Taylor expansions and Pade approximations in finite density QCD

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- Taylor expansion for the QCD equation of state at non-zero chemical potentials $\mu_S = \mu_Q = 0$ and $\mu_Q = 0,\ n_S = 0$
- using Pade approximants to resum Taylor series in finite density QCD
- (constrain) the location of the critical point

based on:

D. Bollweg et al (HotQCD), arXiv:2202.09184

CRC-TR 211 Strong-interaction matter under extreme conditions
DFG Deutsche Forschungsgemeinschaft

Phases of strong-interaction matter

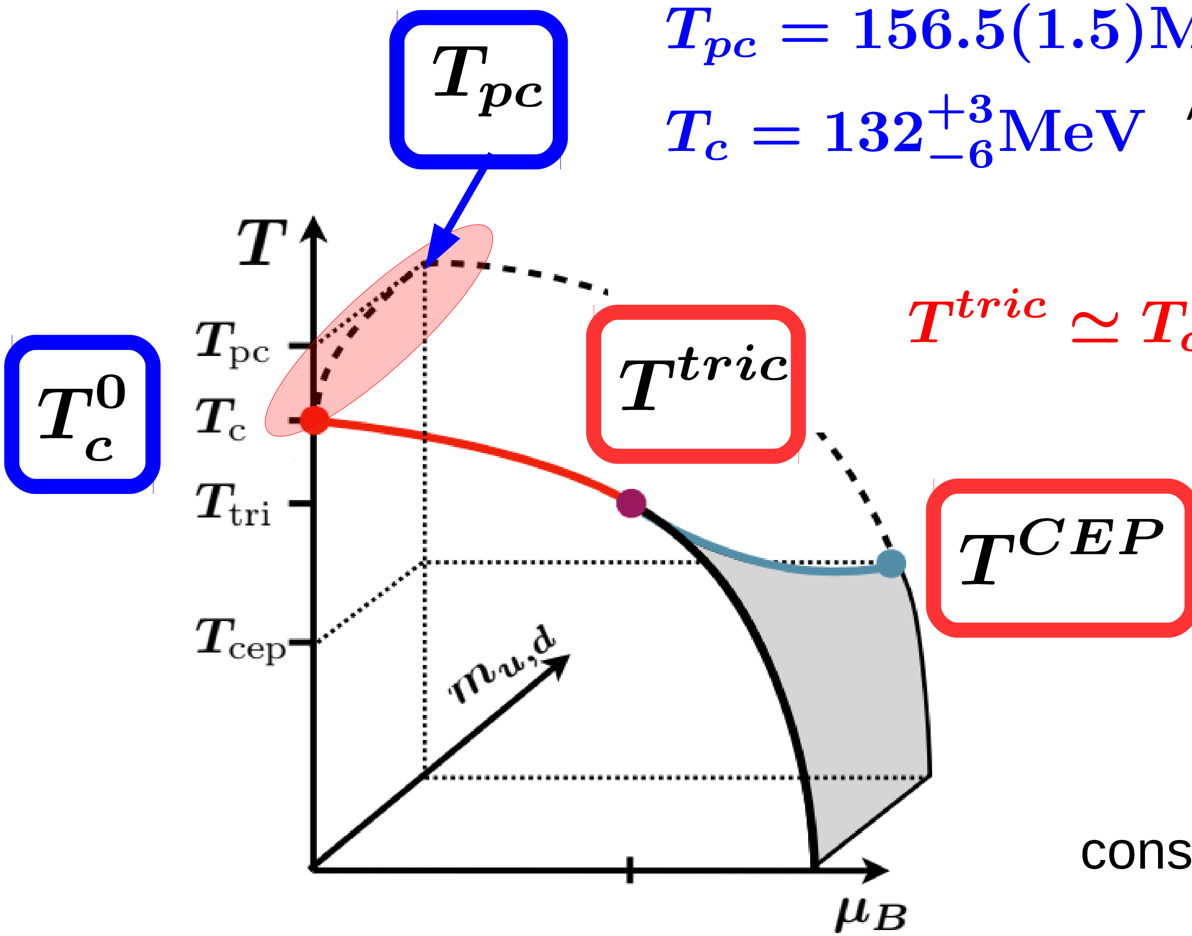
determination of T_c^0 puts an upper limit on T^{CEP}

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

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

A. Bazavov et al (HotQCD), arXiv:1812.08235

H.T. Ding et al (HotQCD), arXiv:1903.04801



$$T^{tric} \simeq T_c - 2\ \mathrm{MeV} \left(\frac{\mu_B}{T_c}\right)^2_{tric}$$

HotQCD@Lattice2021 (M. Sarkar)
arXiv:2112.15398

constraint on the location of the CEP

the temperature range below T_{pc} is most important for getting information on a possible CEP

QCD thermodynamics at non-zero net baryon-density
– Taylor expansion –

Taylor expansion of the **QCD** pressure: $\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T, V, \mu_B, \mu_Q, \mu_S)$

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

cumulants of net-charge fluctuations and correlations:

$$\chi_{ijk}^{BQS} = \left.\frac{\partial^{i+j+k} P/T^4}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k}\right|_{\mu_{B,Q,S}=0} \quad , \quad \hat{\mu}_X \equiv \frac{\mu_X}{T}$$

QCD thermodynamics at non-zero net baryon-density – Taylor expansion –

Taylor expansion of the **QCD** pressure: $\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T,V,\mu_B,\mu_Q,\mu_S)$

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

$$\Downarrow$$

Consider isospin symmetric matter $\Leftrightarrow$ $\mu_Q = 0 \;\Leftrightarrow\; n_Q/n_B = 0.5$

I) $\mu_S = 0 : \tilde{\chi}_0^{B,n} = \chi_{n,00}^{BQS} \equiv \chi_n^B$

II) $n_s = 0 : \hat{\mu}_S \rightarrow \hat{\mu}_S(\hat{\mu}_B) = s_1\hat{\mu}_B + s_3\hat{\mu}_B^3 + \ldots$ such that $n_S = 0$

differences between (II) and conditions met in HIC are small, e.g.

$|\mu_Q/\mu_B| \simeq 0.025$ for $T \simeq T_{pc}$

$$\frac{\Delta P(T,\mu_B)}{T^4} = \frac{P(T,\mu_B) - P(T,0)}{T^4} = \sum_{k=1}^{\infty} \frac{1}{(2k)!} \tilde{\chi}_0^{B,n}(T) \hat{\mu}_B^{2k}$$

QCD thermodynamics at non-zero net baryon-density
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Taylor expansion of the **QCD** pressure: $\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T, V, \mu_B, \mu_Q, \mu_S)$

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

$$\Downarrow$$

Consider isospin symmetric matter $\Leftrightarrow$ $\mu_Q = 0 \;\Leftrightarrow\; n_Q/n_B = 0.5$

$$\frac{P(T,\mu_B)}{T^4} = \frac{P(T,0)}{T^4} + \frac{\tilde{\chi}_0^{B,2}(T)}{2} \left(\frac{\mu_B}{T}\right)^2 + \frac{\tilde{\chi}_0^{B,4}(T)}{24} \left(\frac{\mu_B}{T}\right)^4 + \dots$$

$$\frac{n_B(T,\mu_B)}{T^3} = \frac{\mathrm{d}P/T^4}{\mathrm{d}\hat{\mu}_B} = \tilde{\chi}_0^{B,2}(T) \left(\frac{\mu_B}{T}\right) + \frac{\tilde{\chi}_0^{B,4}(T)}{6} \left(\frac{\mu_B}{T}\right)^3 + \dots$$

Taylor expansion to 8th order in μ_B/T

D. Bollweg et al (HotQCD), arXiv:2202.09184

HotQCD data collection for (2+1)-flavor QCD-EoS

EoS:2017:
arXiv:1701.04325

$N_\tau = 6$				$N_\tau = 8$				$N_\tau = 12$			
β	m_l	T[MeV]	#conf.	β	m_l	T[MeV]	#conf.	β	m_l	T[MeV]	#conf.
5.980	0.00435	135.29	81200	6.245	0.00307	134.64	180320	6.640	0.00196	134.94	5834
6.010	0.00416	139.71	120790	6.285	0.00293	140.45	172110	6.680	0.00187	140.44	5833
6.045	0.00397	145.05	120770	6.315	0.00281	144.95	138150	6.712	0.00181	144.97	13846
6.080	0.00387	150.59	79390	6.354	0.00270	151.00	107510	6.754	0.00173	151.10	14200
6.120	0.00359	157.17	66180	6.390	0.00257	156.78	135730	6.794	0.00167	157.13	15476
6.150	0.00345	162.28	79660	6.423	0.00248	162.25	115850	6.825	0.00161	161.94	16772
6.170	0.00336	165.98	49760	6.445	0.00241	165.98	120270	6.850	0.00157	165.91	19542
6.200	0.00324	171.15	122700	6.474	0.00234	171.02	139980	6.880	0.00153	170.77	21220
6.225	0.00314	175.76	122730	6.500	0.00228	175.64	133070	6.910	0.00148	175.76	12303

added O(10) times new confs.

added O(20) times new confs.

all new

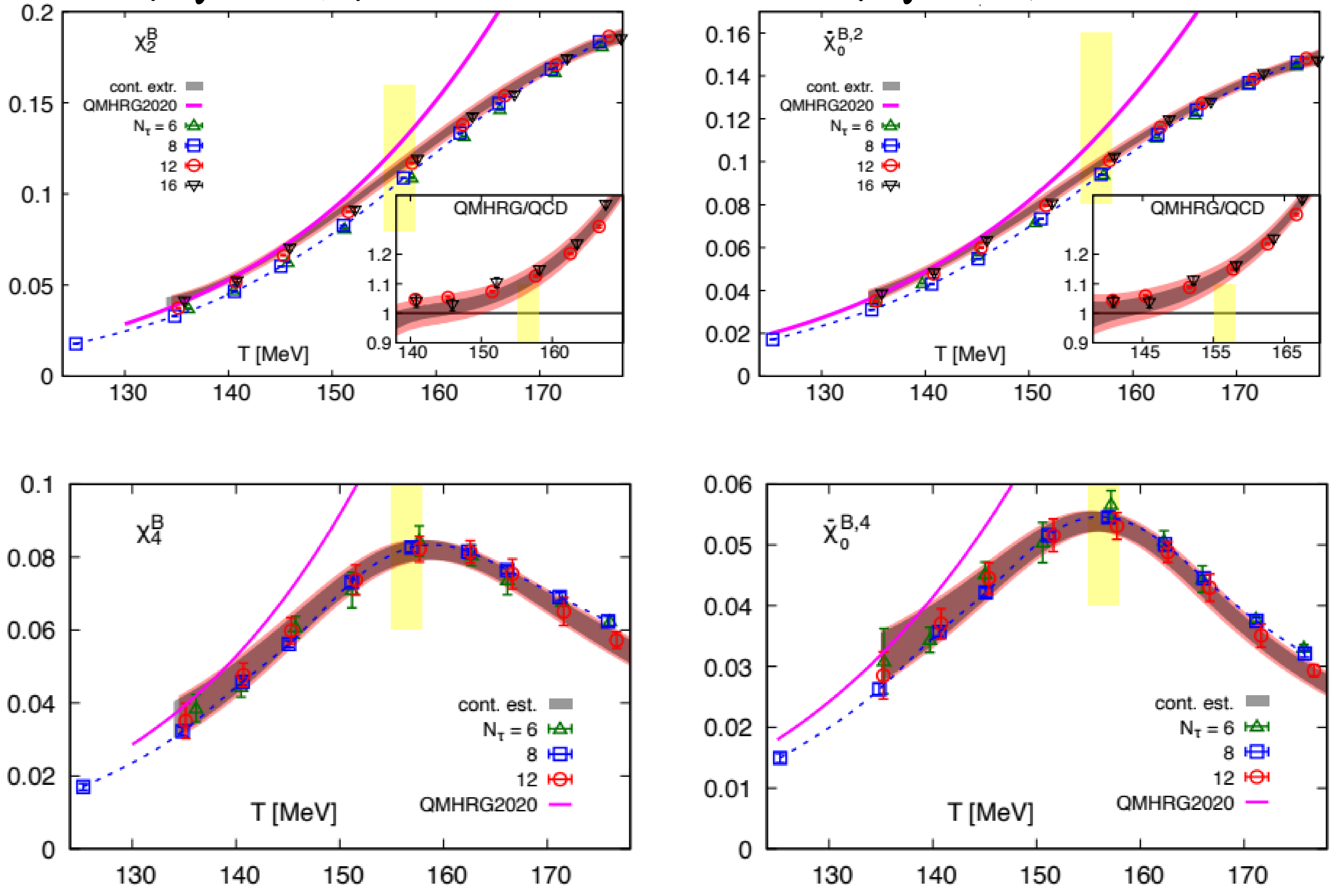
EoS 2022:
arXiv:2202.09184

$N_\tau = 8$				$N_\tau = 12$				$N_\tau = 16$			
β	m_l	T[MeV]	#conf.	β	m_l	T[MeV]	#conf.	β	m_l	T[MeV]	#conf.
6.175	0.003307	125.28	1,471,861								
6.245	0.00307	134.84	1,275,380	6.640	0.00196	135.24	330,447	6.935	0.00145	135.80	17671
6.285	0.00293	140.62	1,598,555	6.680	0.00187	140.80	441,115	6.973	0.00139	140.86	23855
6.315	0.00281	145.11	1,559,003	6.712	0.00181	145.40	416,703	7.010	0.00132	145.95	26122
6.354	0.00270	151.14	1,286,603	6.754	0.00173	151.62	323,738	7.054	0.00129	152.19	26965
6.390	0.00257	156.92	1,602,684	6.794	0.00167	157.75	299,029	7.095	0.00124	158.21	21656
6.423	0.00248	162.39	1,437,436	6.825	0.00161	162.65	214,671	7.130	0.00119	163.50	18173
6.445	0.00241	166.14	1,186,523	6.850	0.00157	166.69	156,111	7.156	0.00116	167.53	19926
6.474	0.00234	171.19	373,644	6.880	0.00153	171.65	144,633	7.188	0.00113	172.60	17163
6.500	0.00228	175.84	294,311	6.910	0.00148	176.73	131,248	7.220	0.00110	177.80	3282

also used in D. Bollweg et al (HotQCD), arXiv:2107.10011

Comparing expansion coefficients for series at

$\mu_Q = 0\ ,\ \mu_S = 0$ **and** $\mu_Q = 0\ ,\ n_S = 0$



Comparing expansion coefficients for series at

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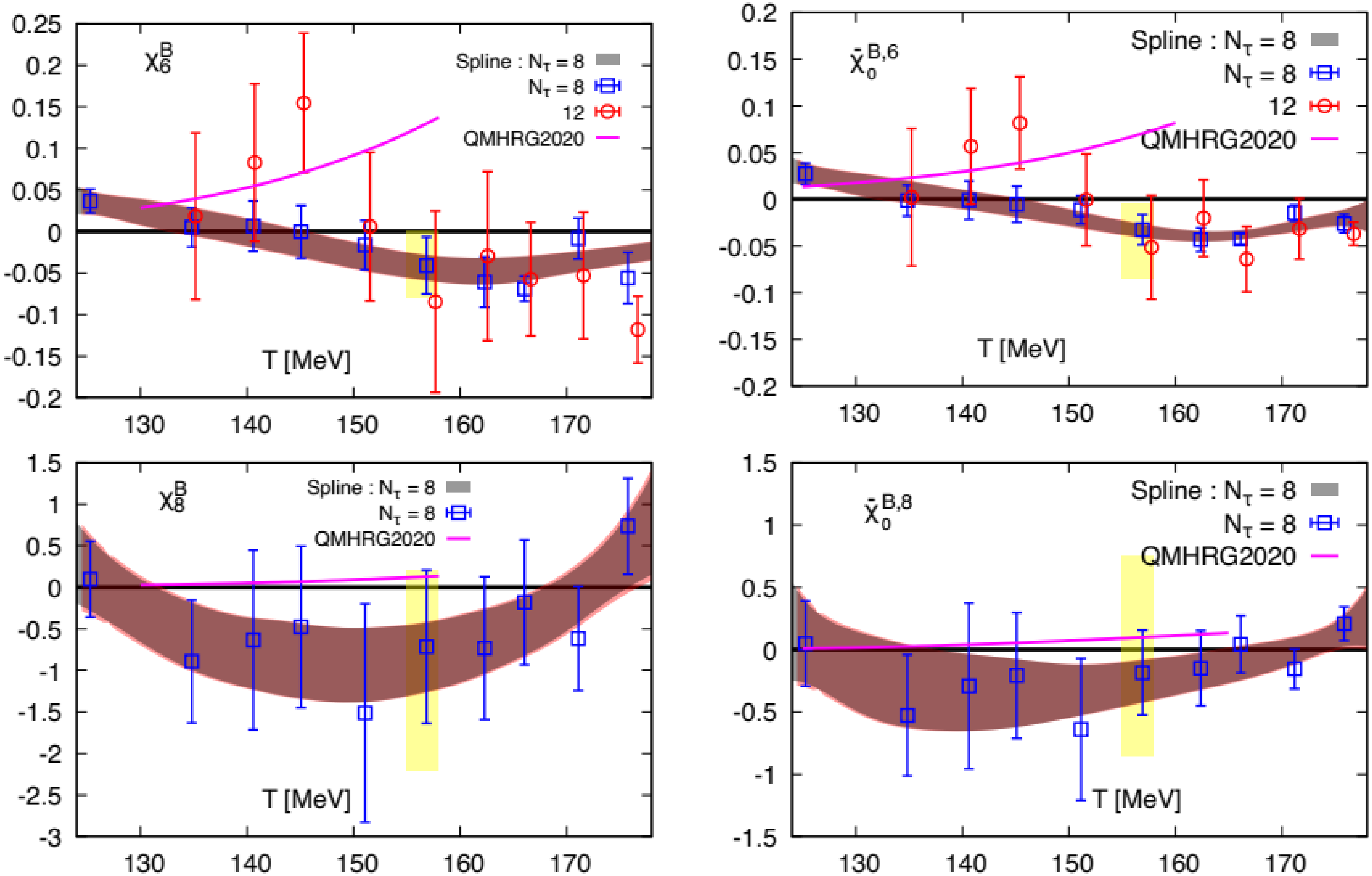


Expansions for $\mu_S = 0$ & $n_S = 0$ are qualitatively similar

Convergence vs. reliability of Taylor series

– given that only a finite number of terms in the expansion is known –

some simple facts: $f(x) = \sum_n c_n\, x^n = c_1 x + c_2 x^2 + c_3 x^3 + \ldots$

$$f'(x) = c_1 + 2c_2 x + 3c_3 x^2 + \ldots$$

$$f''(x) = 2c_2 + 6c_3 x + \ldots$$

radius of convergence: $r_c = \lim_{n\to\infty} r_{c,n} = \lim_{n\to\infty} \left| \frac{c_n}{c_{n+1}} \right|$

$$r'_{c,n} = \left| \frac{n c_n}{(n+1) c_{n+1}} \right| = r_{c,n} \left(1 - \frac{1}{n} \right)$$

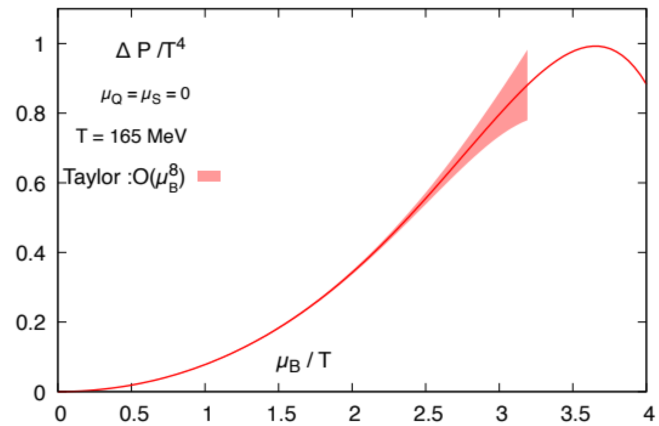
– **all Taylor series for derivatives of f(x) have the same radius of convergence as f(x)**

– higher order expansion coefficients get increasing weight in **higher order derivatives** of f(x) ⇒ **slower convergence**, truncated expansions are less reliable for given x

Corollary: higher order derivatives of finite order Taylor series are reliable only in a smaller range of x-values

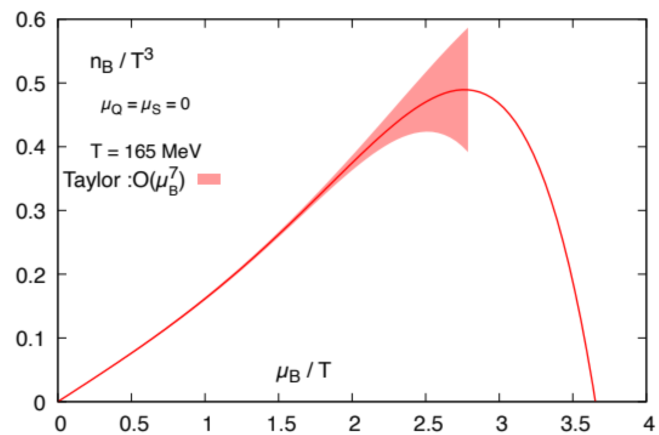
Convergence vs. reliability of Taylor series

$$T = 165\ \mathrm{MeV}:\ \mu_Q = 0\ ,\ \mu_S = 0$$



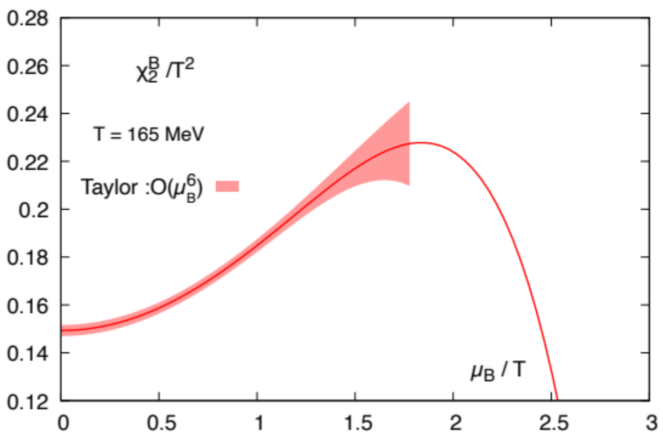
Taylor series for the pressure in the vicinity of T_{cp}

$\chi_6^B < 0\ ,\ \chi_8^B < 0 \Longrightarrow P(T,\mu_B)$ has a maximum at μ_B^{max}



number density is forced to vanish at μ_B^{max}

range of reliability of the 8th order expansion of the number density is reduced relative to that of the pressure



Taylor series for net baryon-number fluctuations vanishes at the maximum of n_B/T^3

at high T, e.g. T>160 MeV, the 8th order Taylor series does provide reliable results for pressure and number density up to $\mu_B/T \simeq 3$

Equation of state of (2+1)-flavor QCD: $\mu_B/T > 0$

– comparing up to 6th order only –

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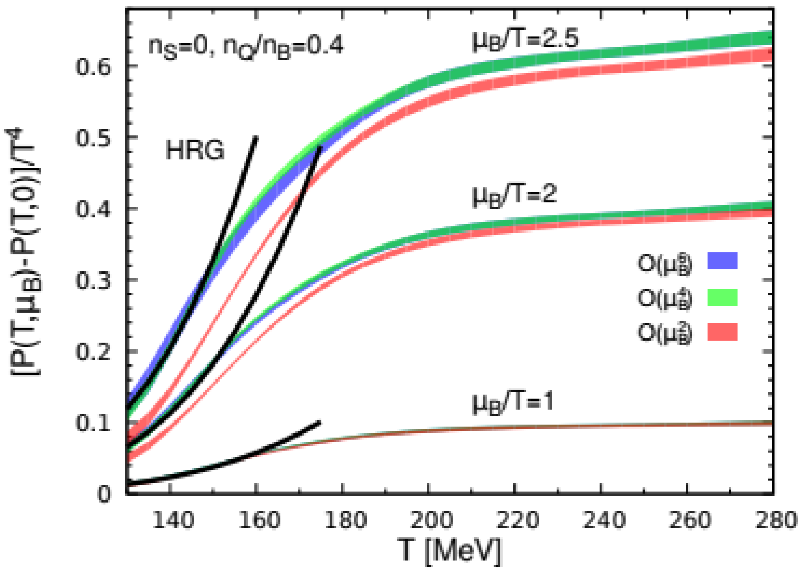
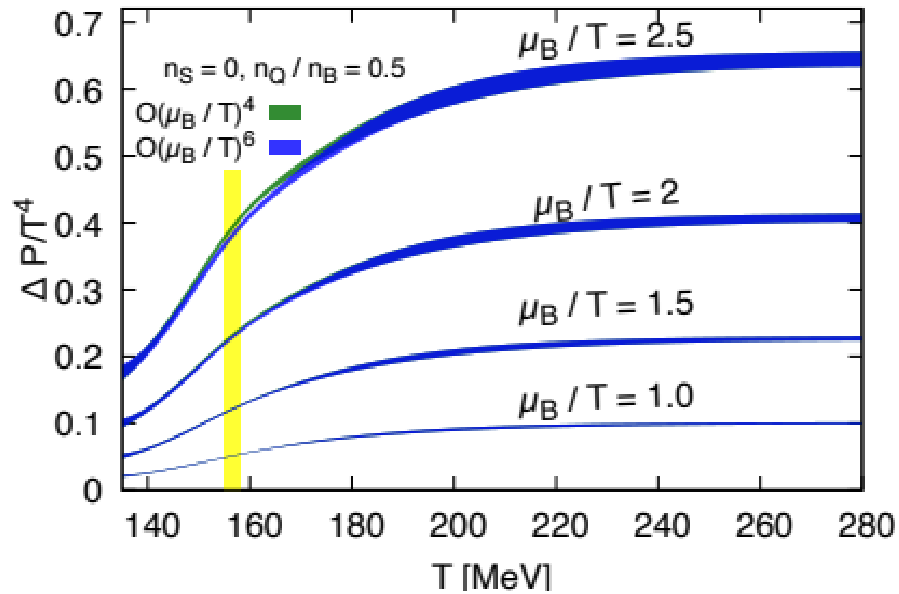
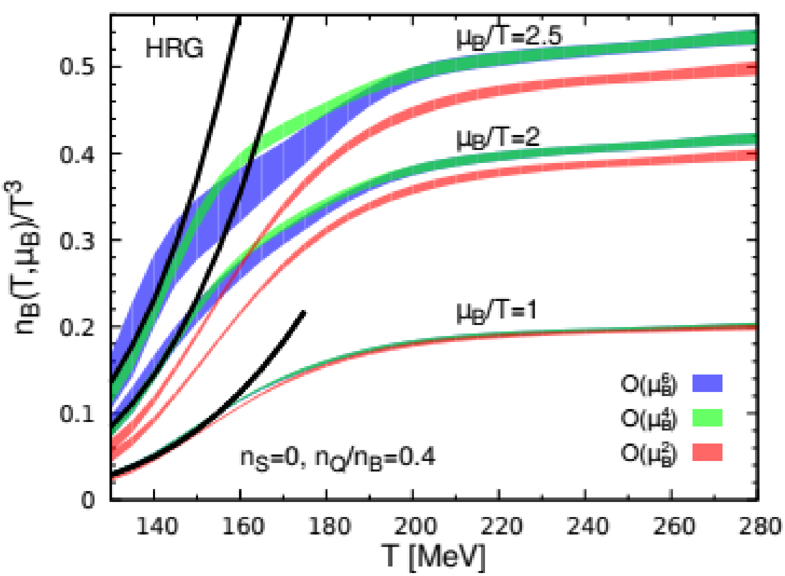
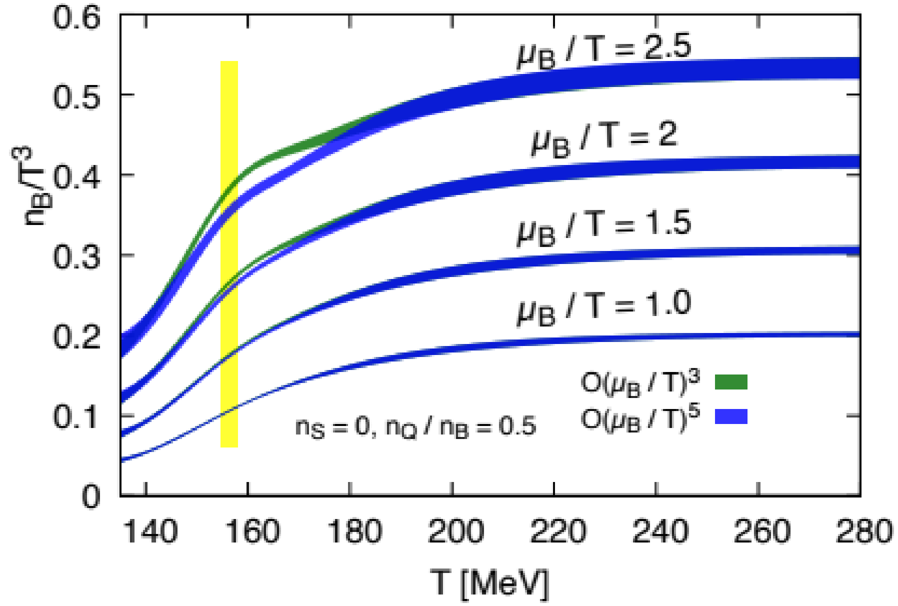


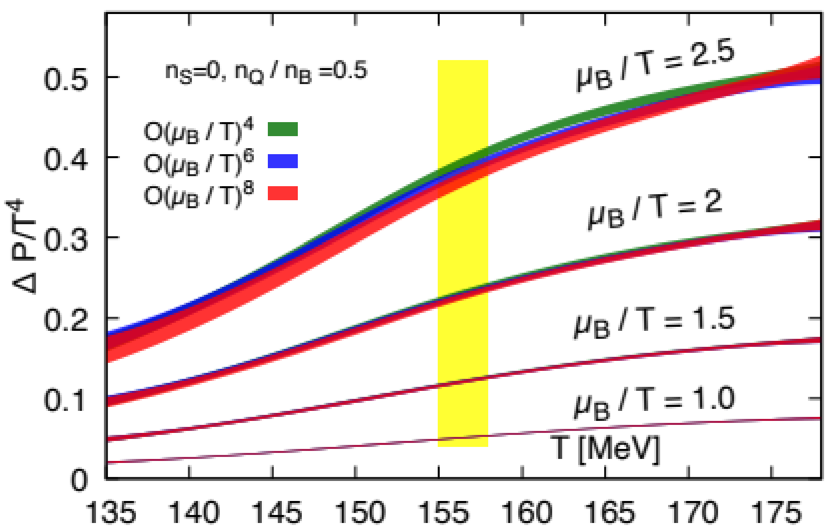




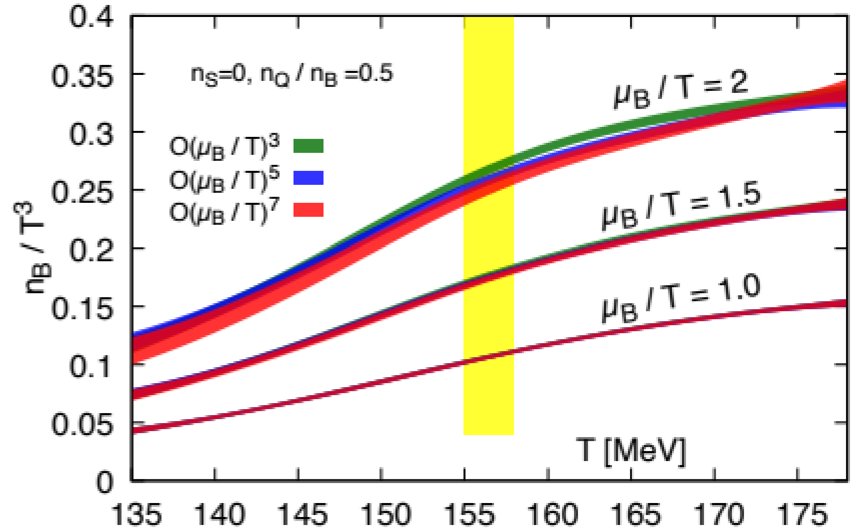


EoS 2022: Taylor series to 8th order

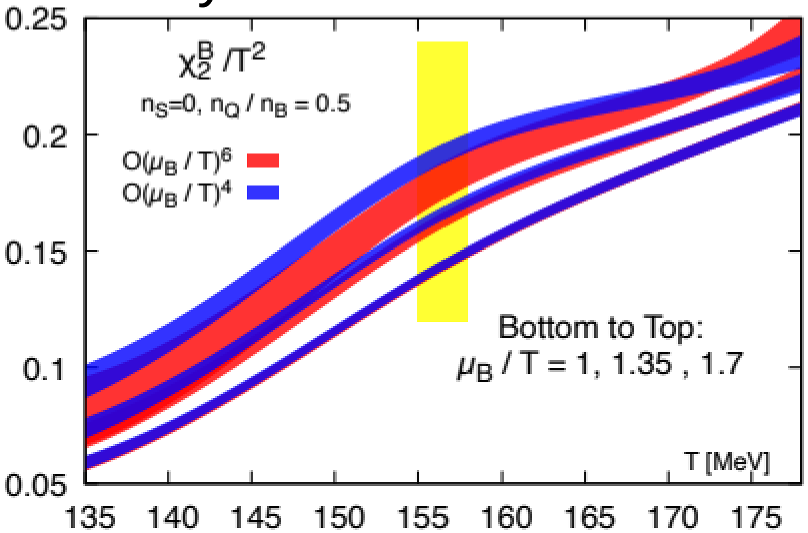
pressure



net baryon-number density



net baryon-number fluctuations



range of reliability of 8th order results in the transition region and below

observable	μ_B/T range
$\boldsymbol{\Delta P/T}4$	$\leq \mathbf{2.5}$
$\boldsymbol{n_B/T^3}$	$\leq \mathbf{2.0}$
$\boldsymbol{\chi_2^B}$	$\leq \mathbf{1.5}$

(see later slides)

Resumming Taylor series with Pade approximants

– conformal mappings — V. Skokov, K. Morita, B. Friman, arXiv:1008.4549
M. Giordano et al., arXiv:2004.10800
G. Basar, arXiv:2105.08080

– partial resummation — S. Modal, S. Mukherjee, P. Hegde , arXiv:2106.03165

– **Pade resummation** — R.V. Gavai and S. Gupta, arXiv:0806.2233
F.K. et al., arXiv:1009.5211
D. Bollweg et al (HotQCD), arXiv:2202.09184

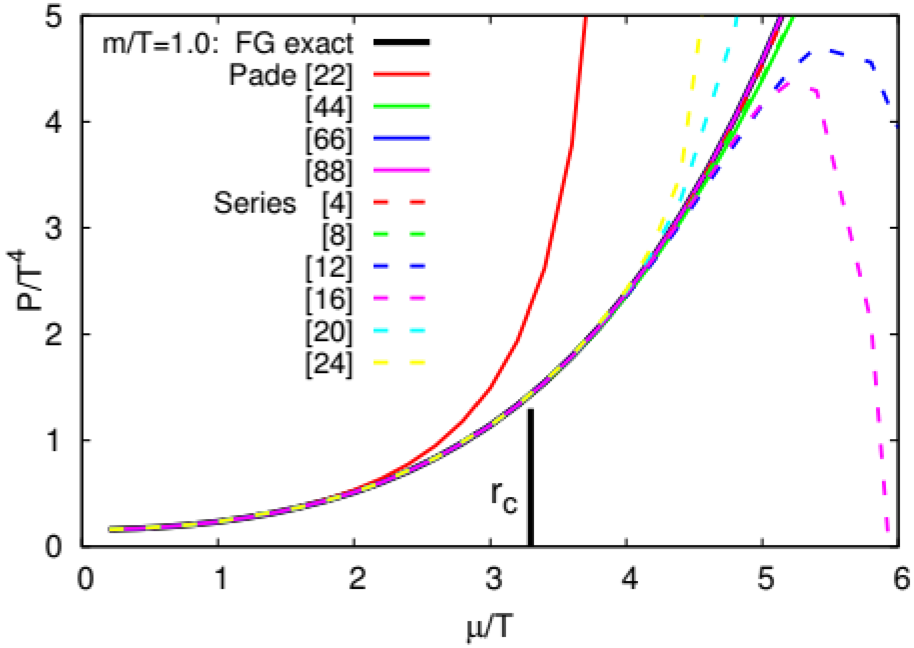
see also next talk by C. Schmidt

At high density QCD is dominated by properties of a Fermi gas at low as well as at high temperature:

– Taylor series for a relativistic Fermi gas as function of chemical potential has a radius of convergence controlled by a complex pole at $\mu_c/T = i\pi \pm m/T$
– series expansions in real μ break down at $r_c = \sqrt{\pi^2 + (m/T)^2}$

– diagonal Pades, P[n,n], have no problem avoiding the influence of such a singularity, which is far away from the real axis

– phase transitions are signaled by (stable) poles in Pade approximants on the real axis



QCD thermodynamics at non-zero net baryon-density – Taylor expansion and Pade resummation –

R.V. Gavai and S. Gupta, arXiv:0806.2233
F.K. et al., arXiv:1009.5211
D. Bollweg et al (HotQCD), arXiv:2202.09184

$$\frac{\Delta P}{T^4} = \sum_{k=1}^{n} P_{2k} \hat{\mu}_B^{2k}$$

$$\frac{n_B}{T^3} = \sum_{k=1}^{n} N_{B,2k-1} \hat{\mu}_B^{2k-1}$$

with $N_{B,2k-1} = (2k-1) P_{2k}$

for $\mu_Q = \mu_S = 0$

as well as $\mu_Q = n_S = 0$

$\Delta P/T^4$ and n_B/T^3 have identical radii of convergence

$$P[n,n] = \frac{\sum_{k=1}^{n} a_{k,0} \hat{\mu}_B^k}{\sum_{k=1}^{n} b_{k,0} \hat{\mu}_B^k}$$

$$P[n-1,n] = \frac{\sum_{k=1}^{n-1} a_{k,1} \hat{\mu}_B^k}{\sum_{k=1}^{n} b_{k,1} \hat{\mu}_B^k}$$

$P[n-1,n]$ and

$$P'[n,n] = \frac{\mathrm{d}P[n,n]}{\mathrm{d}\hat{\mu}_B}$$

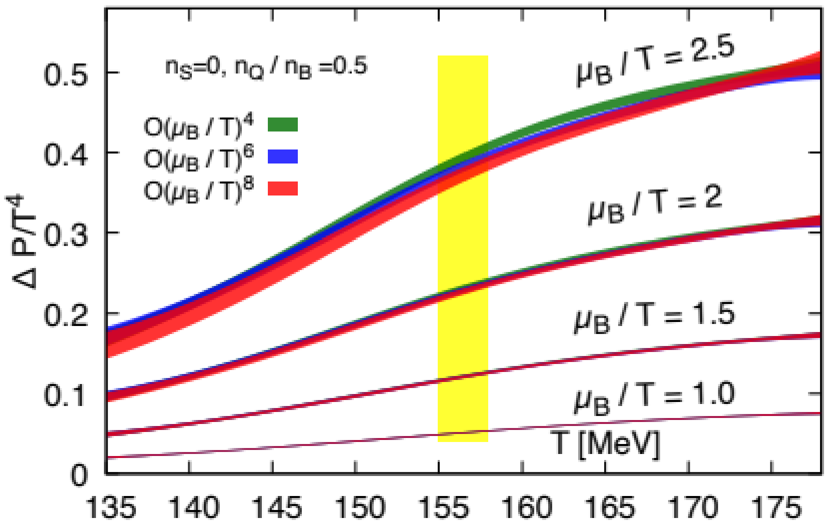
reproduce Taylor series of $\frac{n_B}{T^3}$

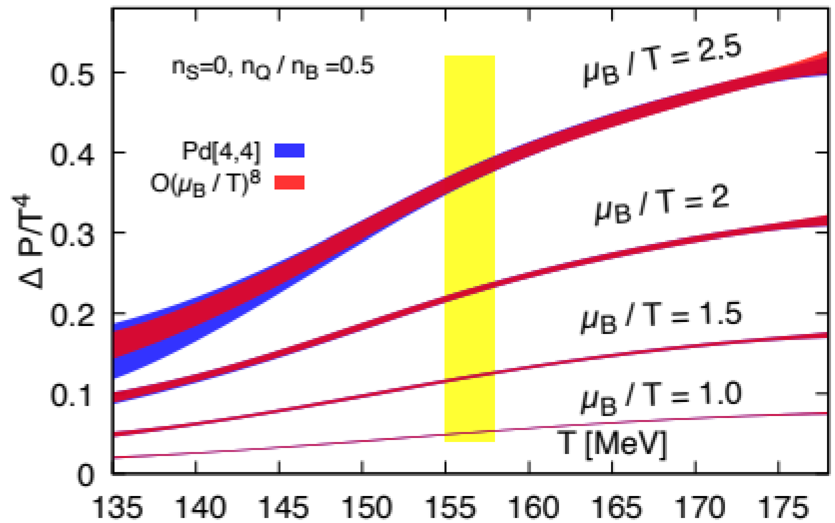
P[n,n] and P'[n,n] have identical pole structure

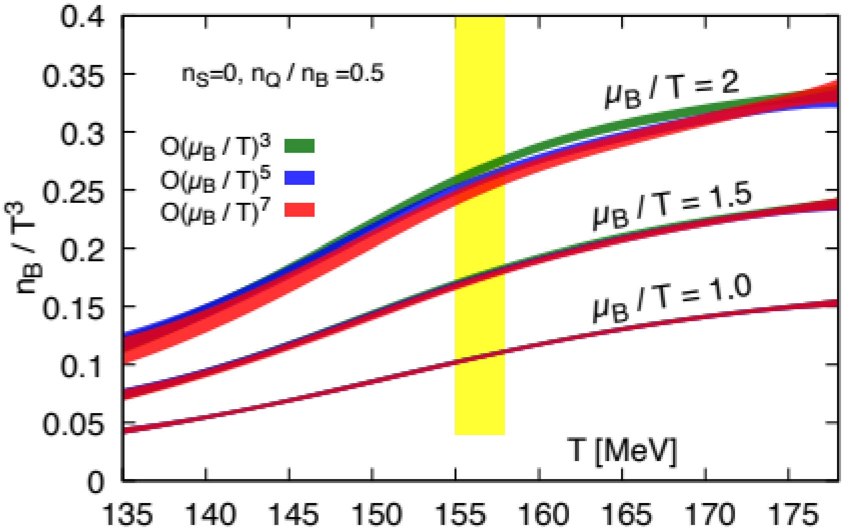
Comparing Taylor series and Pade resummation

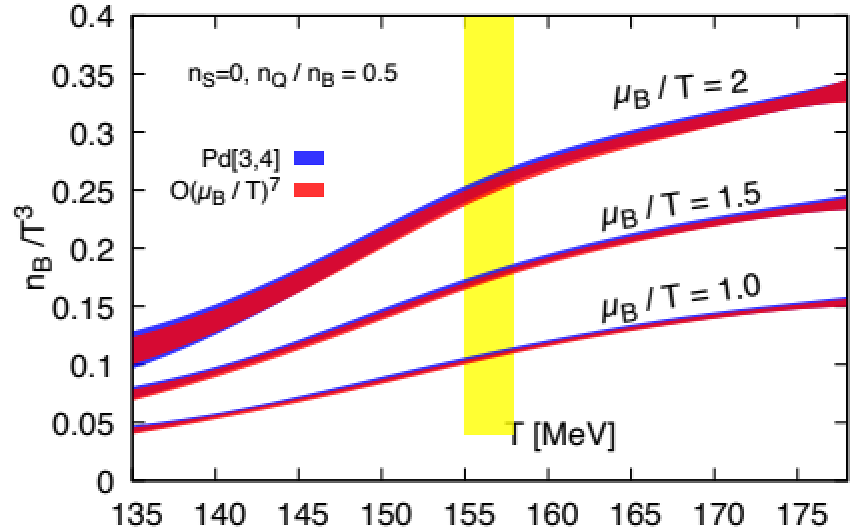
Taylor: $\mathcal{O}(\mu_B^n)$, $n = 4, 6, 8$

Taylor $\mathcal{O}(\mu_B^8)$ vs. [4,4] Pade

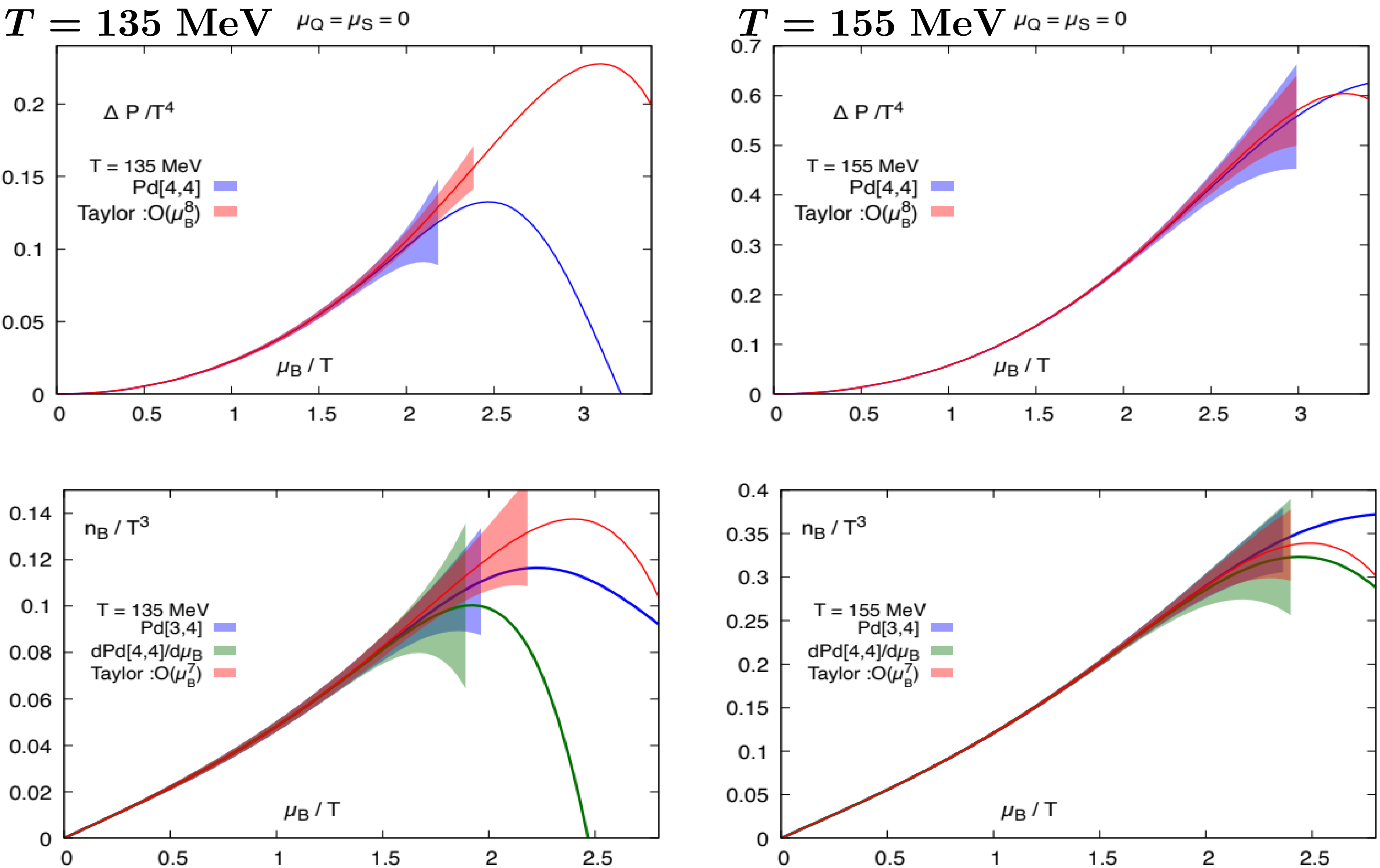








Comparing Taylor series and Pade resummation



agreement between Taylor series and Pade approximants in a larger μ_B range at higher temperature; qualitatively similar μ_B dependence

Analytic structure of the [n,n] Pade approximants

Pade resummation

HotQCD,
arXiv:2202.09184

$$\Delta P(T,\mu_B)/T^4 = P_2(T)\hat{\mu}_B^2 + P_4(T)\hat{\mu}_B^4 + P_6(T)\hat{\mu}_B^6 + P_8(T)\hat{\mu}_B^8 + \dots$$

$$P_n = \tilde{\chi}_0^{B,n}/n!$$

Note: $P_2 > 0\ ,\ P_4 > 0\ \forall\ T$ ⇒ suggests variable transformation

$$\bar{x} = \sqrt{\frac{P_4}{P_2}}\hat{\mu}_B = \sqrt{\frac{\tilde{\chi}_0^{B,4}}{12\tilde{\chi}_0^{B,2}}}\ \hat{\mu}_B$$

$$\Rightarrow \frac{\Delta P(T,\mu_B)}{T^4}\frac{P_4}{P_2^2} = \sum_{k=1}^{\infty} c_{2k,2}\bar{x}^{2k} = \bar{x}^2 + \bar{x}^4 + c_{6,2}\bar{x}^6 + c_{8,2}\bar{x}^8 + \dots$$

$$c_{2k,2} = \frac{P_{2k}}{P_2}\left(\frac{P_2}{P_4}\right)^{k-1} = \frac{1}{6}\frac{12^k}{(2k)!}\frac{\tilde{\chi}_0^{B,2k}}{\tilde{\chi}_0^{B,2}}\left(\frac{\tilde{\chi}_0^{B,2}}{\tilde{\chi}_0^{B,4}}\right)^{k-1}$$

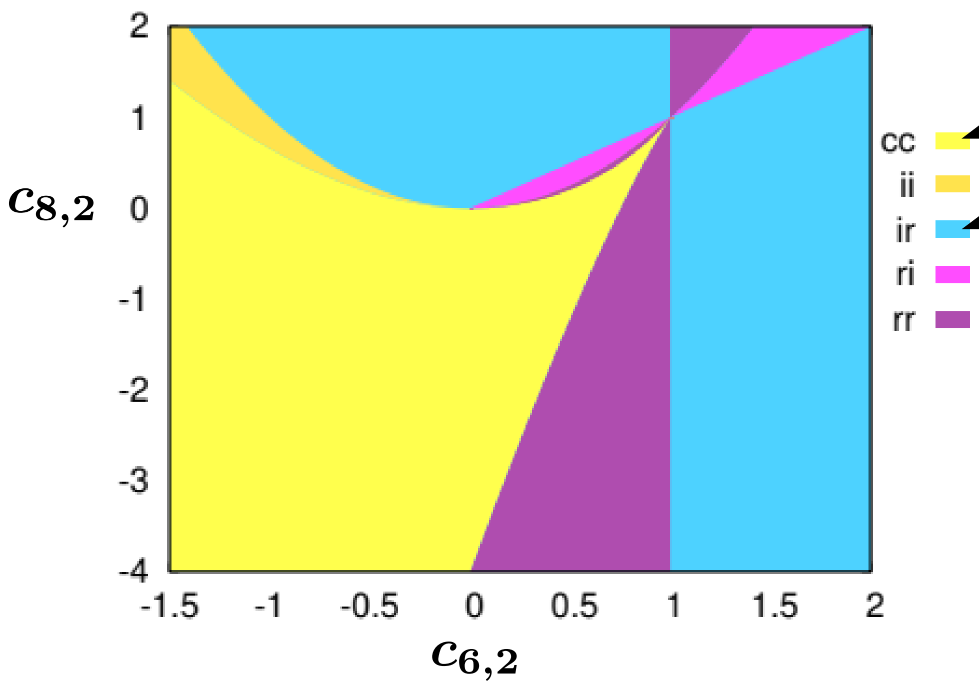
Poles of [n,n] Pade approximants in QCD

– P[2,2] poles on real axis at $\bar{x} = \pm 1$ ⇐ consequence of $\tilde{\chi}_0^{B,2} > 0\ ,\ \tilde{\chi}_0^{B,4} > 0\ \forall\ T$

$$P[2,2] \ = \ \frac{\bar{x}^2}{1-\bar{x}^2}$$

– poles of P[4,4] are controlled by $c_{6,2}$ and $c_{8,2}$ only

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



2 pairs of complex poles

1 pair of purely imaginary poles
1 pair of real poles
imag. pole is closest to origin

in most of the parameter space the radius of convergence is controlled by a complex or even purely imaginary pole

Poles of [n,n] Pade approximants in QCD

– P[2,2] poles on real axis at $\bar{x} = \pm 1$ ⇦ consequence of $\tilde{\chi}_0^{B,2} > 0\ ,\ \tilde{\chi}_0^{B,4} > 0\ \forall\, T$

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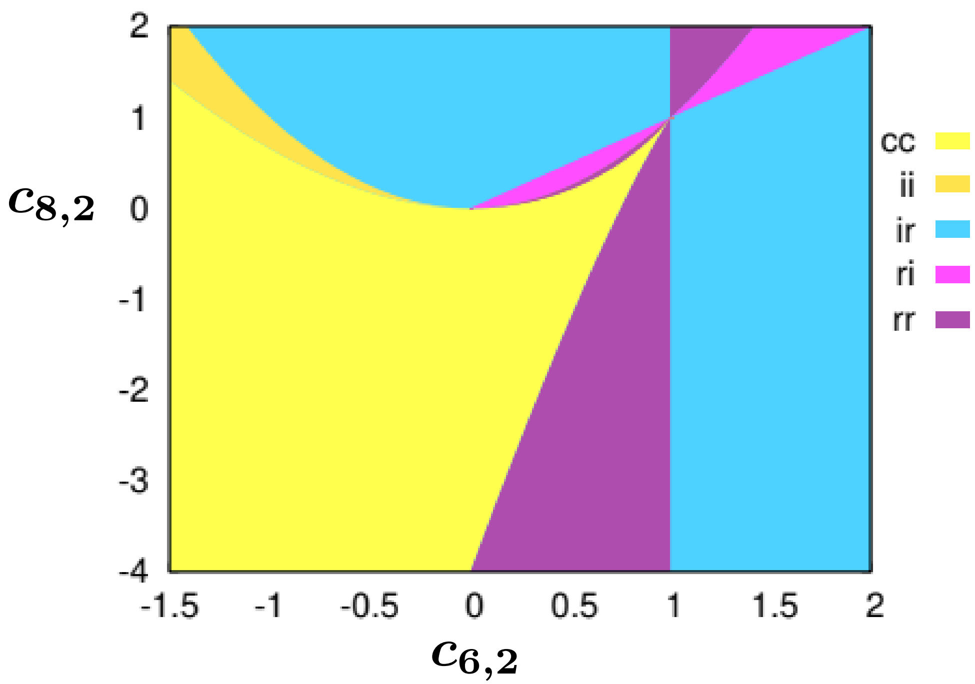
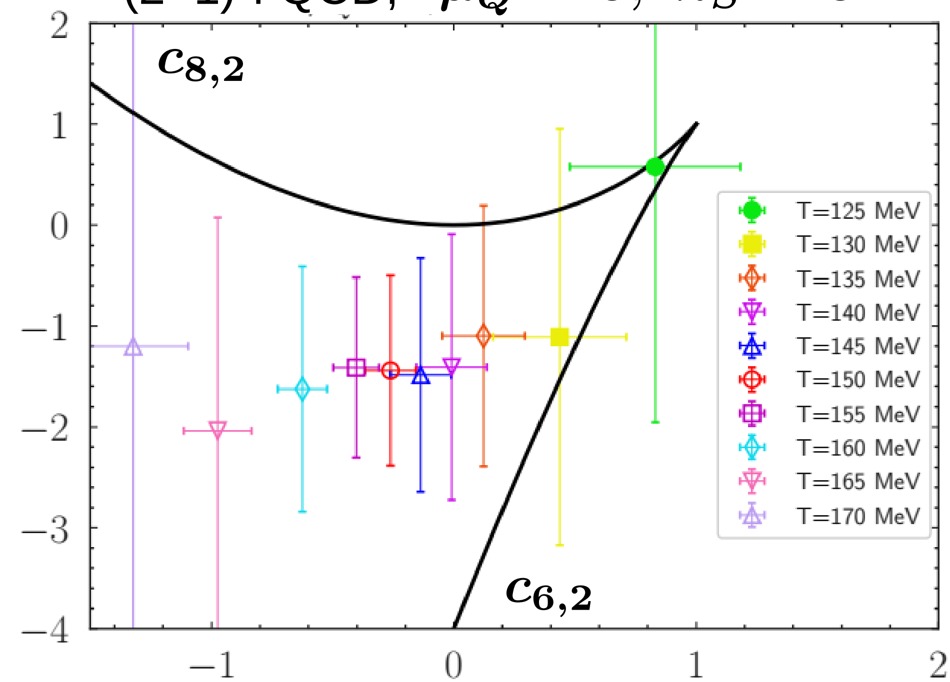


(2+1)-f QCD, $\mu_Q = 0,\ n_S = 0$



complex poles for T> 135 MeV

Poles of [n,n] Pade approximants in QCD

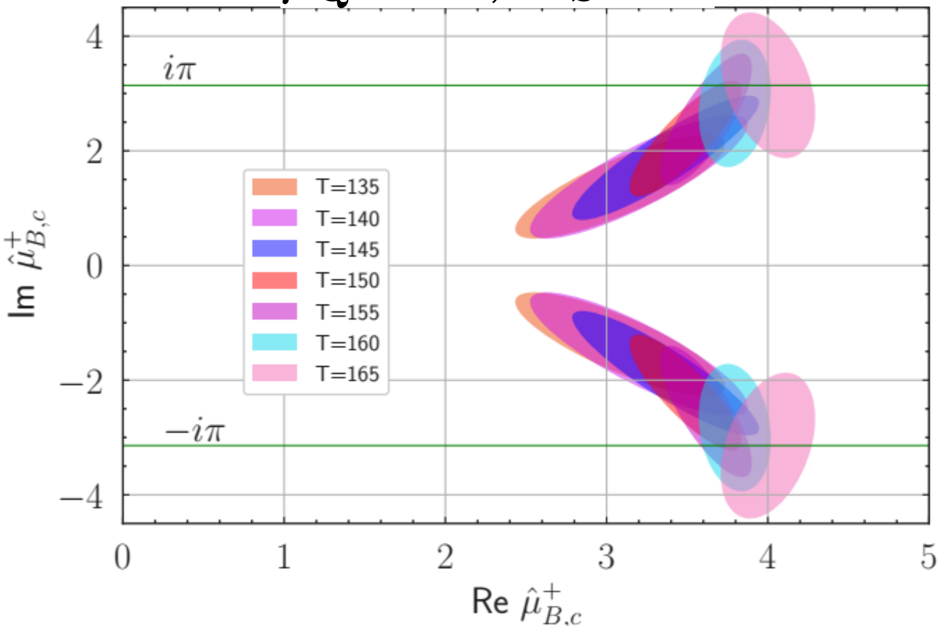
complex poles move to real axis as temperature decreases

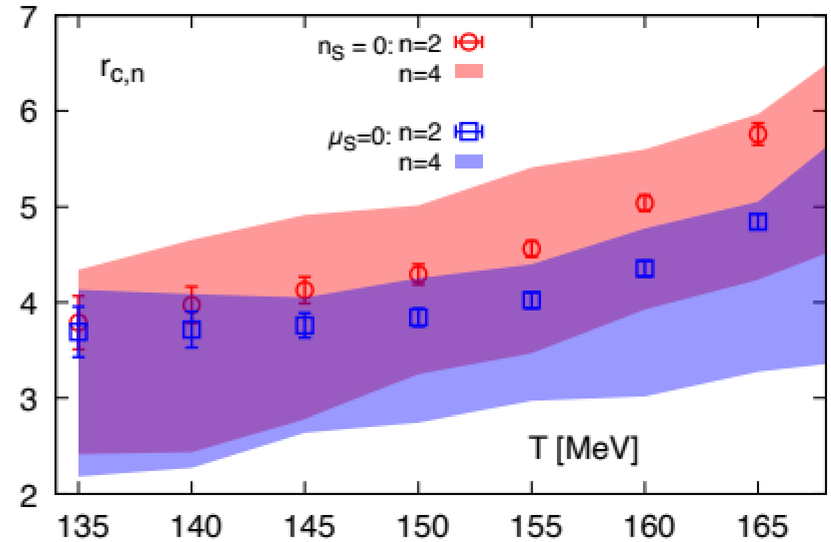
$$\hat{\mu}^{\pm}_{B,c} = \pm r_{c,4} e^{\pm i\Theta_{c,4}}$$

distance of complex poles from the origin is given by the **Mercer-Roberts estimator** for the radius of convergence

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

$$\mu_Q = 0\ ,\ n_S = 0$$



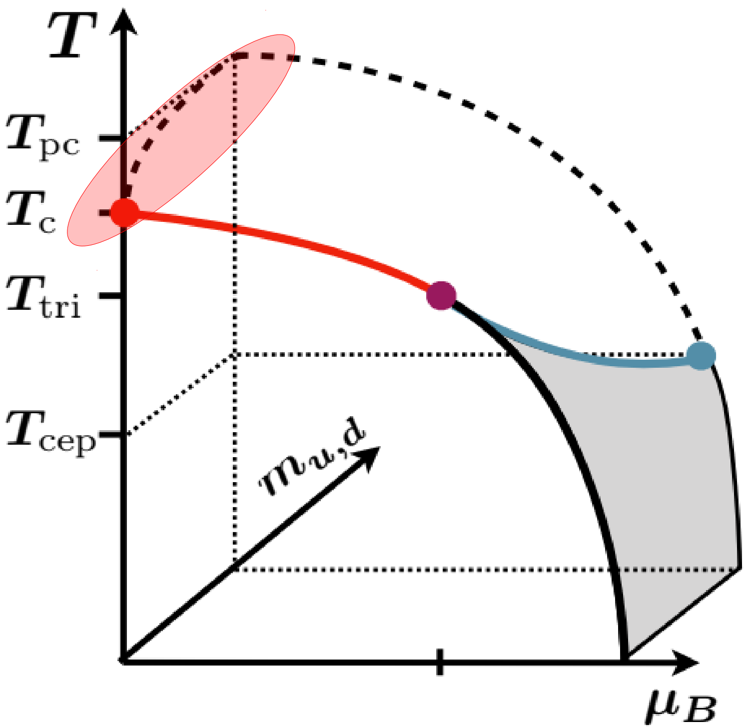


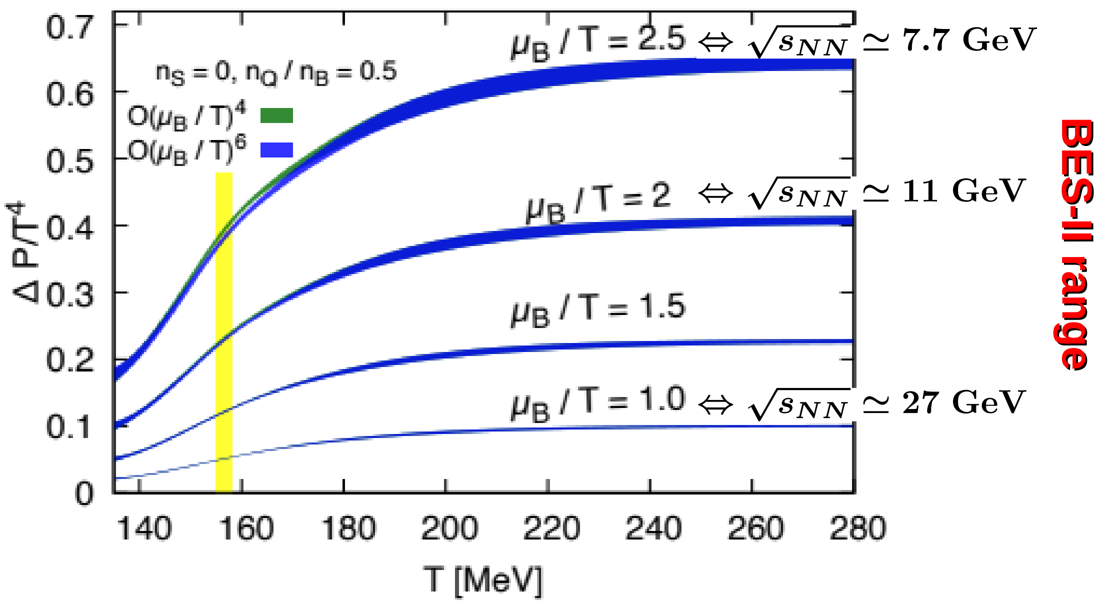
within current errors poles on the real axis (critical point) are possible only for

$$T \leq 135\mathrm{MeV}\ ,\ \mu_B/T > 2.5$$

higher statistics will sharpen the constraint

Conclusions





What we learned so far about the CEP in QCD from lattice QCD calculations:

I) the critical temperature is below $T_c = 132^{+3}_{-6}$ MeV

II) the corresponding critical chemical potential is likely to be above 400 MeV

→ Taylor expansions need to be resummed in order to reach CEP

– no CEP for $\mu_B/T \le 2.5$

– CEP not in the BES-II range

– EoS (pressure & number density) well controlled for
$\mu_B/T \le 2.0\ \forall T > 135$ MeV
(large range for higher T)

– reliable μ_B - range is smaller for higher order cumulants, given only an 8th order Taylor series for the pressure