Lattice QCD equation of state at finite chemical potential from an alternative expansion scheme

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Strangeness in Quark Matter 2021

with:

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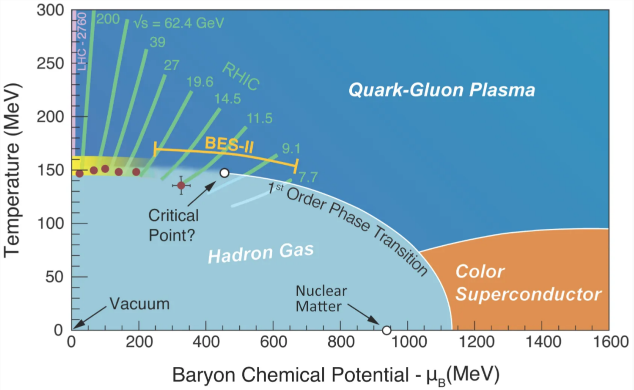
The phase diagram of QCD

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)
- Transition form hadron gas to QGP at $\mu_B = 0$ is **a smooth crossover** at $T \simeq 155 - 160\,\text{MeV}$
- At larger μ_B, the transition is believed to become of first order $\rightarrow$ **critical point**
- Investigations from first principles:
    - **Lattice QCD**
    - Perturbative methods (HTL, etc.)
    - Functional methods (FRG, DSE, etc.)

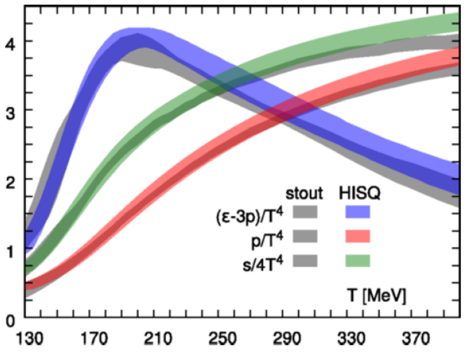


Lattice QCD: equation of state (EoS)

- ★ Completely describes equilibrium properties of QCD matter, and is a crucial input to hydrodynamic simulations
- ★ Known at $\mu_B = 0$ to high precision for a few years now (continuum limit, physical quark masses) $\longrightarrow$ Agreement between different calculations

From grancanonical partition function $\mathcal{Z}$

- ∗ **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**: $\epsilon = Ts - p + \sum_i \mu_i n_i$
- ∗ More (**Fluctuations**, etc...)



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**)

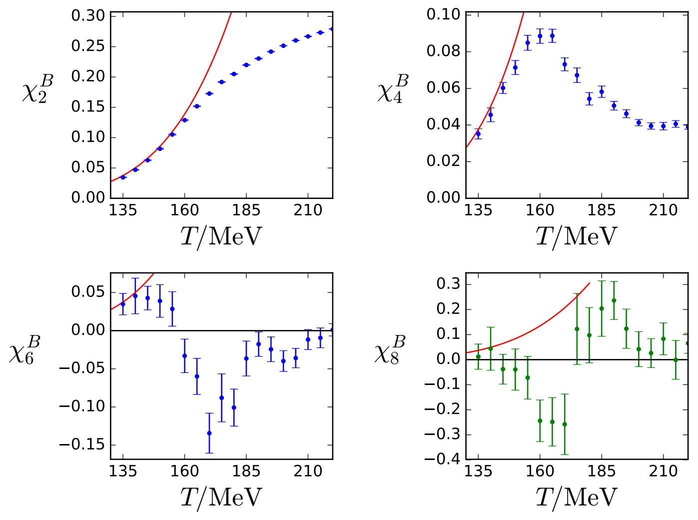
Lattice QCD at finite μ_B - Taylor coefficients

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

$$\chi_{ijk}^{BQS}(T) = \frac{\partial^{i+j+k} p/T^4}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k}\bigg|_{\vec{\mu}=0}$$

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

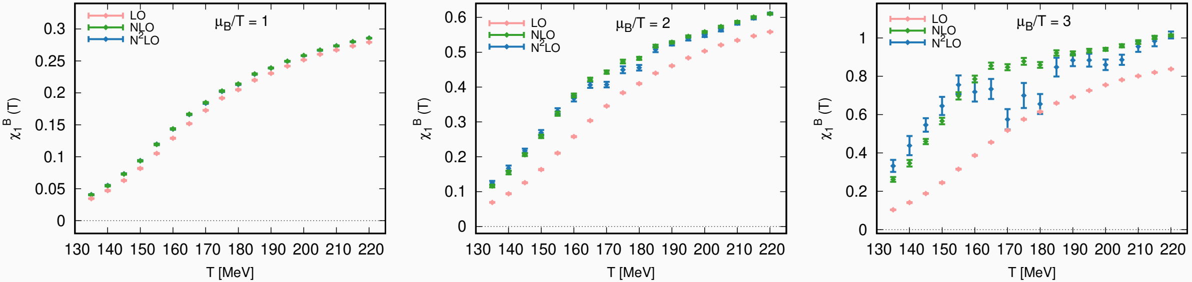
- Higher order coefficients present a more complicated structure



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



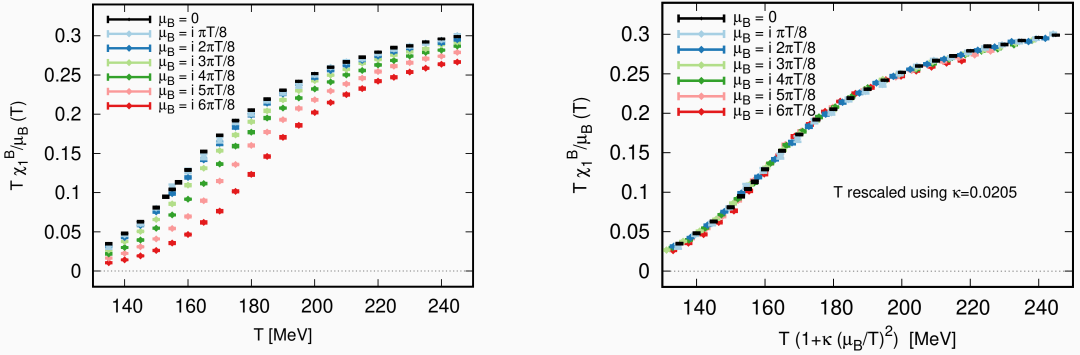
- Inherent problem with Taylor expansion: carried out at $T = \text{const}$. This doesn't cope well with $\hat{\mu}_B-$dependent transition temperature
- Can we find an alternative expansion to improve finite-$\hat{\mu}_B$ behavior?

Borsányi, PP *et al.* 2102.06660 [hep-lat]

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 rescaling of T:

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



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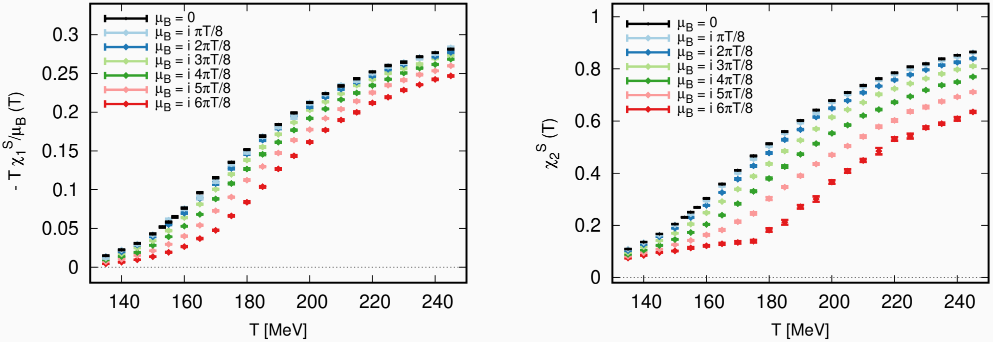
An alternative approach

The other (BS) second order susceptibilities display a very similar scenario:

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



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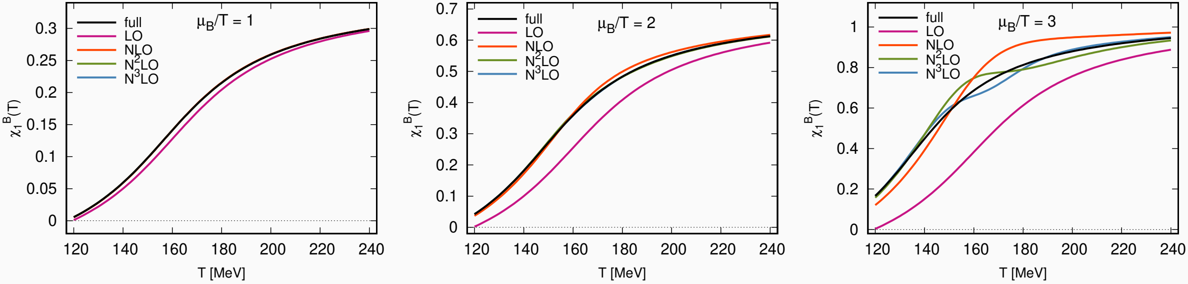
Taylor expanding a (shifting) sigmoid

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



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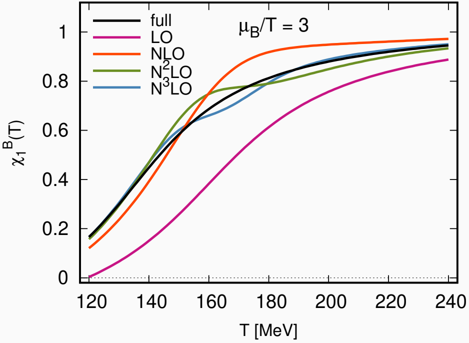
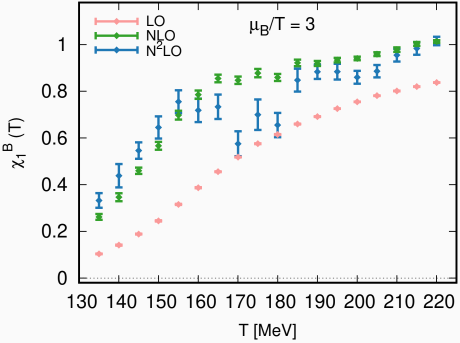
Taylor expanding a (shifting) sigmoid

- The Taylor expansion seems to have problems reproducing the original function (left)
- Quite suggestive comparison with actual Taylor-expanded lattice data (right)





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

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Rigorous formulation

- We have observed the $\hat{\mu}_B$-dependence seems to amount to a simple T- rescaling
- A simplistic scenario with a single T- independent parameter κ does not provide a systematic treatment which can serve as an alternative expansion scheme
- We allow for more than $\mathcal{O}(\hat{\mu}^2)$ expansion of T' and let 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 in the shift

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

- Comparing the (Taylor) expansion in $\hat{\mu}_B$ and our expansion in ΔT order by order, we can relate $\chi_n^B(T)$ and $\kappa_n(T)$

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Rigorous formulation

Equating same-order terms one finds:

$$\kappa_2(T) = \frac{1}{6T}\frac{\chi_4^B(T)}{\chi_2^{B\prime}(T)}$$
$$\kappa_4(T) = \frac{1}{360\chi_2^{B\prime}(T)^3}\left(3\chi_2^{B\prime}(T)^2\chi_6^B(T) - 5\chi_2^{B\prime\prime}(T)\chi_4^B(T)^2\right)$$

and similar relations for κ_n^{BS} and κ_n^{SS}.

- In principle, the procedure can be carried over systematically, however higher order terms still suffer from cancellations and can prove challenging
- Instead, we only use the first relation and combine it with simulations at imaginary-$\hat{\mu}_B$ to extract $\kappa_2^{ij}(T)$, $\kappa_4^{ij}(T)$

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Determine κ_n

I. Directly determine $\kappa_2^{ij}(T)$ at $\hat{\mu}_B = 0$ from the previous relation

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

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

III. Calculate the quantity $\Pi(T, N_\tau, \hat{\mu}_B^2)$ for several $\hat{\mu}_B^2$ and N_τ values

IV. Perform a combined fit of the $\hat{\mu}_B^2$ and $1/N_\tau^2$ dependence of $\Pi(T)$ 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 $\kappa_2^{ij}(T)$ and $\kappa_4^{ij}(T)$

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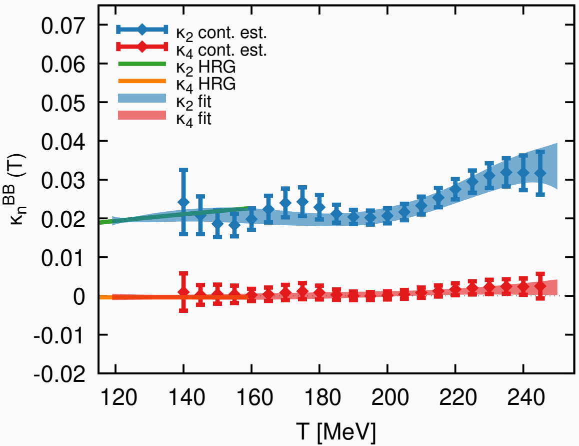
The results for $\kappa_2(T)$, $\kappa_4(T)$

Our initial guess was not far-off:

- Fairly constant $\kappa_2(T)$ over a large T-range
- Clear separation in magnitude between $\kappa_2(T)$ and $\kappa_4(T)$ hints at better convergence
- Agreement with the HRG model results at low temperatures
- Polynomial fits of $\kappa_2(T)$ and $\kappa_4(T)$ before use in thermodynamics (good fit qualities)



NOTE: polynomial fits take into account both statistical and systematic correlations.

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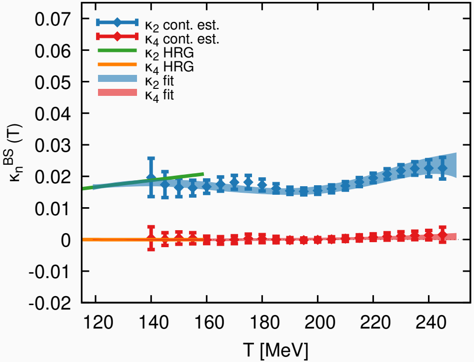
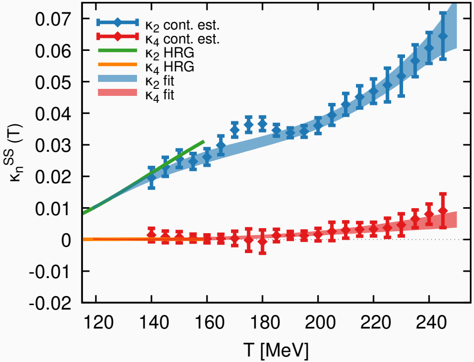
The results for $\kappa_2(T)$, $\kappa_4(T)$

A similar picture appears for κ_n^{BS} and κ_n^{SS}





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Thermodynamics at finite (real) μ_B

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

$$\frac{n_B(T,\,\hat{\mu}_B)}{T^3} = \hat{\mu}_B \chi_2^B(T',0)$$

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

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:

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

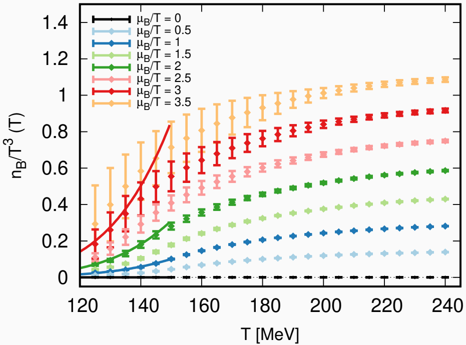
$$\frac{\epsilon(T,\,\hat{\mu}_B)}{T^4} = \frac{s(T,\,\hat{\mu}_B)}{T^3} - \frac{p(T,\,\hat{\mu}_B)}{T^4} + \hat{\mu}_B \frac{n_B(T,\,\hat{\mu}_B)}{T^3}$$

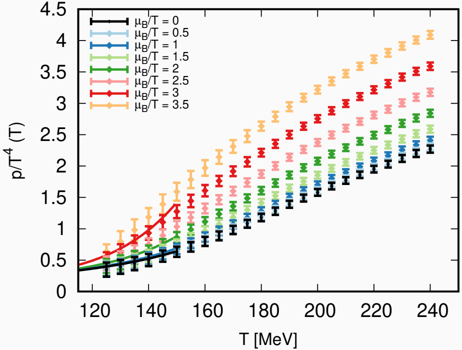
And similarly for strangeness-related quantities:

$$\frac{n_S(T,\,\hat{\mu}_B)}{T^3} = \hat{\mu}_B \chi_{11}^{BS}(T',0) \qquad \chi_2^S(T,\,\hat{\mu}_B) = \chi_2^S(T',0)$$

Thermodynamics at finite (real) μ_B

- We reconstruct thermodynamic quantities up to $\hat{\mu}_B \simeq 3.5$ with uncertainties well under control
- Agreement with HRG model calculations at small temperatures
- No pathological (non-monotonic) behavior is present





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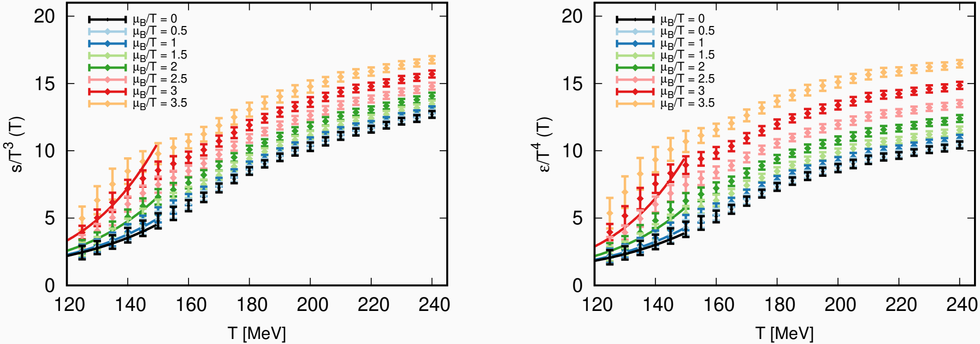

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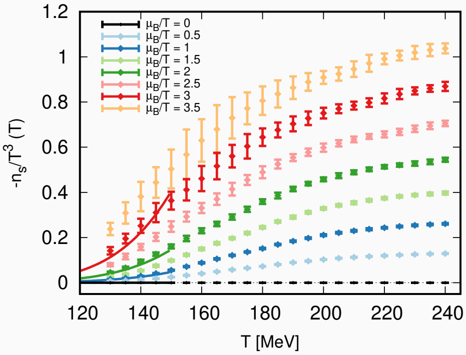

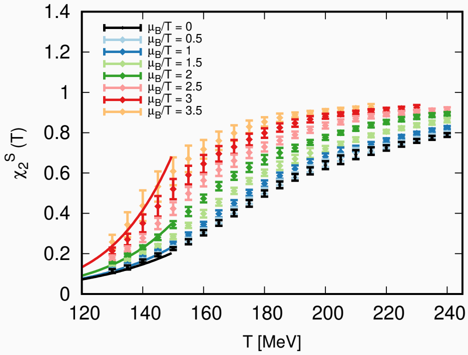

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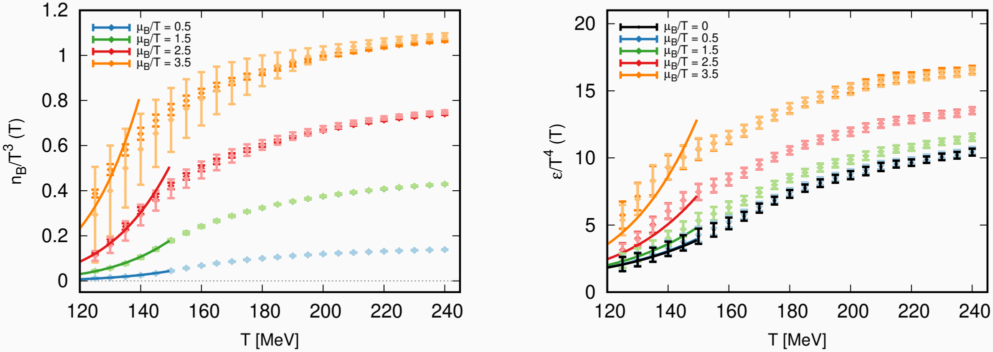
Thermodynamics at finite (real) μ_B

- We also check the results without the inclusion of $\kappa_4(T)$ (darker shades)
- Including $\kappa_4(T)$ only results in added error, but does not "move" the results

$\longrightarrow$ Good convergence



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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 (better convergence)
- Thermodynamic quantities up to $\hat{\mu}_B \simeq 3.5$ have very reasonable uncertainties
- Just as Taylor, systematically improvable if given sufficient computing power

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THANK YOU!

BACKUP

Rigorous 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:

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

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

$$\kappa_4^{S}(T) = \frac{1}{24\chi_{2}^{S\prime}(T)^3}\Big(\chi_{2}^{S\prime}(T)^2\chi_{42}^{BS}(T) - 3\chi_{2}^{S\prime\prime}(T)\chi_{22}^{BS}(T)^2\Big)$$