Novel extrapolation scheme for lattice QCD equation of state

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with:
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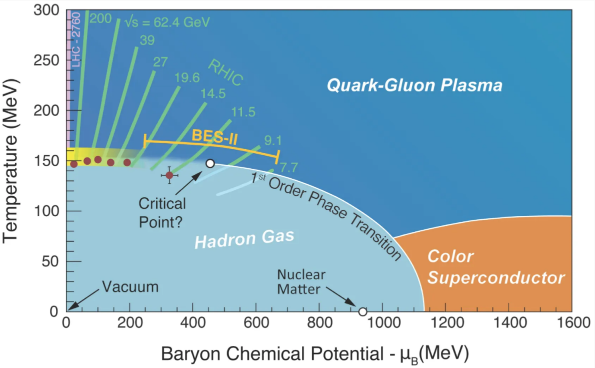
Introduction - The phase diagram of QCD

Different phases of QCD matter (in equilibrium) are depicted in (temperature vs baryo-chemical potential) phase diagram

- Early Universe-like conditions at $\mu_B = 0$ (matter-anti-matter symmetry)
- At $T \simeq 0$ and $\mu_B \simeq 922\,\mathrm{MeV}$ sits "ordinary nuclear matter" (e.g. a proton), while at much larger μ_B might sit **neutron stars** (cores)
- Transition form hadron gas to QGP at $\mu_B = 0$ is **a smooth crossover** at $T \simeq 155 - 160\,\mathrm{MeV}$
- At larger μ_B, the transition is believed to become of first order → **critical point**



Study of the QCD phase diagram

Theoretical investigation of the phase diagram make use of different methods and tools

From first principles:

- **Lattice QCD**
- Perturbation theory
- Functional methods (functional renormalization group - FRG, Dyson-Schwinger equations, etc...)

Models:

- Nambu-Jona-Lasinio (NJL) -type models (**Nambu and Jona-Lasinio, Phys. Rev. 122 (1961) 345, Phys. Rev. 124 (1961) 246**)
- Hadron Resonance Gas (HRG) -type models (**Hagedorn, Nuovo Cim. Suppl. 3 (1965), 147**)
- ...

Thermodynamic description of QCD

Thermodynamics of QCD is commonly investigated in grancanonical ensemble

$$\mathcal{Z} = \sum_N Z_N e^{\mu N}$$

- **Equation of State (EoS)** is extremely important since it completely describes the equilibrium properties of QCD matter
- One of the main inputs to hydro and several other tools for calculations in heavy-ion collisions and higher-density physics.
- Thermodynamic quantities follow directly from the grancanonical partition function $\mathcal{Z}$ and the relation:

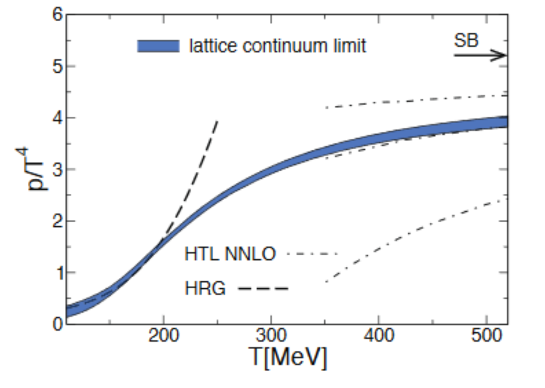
$$-k_B T \ln \mathcal{Z} = U - TS - \mu N$$

  - **Pressure**: $p = -k_B T \frac{\partial \ln \mathcal{Z}}{\partial V}$
  - **Entropy density**: $s = \left(\frac{\partial p}{\partial T}\right)_{\mu_i}$
  - **Charge densities**: $n_i = \left(\frac{\partial p}{\partial \mu_i}\right)_{T,\mu_{j\neq i}}$
  - **Energy density**: $\epsilon = Ts - p + \sum_i \mu_i n_i$
  - **Speed of sound**: $c_s^2 = \left(\frac{\partial p}{\partial \epsilon}\right)_{s/n_B}$
  - More (**Fluctuations**, etc...)

EoS at $\mu_B = 0$

A combination of methods gives us good understanding of the EoS at $\mu_B = 0$ at all temperatures

- Perturbative QCD at high temperature
  → "pure quark-gluon phase"
- Hadron Resonance Gas (HRG) model at low temperature
  → "pure hadron phase"
- **Lattice QCD bridges between regimes and captures the transition**

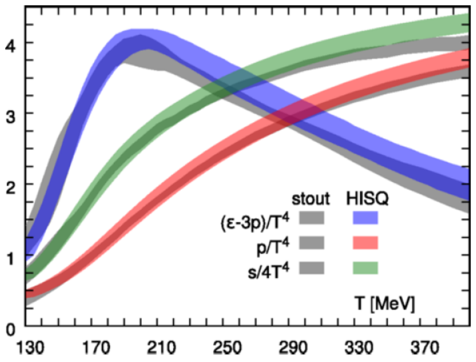


WB: Borsányi *et al.*, PLB 370 (2014) 99-104

Lattice QCD: equation of state at $\mu_B = 0$

- EoS at vanishing chemical potential known to high precision for a few years now (continuum limit, physical quark masses)
- Great agreement between different collaborations

$\Rightarrow$ Systematics are well under control and results are extremely reliable



WB: Borsányi *et al.*, PLB 370 (2014) 99-104, HotQCD: Bazavov *et al.* PRD 90 (2014) 094503

Lattice QCD at finite μ_B

Lattice QCD suffers from the **sign problem** at finite chemical potential

- Taylor expansion around $\mu_B = 0$

$$\frac{p(T,\mu_B)}{T^4} = \sum_{n=0}^{\infty} c_{2n}(T) \left(\frac{\mu_B}{T}\right)^{2n} \quad , \qquad c_n(T) = \frac{1}{n!}\chi_n^B(T,\mu_B = 0)$$

- Analytical continuation from imaginary μ_B
- Other methods to work around the sign problem still in exploratory stages
  - Reweighting techniques
  - Complex Langevin
  - Lefschetz thimbles
  - ...
- **The equation of state:** lattice results for the Taylor coefficients are currently available up to $\mathcal{O}(\hat{\mu}_B^8)$, but the reach is still limited to $\hat{\mu}_B \lesssim 2 - 2.5$ despite great computational effort (**WB: Borsányi *et al.* JHEP 10 (2018) 205, HotQCD: Bazavov *et al.* PRD101 (2020), 074502**)

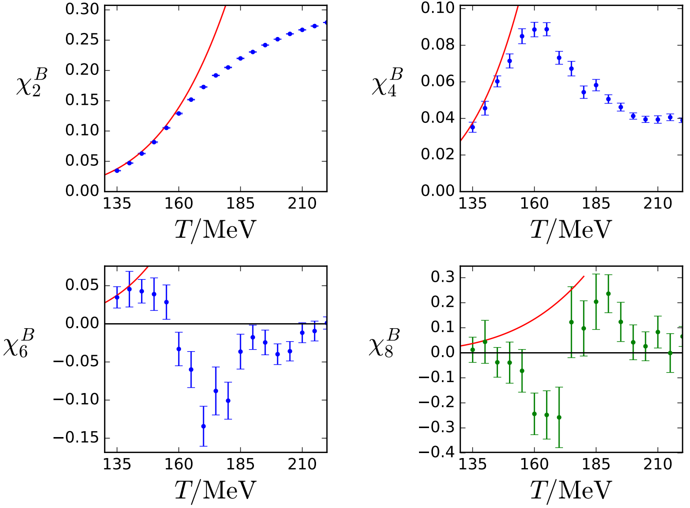
Lattice QCD at finite μ_B - Taylor coefficients

- Fluctuations of baryon number are the Taylor expansion coefficients of the pressure

$$\chi^{BQS}_{ijk}(T) = \left.\frac{\partial^{i+j+k} p/T^4}{\partial\hat\mu^i_B \partial\hat\mu^j_Q \partial\hat\mu^k_S}\right|_{\vec\mu=0}$$

- Signal extraction is increasingly difficult with higher orders, especially in the transition region

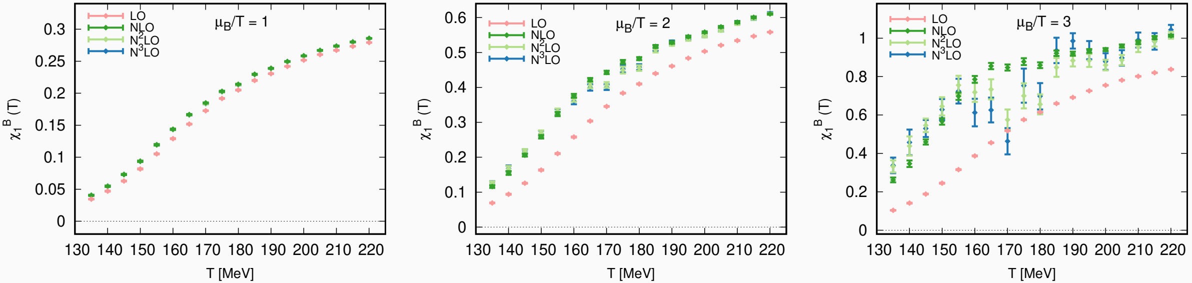
- Higher order coefficients present a more complicated structure



WB: Borsányi *et al.* JHEP 10 (2018) 205; (also e.g., HotQCD: Bazavov *et al.* PRD101 (2020), 074502)

Lattice QCD at finite μ_B - Taylor expansion

- Thermodynamic quantities at large chemical potential become problematic
- Higher orders do not help with the convergence of the series



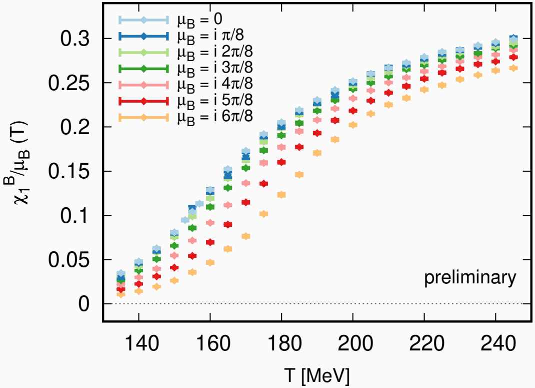
- Inherent problem with Taylor expansion: carried out at $T = \text{const}$. This doesn't cope well with $\hat{\mu}_B-$dependent transition temperaure
- Can we find an alternative expansion to improve finite-$\hat{\mu}_B$ behavior?

An alternative approach

From simulations at imaginary μ_B we *observe* that $\chi_1^B(T, \hat{\mu}_B)$ at (imaginary) $\hat{\mu}_B$ appears to be differing from $\chi_2^B(T, 0)$ mostly by a shift in T:

$$\frac{\chi_1^B(T, \hat{\mu}_B)}{\hat{\mu}_B} = \chi_2^B(T', 0) \ , \quad T' = T\left(1 + \kappa\, \hat{\mu}_B^2\right)$$

- More apparent close to the transition
- **Important note:** We can't expect this simple description to work at high-T. However:
  - At high-T Taylor expansion has no problems ($\chi_n^B \simeq 0 \ \forall n > 4$)
  - We don't need EoS from lattice at high-T
- We extend the formalism of "lines of constant physics" from **HotQCD: Bazavov *et al.* PRD 95 (2017) 054504**

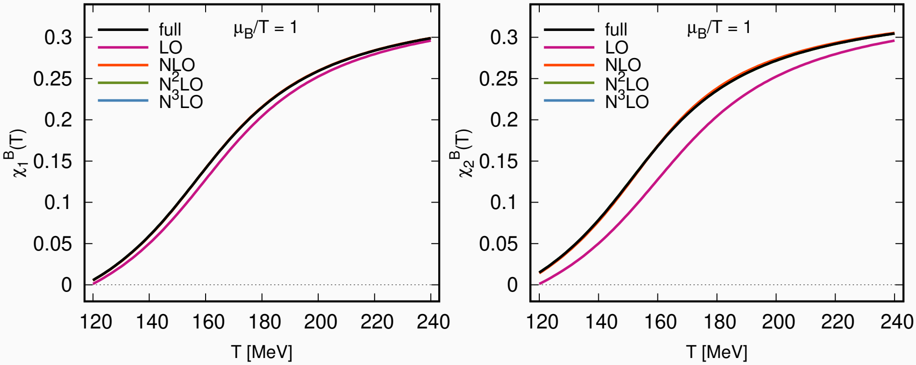


Taylor expanding a (shifting) sigmoid

Assume we have a sigmoid function $f(T)$ which shifts with $\hat{\mu}$, with a simple T-independent shifting parameter κ. How does Taylor cope with it?

$$f(T,\,\hat{\mu}) = f(T',0)\;, \qquad\qquad T' = T(1+\kappa\,\hat{\mu}^2)\;,$$

We fitted $f(T,0) = a + b\,\arctan(c(T-d))$ to $\chi_2^B(T,0)$ data for a 48×12 lattice



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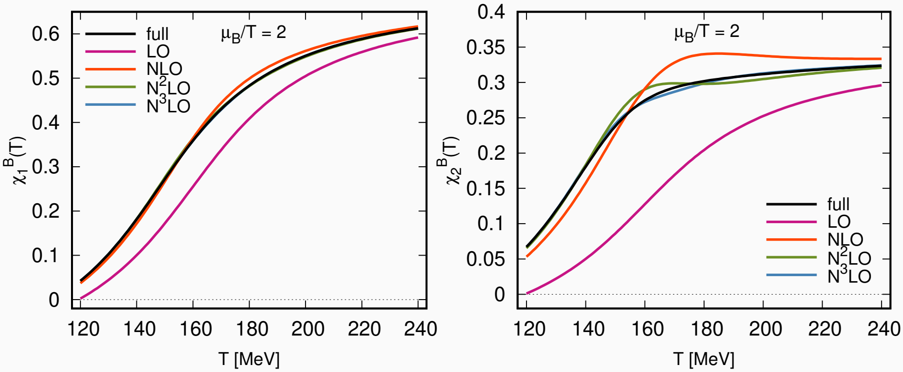

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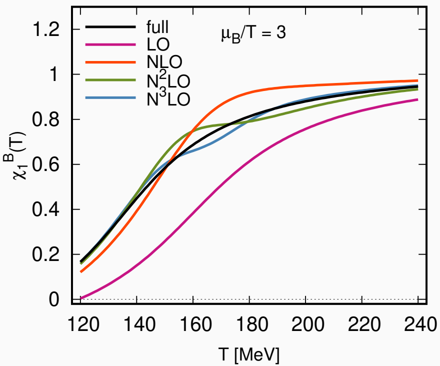
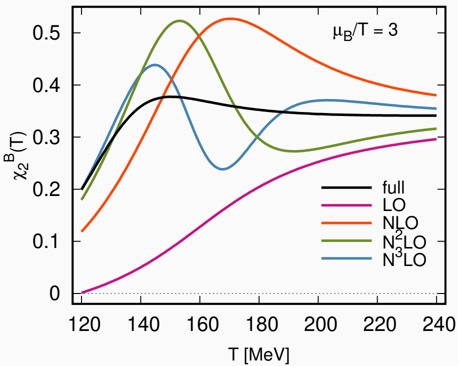
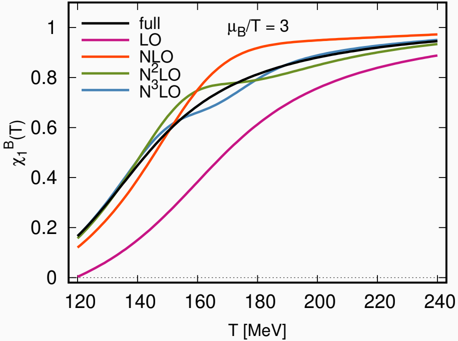
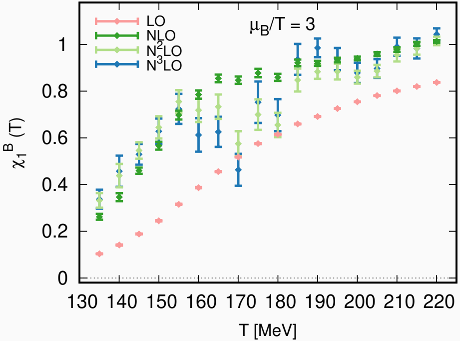




Taylor expanding a sigmoid

- The Taylor expansion seems to have problems reproducing the original function (left)
- A similar picture arises from actual lattice data (right)



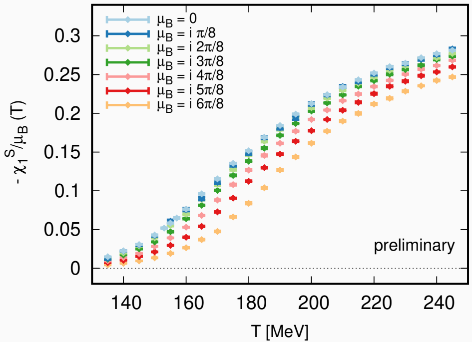


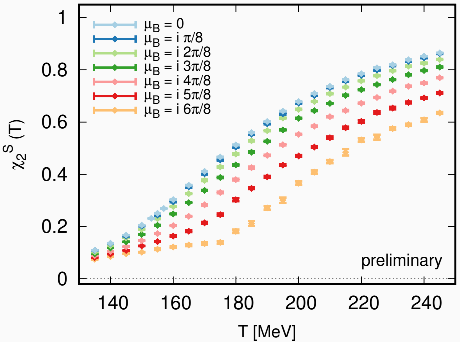
- Problems at T slightly larger than T_{pc} $\Rightarrow$ influence from structure in χ_6^B and χ_8^B

An alternative approach

We also notice that a very similar scenario appears for:

$$\frac{\chi_1^S}{\hat{\mu}_B}(T,\, \hat{\mu}_B) = \chi_{11}^{BS}(T', 0)\ , \qquad \chi_2^S(T,\, \hat{\mu}_B) = \chi_2^S(T', 0)$$





Formulation

- We have observed the $\hat{\mu}_B$-dependence seems to amout to a simple T-shift
- However, a simplistic scenario with a single T- independent parameter κ cannot be sufficient, hence we seek a systematic treatment which can serve as an alternative to Taylor expansion
- We allow for more than $\mathcal{O}(\hat{\mu}^2)$ expansion of T' and letting the coefficients be $T-$dependent:

$$\frac{\chi_1^B(T, \hat{\mu}_B)}{\hat{\mu}_B} = \chi_2^B(T', 0) \ , \quad T' = T \left(1 + \kappa_2(T)\, \hat{\mu}_B^2 + \kappa_4(T)\, \hat{\mu}_B^4 + \mathcal{O}(\hat{\mu}_B^6)\right)$$

- **Important:** we are simply re-organizing the Taylor expansion via an expansion of the shift

$$\Delta T = T - T' = \left(\kappa_2(T)\, \hat{\mu}_B^2 + \kappa_4(T)\, \hat{\mu}_B^4 + \mathcal{O}(\hat{\mu}_B^6)\right)$$

HotQCD: Bazavov *et al.* PRD 95 (2017) 054504

Formulation

1. With a Taylor expansion one has:

$$\frac{\chi_1^B(T,\,\hat{\mu}_B)}{\hat{\mu}_B} = \chi_2^B(T,0) + \frac{1}{3!}\chi_4^B(T,0)\,\hat{\mu}_B^2 + \frac{1}{5!}\chi_6^B(T,0)\,\hat{\mu}_B^4 + \mathcal{O}(\,\hat{\mu}_B^6)$$

2. On the other hand, with an expansion in $\Delta T = T - T'$ one can write:

$$\begin{aligned}\frac{\chi_1^B(T,\,\hat{\mu}_B)}{\hat{\mu}_B} &= \chi_2^B(T,0) + \Delta T\frac{d\chi_2}{dT} + \frac{1}{2}\Delta T^2\frac{d^2\chi_2}{dT^2} + \mathcal{O}(\Delta T^3) = \\ &= \chi_2^B(T,0) + \kappa_2(T)\,T\frac{d\chi_2}{dT}\,\hat{\mu}_B^2 + \left[\frac{T^2}{2}\kappa_2^2(T)\frac{d^2\chi_2}{dT^2} + T\kappa_4(T)\frac{d\chi_2}{dT}\right]\hat{\mu}_B^4 + \mathcal{O}(\,\hat{\mu}_B^6)\end{aligned}$$

since $\Delta T = T\left(\kappa_2(T)\,\hat{\mu}_B^2 + \kappa_4(T)\,\hat{\mu}_B^4\right)$.

Formulation

Equating same-order terms in the previous expansions one can easily show that:

$$\kappa_2(T) = \frac{1}{6T}\frac{\chi_4^B(T)}{\chi_2^{B\prime}(T)}$$

$$\kappa_4(T) = \frac{1}{360\chi_2^{B\prime}(T)^3}\left(3\chi_2^{B\prime}(T)^2\chi_6^B(T) - 5\chi_2^{B\prime\prime}(T)\chi_4^B(T)^2\right)$$

$$\dots$$

- The procedure can in principle be carried over systematically
- Higher order terms still suffer from cancellations and can be challenging
- **However** we can exploit imaginary- $\hat{\mu}_B$ simulations to extract $\kappa_n(T)$

Formulation

Similar relations can be derived analogously from:

$$\frac{\chi_1^S}{\hat{\mu}_B}(T,\,\hat{\mu}_B) = \chi_{11}^{BS}(T',0)\ , \qquad \chi_2^S(T,\,\hat{\mu}_B) = \chi_2^S(T',0)$$

yielding:

$$\kappa_2^{BS}(T) = \frac{1}{6T}\frac{\chi_{31}^{BS}(T)}{\chi_{11}^{BS\prime}(T)} \qquad \kappa_2^{S}(T) = \frac{1}{2T}\frac{\chi_{22}^{BS}(T)}{\chi_{2}^{S\prime}(T)}$$

$$\kappa_4^{BS}(T) = \frac{1}{360\chi_{11}^{BS\prime}(T)^3}\Big(3\chi_{11}^{BS\prime}(T)^2\chi_{51}^{BS}(T) - 5\chi_{11}^{BS\prime\prime}(T)\chi_{31}^{BS}(T)^2\Big) \qquad \kappa_4^{S}(T) = \frac{1}{24\chi_{2}^{S\prime}(T)^3}\Big(\chi_{2}^{S\prime}(T)^2\chi_{42}^{BS}(T) - 3\chi_{2}^{S\prime\prime}(T)\chi_{22}^{BS}(T)^2\Big)$$

Determine κ_n

I. Directly determine $\kappa_2(T)$ at $\hat{\mu}_B = 0$ from:

$$\kappa_2(T) = \frac{1}{6T} \frac{\chi_4^B(T)}{\chi_2^{B\prime}(T)}$$

II. From our imaginary-$\hat{\mu}_B$ simulations ($\hat{\mu}_Q = \hat{\mu}_S = 0$) we calculate:

$$\frac{T' - T}{T\,\hat{\mu}_B^2} = \kappa_2(T) + \kappa_4(T)\,\hat{\mu}_B^2 + \mathcal{O}(\hat{\mu}_B^4) = K(T)$$

III. Calculate the quantity $K(T, N_\tau, \hat{\mu}_B^2)$ for several $\hat{\mu}_B^2$ and for $N_\tau = 8, 10, 12$

IV. Perform a combined fit of the $\hat{\mu}_B^2$ and $1/N_\tau^2$ dependence of $K(T)$ at each temperature, yielding a continuum estimate for the coefficients

$\Rightarrow$ The $\mathcal{O}(1)$ and $\mathcal{O}(\hat{\mu}_B^2)$ coefficients of the fit are $\kappa_2(T)$ and $\kappa_4(T)$

Systematics

For an analysis of the systematic uncertainties, we consider:

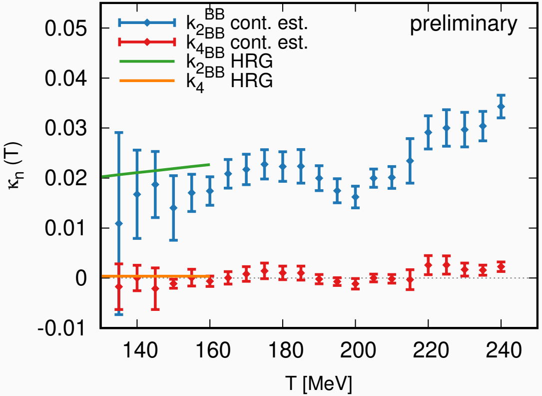
- 2x scale settings
- 2x choices of $\hat{\mu}_B$ fitting range ($\hat{\mu}_B = in\pi/8$ with $n \in \{0, 3-5\}$ or $n \in \{0, 3-6\}$)
- 3x fit functions. Always linear in $1/N_\tau^2$, and linear, parabolic or 1/linear in $\hat{\mu}_B^2$
- 2x splines at $\hat{\mu}_B = 0$

for a total of 24x analyses for each T.

At each temperature, the 24x analyses are combined with Akaike weights.

The results for $\kappa_2(T)$, $\kappa_4(T)$

- At low temperatures, there is agreement with the HRG model result
- As expected, at high temperatures κ_2 increases
- The values of κ_4 are always compatible with 0 $\rightarrow$ we have indication on the oder of magnuitude



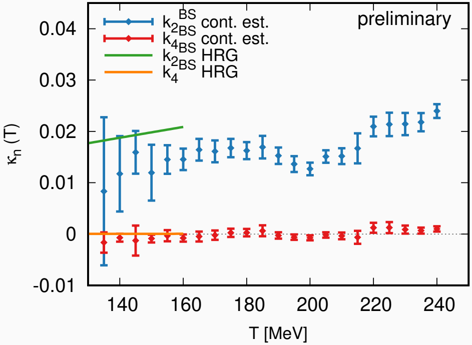
From the results we can tell our initial guess was not far-off:

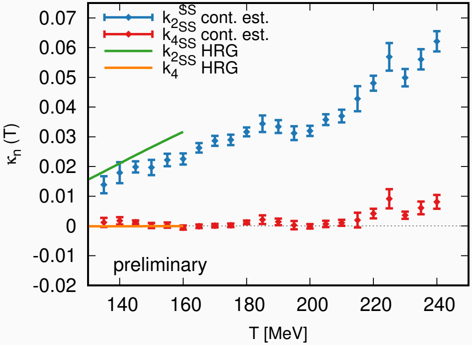
- $\kappa_2(T)$ does not vary much over a large T-range
- $\kappa_4(T)$ is indeed very small

HotQCD: Bazavov *et al.* PRD 95 (2017) 054504

The results for $\kappa_2(T)$, $\kappa_4(T)$

A similar picture appears for κ_n describing the shift in χ_{11}^{BS} and χ_2^S





Thermodynamics at finite (real) μ_B

Thermodynamic quantities at finite (real) μ_B can be reconstruted from the same ansazt:

$$\frac{n_B(T,\,\hat{\mu}_B)}{T^3} = \chi_B^2(T',0)$$

with $T' = T(1+\kappa_2(T)\,\hat{\mu}_B^2 + \kappa_4(T)\,\hat{\mu}_B^4)$.

From the baryon density n_B one finds the pressure:

$$\frac{p(T,\,\hat{\mu}_B)}{T^4} = \frac{p(T,0)}{T^4} + \int_0^{\hat{\mu}_B} \mathrm{d}\hat{\mu}'_B \frac{n_B(T,\,\hat{\mu}'_B)}{T^3}$$

then the entropy, energy density:

$$\frac{s(T,\,\hat{\mu}_B)}{T^4} = 4\frac{p(T,\,\hat{\mu}_B)}{T^4} + T\,\left.\frac{\partial p(T,\,\hat{\mu}_B)}{\partial T}\right|_{\hat{\mu}_B} - \,\hat{\mu}_B\frac{n_B(T,\,\hat{\mu}_B)}{T^3}$$

$$\frac{\epsilon(T,\,\hat{\mu}_B)}{T^4} = \frac{s(T,\,\hat{\mu}_B)}{T^3} - \frac{p(T,\,\hat{\mu}_B)}{T^4} + \,\hat{\mu}_B\frac{n_B(T,\,\hat{\mu}_B)}{T^3}$$

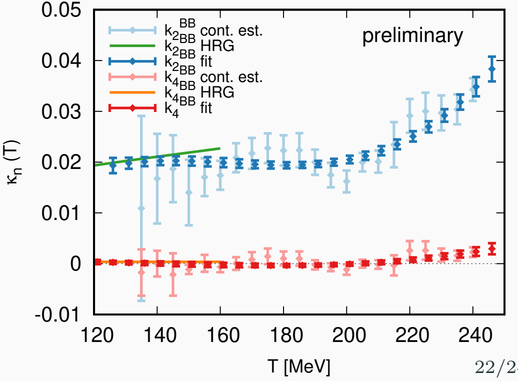
Thermodynamics at finite (real) μ_B

For our extrapolation at finite (real) chemical potential we use:

- Continuum extrapolated pressure and entropy density at $\hat{\mu}_B = 0$ (from **Borsányi *et al.* PLB 730 (2014) 99**)
- Continuum $\chi_2^B(T)$ at $\hat{\mu}_B = 0$ (from **Bellwied *et al.* PRD 92 (2015) 114505**)

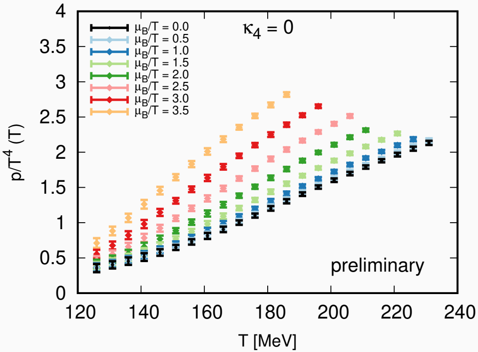
The last ingredients are the coefficients $\kappa_n(T)$:

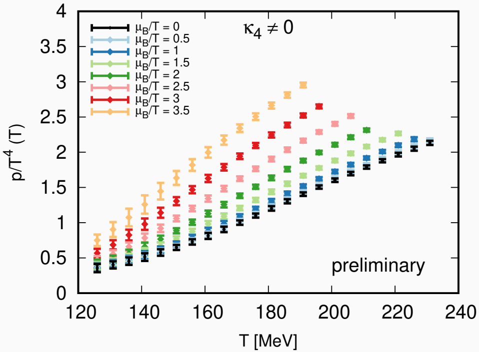
- The curves for $\kappa_2(T)$ and $\kappa_4(T)$ are the result of a fit (3^{rd} order polynomial)
- At low-T ($T < 135\,\text{MeV}$) we included a few HRG points to constraint the fit



Thermodynamics at finite (real) μ_B

- Including $\kappa_4(T)$ results in added error, but doesn't affect the results sensibly
- In any case, errors are under control up to $\hat{\mu}_B \simeq 3.5$
- At the level of the pressure, errors are extremely small (unsurprinsignly)





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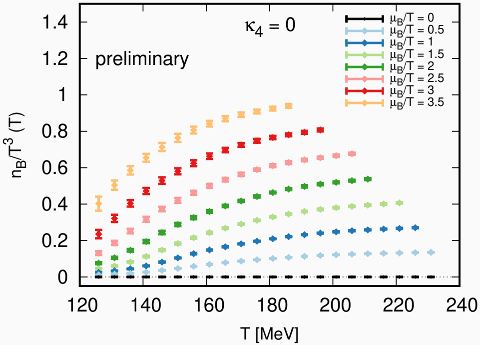

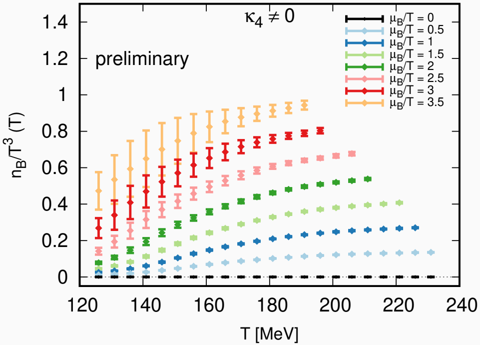

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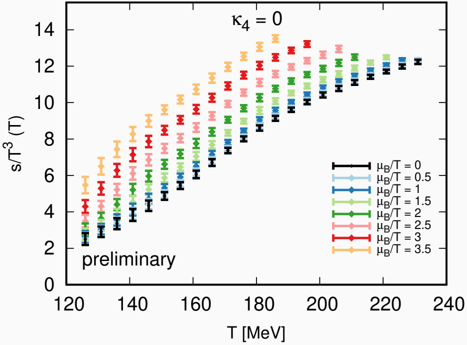

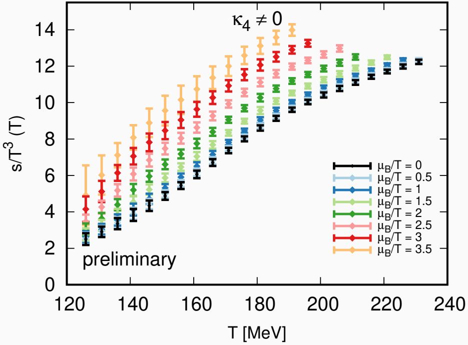

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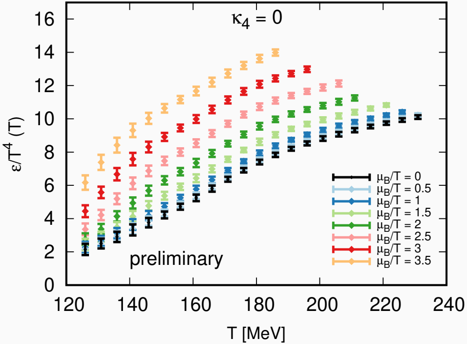

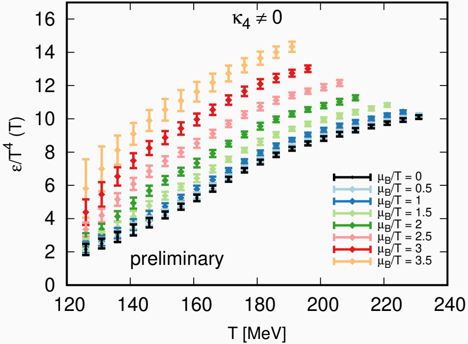

Summary

- The EoS for QCD at large chemical potential is highly demanded in HIC community, especially for hydrodynamic simulations
- Historical approach of Taylor expansion for EoS has shortcomings
  - Because of technical/numerical challenges
  - Because of phase structure of the theory
- An alternative summation scheme tailored to the specific behavior of relevant observables seems a better approach
- Just as Taylor, systematically improvable if given sufficient computing power

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THANK YOU!

BACKUP

The results for $\kappa_2(T)$, $\kappa_4(T)$

The coefficients $\kappa_2(T)$ and $\kappa_4(T)$ calculated on a $24^3 \times 8$ lattice vs. our polynomial fit