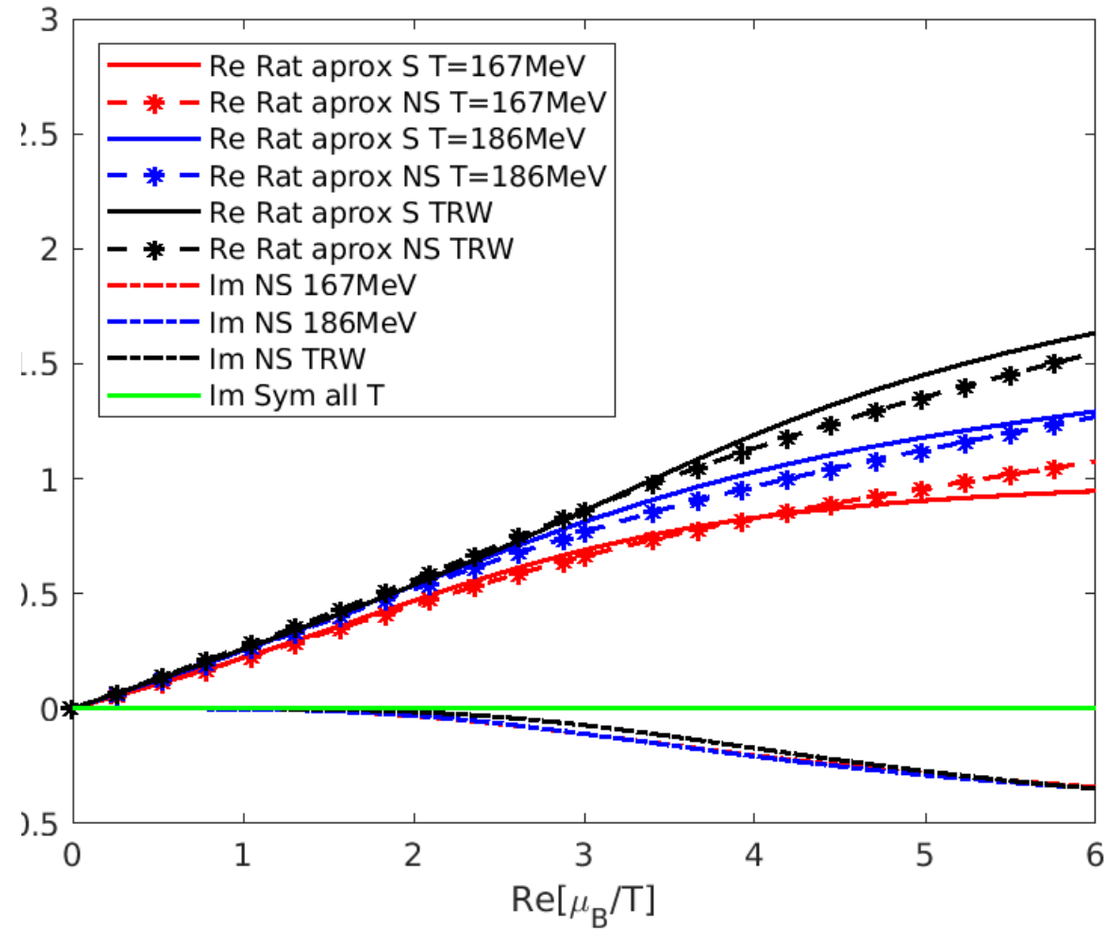




- Expected symmetries are observed

Free energy and analytic continuation





- Free energy develops a non-analyticity close to the Roberge-Weiss transition
- Analytic continuation of the baryon number density. Without enforcing symmetries, the imaginary part states zero for $\mu_B/T < 2$

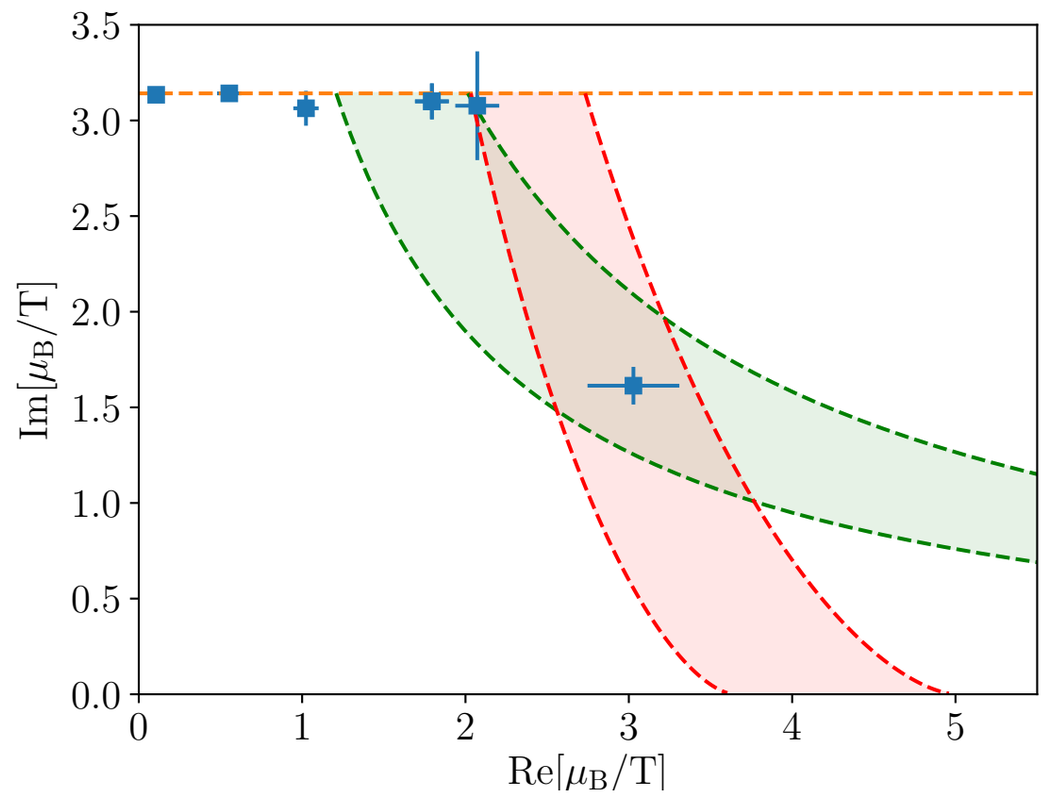
Lee-Yang Edge Singularities

- From Lee-Yang (1952) and Fisher (1978) we know How zeros of the partition functions (poles of susceptibilities) are expected to behave in the vicinity of a critical point.
- The can be found at a universal value of the scaling variable $z = z_c$. They indicate the edge of a branch cat in the universal scaling functions.
- The universal value as recently been determined from RG-study, in particular for Z(2), O(2) and O(4)

A. Connelly, G. Johnson, F. Rennecke, and V. Skokov, Phys. Rev. Lett. 125, 191602 (2020), arXiv:2006.12541 [cond-mat.stat-mech].

- Consider universal critical behaviour in the vicinity of the Roberge-Weiss (RW), the chiral transition or even in the vicinity of the QCD critical end-point.

- Data points indicate our preliminary results on the Lee-Yang Edge singularities

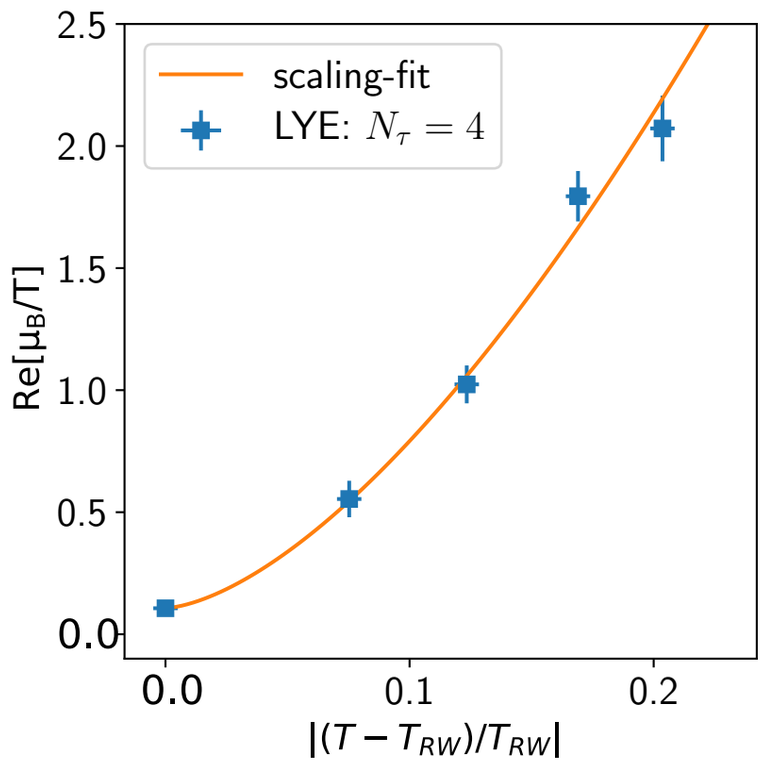


Nicotra et al (Bi-Param Collaboration) Lattice 2021

Scaling analysis

RW-transition Z(2)

$$\mathrm{Re}[\boldsymbol{\mu_B/T}] \sim \mathrm{Im}[\boldsymbol{h}]$$



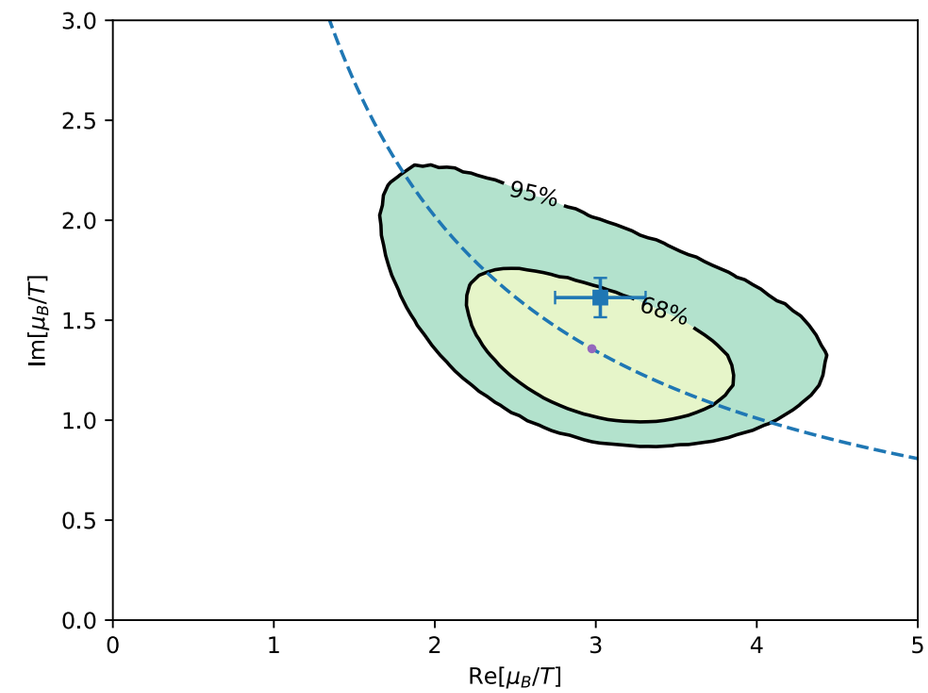
- Scaling of the LYE is in accordance with the expected universal behaviour

$$\mathrm{Re}[\mu_B/T] = \pm\pi \left(\frac{z_0}{|z_c|}\right)^{\beta\delta} \left(\frac{T_{RW} - T}{T_{RW}}\right)^{\beta\delta},$$

$$\mathrm{Im}[\mu_B/T] = \pm\pi\,,$$

Chiral transition O(4)

$$\boldsymbol{T = 145}\ \mathrm{MeV}$$



- LEY is at $T = 145$ MeV is in good agreement with the expected position determined by the non-universal parameter previously found by HotQCD: T_c, k_2, z_0

Summary and outlook

- Universal critical behaviour is observed in lattice QCD data and guided our thinking on the QCD phase diagram
- Pseudocritical and critical temperatures as well as some non-universal constants are known to quite some precision.

- The calculation for high order cumulants is numerical very challenging
- Lattice QCD calculations show a significant increase in precision for cumulant ratios along the crossover line in the QCD phase diagram for $\mu_B/T \leq 1.2$ due to increase in the statistics and thus also the order of the expansion.
- Presented first calculations of R^B_{51} and R^B_{62} along the crossover line.
- From preliminary data at imaginary chemical potential we could identify LYE singularities, wich behave also in accordance with the expected universal behaviour

- **Outlook:**
  - Need to increase statistics for ($N_\tau = 12$)- and ($N_\tau = 16$)-lattices further.
  - Investigate resummation schemes to push Taylor expansion results to larger μ_B/T.
  - Try to follow LYE to even lower temperature.

Backup

The Taylor expansion method

- Compute expansion coefficients of the pressure

$$\frac{p}{T^4} = \frac{\ln Z}{T^3 V} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk,0}^{BQS} \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

Gavai, Gupta (2001)
Bielefeld-Swansea (2002)

- **Notation:** relevant operators are derivatives of the determinant

$$D_i^f = \frac{\partial^i}{\partial \mu_f^i} \det\left[M_f(\mu_f)\right]^{1/4} = \frac{\partial^i}{\partial \mu_f^i} e^{\frac{1}{4}\mathrm{Tr}\ln M_f(\mu_f)}, \quad f \in \{u, d, s\}$$

up to 4th-order in μ:

exponential dependence:

$$D_1^f = \mathrm{Tr}\left[M_f^{-1} M_f^{(1)}\right]$$

$$D_2^f = -\mathrm{Tr}\left[M_f^{-1} M_f^{(1)} M_f^{-1} M_f^{(1)}\right] + \mathrm{Tr}\left[M_f^{-1} M_f^{(2)}\right]$$

$$\vdots$$

from 6th-order in μ onwards:

linear dependence:

$$D_1^f = \mathrm{Tr}\left[M_f^{-1} M_f^{(1)}\right]$$

$$D_2^f = -\mathrm{Tr}\left[M_f^{-1} M_f^{(1)} M_f^{-1} M_f^{(1)}\right]$$

all $M_f^{(k)} = 0$, for k>1

⇒ much less operators to measure!

Gavai, Sharma 2015

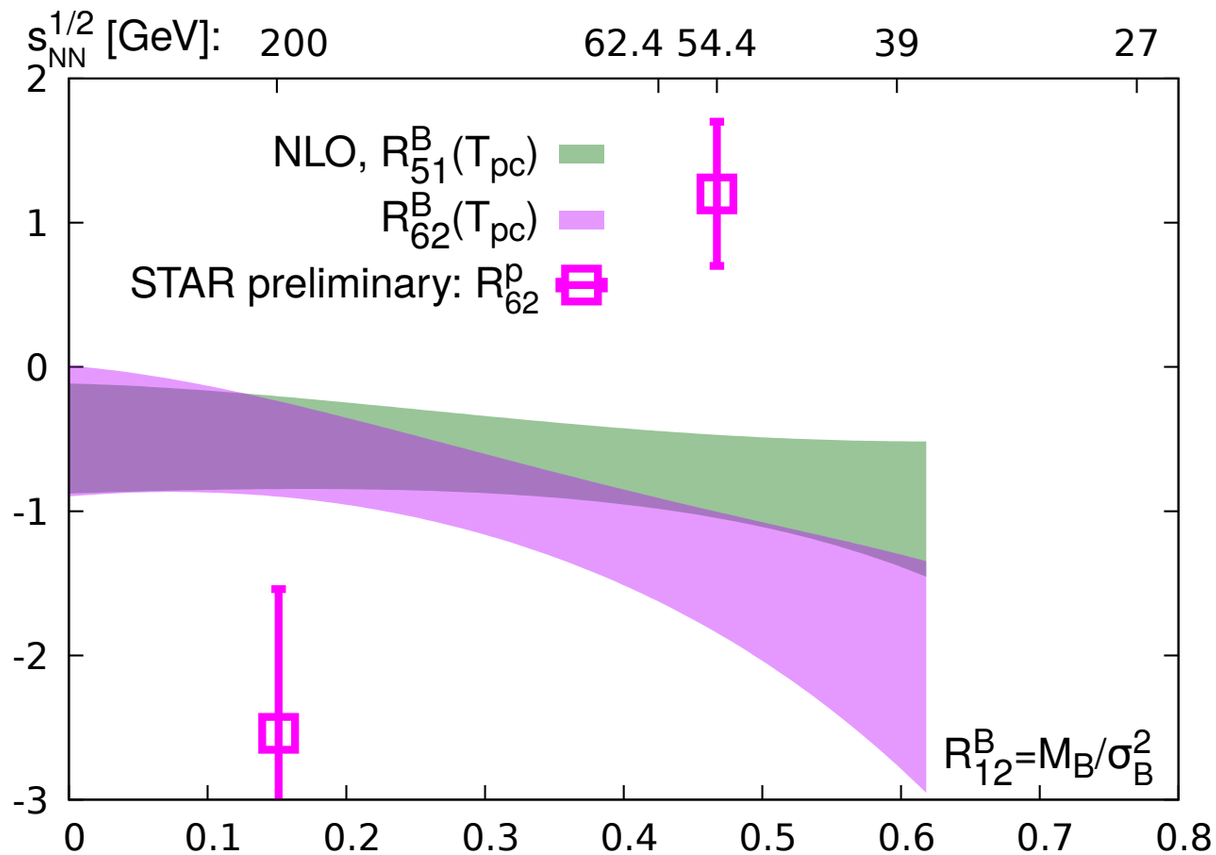
Lattice setup and statistics

- Use (2+1)-flavor of HISQ-fermions, with physical strange and light quark masses.
- **Lattices sizes** are $32^3 \times 8,\ 48^3 \times 12,\ 64^3 \times 16$, at 9 different temperature values.
- **Statistics:** Compared to our previous analysis of skewness and kurtosis [HotQCD, PRD 96 (2017) 074510] we increased the statistics on ($N_\tau = 8$)-lattices by a factor 3-4 and on ($N_\tau = 12$)-lattices by a factor 6-8. I.e. we have now

N_τ	8	12	16
#conf.	$1.2 \cdot 10^6$	$(2-3) \cdot 10^5$	10^4

- **Order of the expansion:** We can now go to N^{3}LO, compared to NLO in our previous study. I.e., we include 8-th order expansion coefficients of the pressure.
- Recent Calculations were performed on Summit, using Nvidia's V100 GPU's.

Results: Fifth and sixth order cumulant ratios R^B_{51} and R^B_{62}



- R^B_{51} and R^B_{62} on ($N_\tau = 8$)-lattices
- Not consistent with STAR data:
  - ➡ A. Pandav@SQM19

$$\sqrt{s_{NN}} = 200 \text{ GeV}: R^P_{62} < 0$$

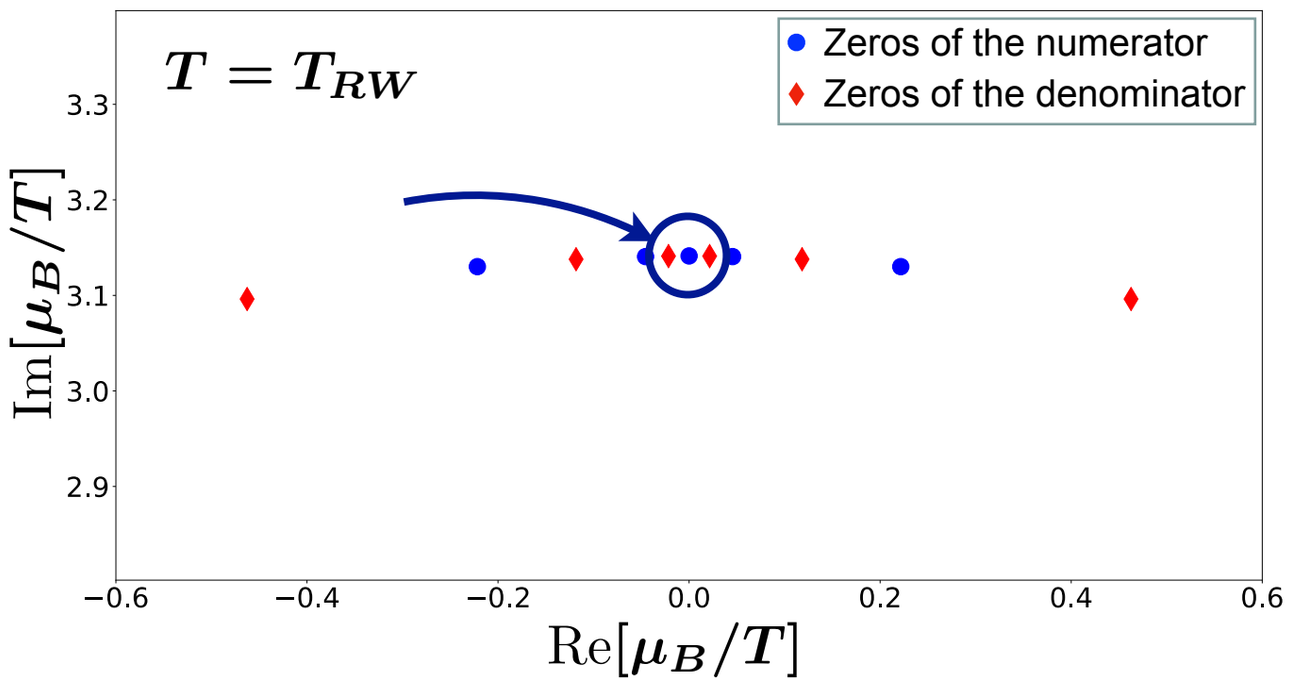
$$\sqrt{s_{NN}} = 54.4 \text{ GeV}: R^P_{62} > 0$$

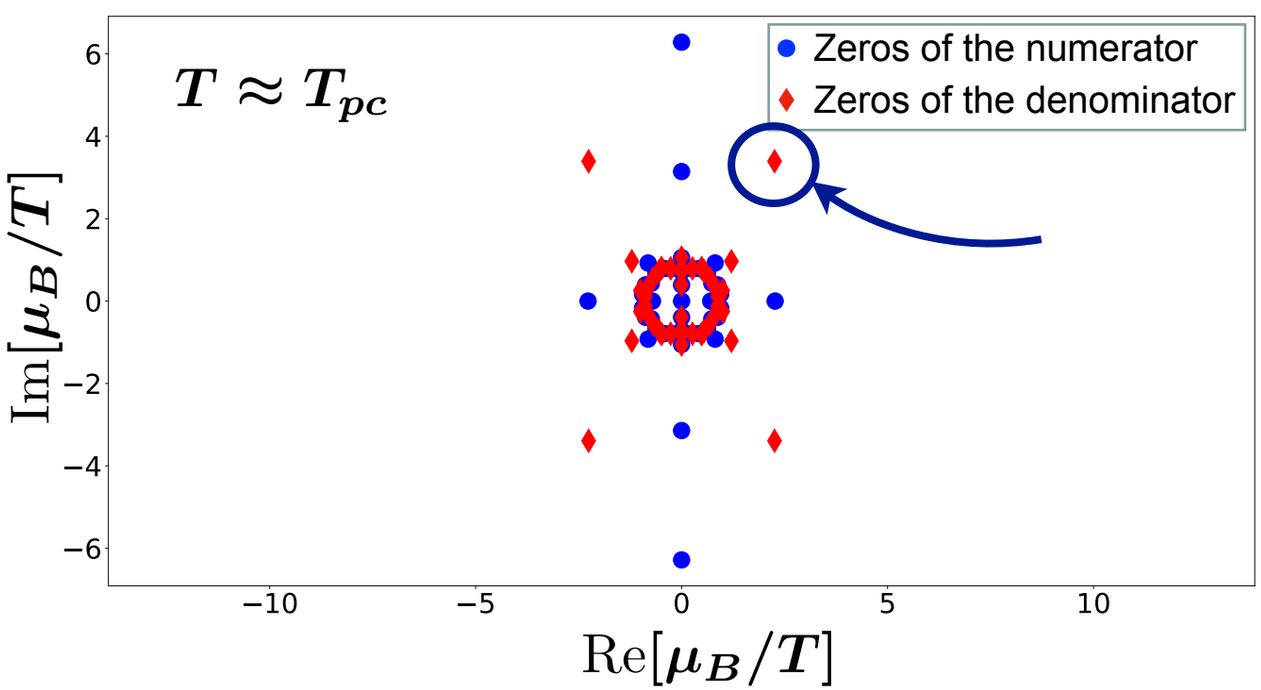
  - ➡ Lattice QCD predictions

$\sqrt{s_{NN}}$	R^B_{51}	R^B_{62}
200	$-0.5(3)$	$-0.7(3)$
54.4	$-0.7(4)$	$-2(1)$

Singularities in the complex plane

Bielefeld-Parma (preliminary)





- Obtain zeros of the numerator and denominator
- Some zeros match to high precision, for others its not so clear…
- The RW-singularity seems to be stable
- Other singularities need further investigations…work in progress.
- Singularities may also be understood in terms of the Fourier coefficients of the $\mathrm{Im}[\chi_1^B]$

[Vovchenko et al, PRD 97, 114030 (2018)]

[Almási et al, PRD 100, 016016 (2019)]

[Almási et al, PLB 793 (2019)]