Lattice QCD at finite temperature and density: present and future

Paolo Parotto, Pennsylvania State University

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Paralia (Pieria, Greece)

QCD Lagrangian

Quantum Chromodynamics (QCD) is a gauge theory with color $SU(3)_c$ symmetry:

$$\boxed{\mathcal{L}_{\text{QCD}} = \sum_f \bar{\psi}_f (i\gamma^\mu D_\mu - m_f)\psi_f - \frac{1}{4} G^a_{\mu\nu} G_a^{\mu\nu}}$$

where:

$$G^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g_S\, f^{abc} A^b_\mu A^c_\nu$$
$$D_\mu = \partial_\mu + i\, g_S\, t^a A^a_\mu$$

Problem: perturbation theory for QCD is not feasible in the regime around the QCD transition because g_S is not small

Solution: the path integral formulation does not rely on a perturbative approach, and gives us the partition function:

$$\mathcal{Z}[A, \bar{\psi}, \psi] = \int \mathcal{D}A^a_\mu(x)\, \mathcal{D}\bar{\psi}(x)\, \mathcal{D}\psi(x)\, e^{-\int d^4x\, \mathcal{L}_E[A, \bar{\psi}, \psi]}$$

where $S_E = \int d^4x\, \mathcal{L}_E$ is the *euclidean* QCD action. Lattice QCD starts from here.

Lattice formulation of QCD

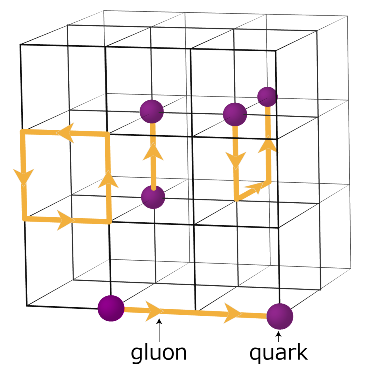
Problem: we cannot calculate the full integral for $\mathcal{Z}[A, \bar{\psi}, \psi]$.

Solution: define the theory on a discretized 3+1d lattice of size $N_s^3 \times N_\tau$, with lattice spacing a. This allows us to reduce the (otherwise infinite) dimensionality of the problem.

- The quark fields $\bar{\psi}, \psi$ are defined on the lattice sites, the gauge fields A_μ are defined on the lattice links as $U_\mu = \exp[iaA_\mu]$
- Now, one can calculate a *finite* number of integrals to evaluate expressions of the like:

$$Z[U, \bar{\psi}, \psi] = \int \mathcal{D}U \, \mathcal{D}\bar{\psi} \, \mathcal{D}\psi \, e^{-S_G[U,\bar{\psi},\psi] - S_F[U,\bar{\psi},\psi]}$$

where S_G and S_F are the gauge (gluonic) and fermionic actions



Lattice formulation of QCD

Actually, we can analytically perform the integral over the quark fields, and remain with:

$$Z[U, \bar{\psi}, \psi] = \int \mathcal{D}U \; \det M[U] \, e^{-S_G[U]}$$

and any observable $\hat{O}$ can then be calculated as:

$$\left\langle \hat{O} \right\rangle = \frac{1}{Z} \int \mathcal{D}U \, \hat{O} \; \det M[U] \, e^{-S_G[U]}$$

Problem: the integrals cannot be calculated by brute force. Even for a small 10^4 lattice, integral is 320000-dimensional!

Solution:

- Monte Carlo integration with **importance sampling**: interpret the factor $\det M[U] \, e^{-S_G[U]}$ as a weight for the configuration U, and reduce the sum only to the most "likely" configurations

Lattice formulation of QCD

- The finiteness of the lattice spacing a serves as a *regulator* for the theory. At the end one wishes to recover the continuum theory with $\lim_{a\to 0}$ ($\lim_{N_\tau\to\infty}$): **continuum limit** $\to$ very delicate business!

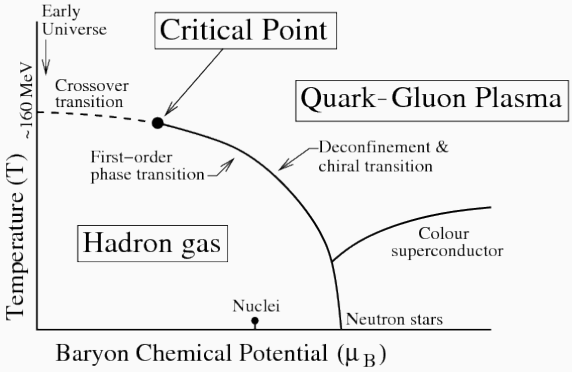
- Calculations are done in a finite volume. When possible, one wishes to study the thermodynamic limit $\lim_{V\to\infty}$: a.k.a. **infinite volume limit**

- **Scale setting:** eventually, we have to express a in physical units. We calculate some quantity whose value is well known, and use it to set the scale (e.g. pion decay constant, pion mass, kaon mass, etc.)

The phase diagram of QCD

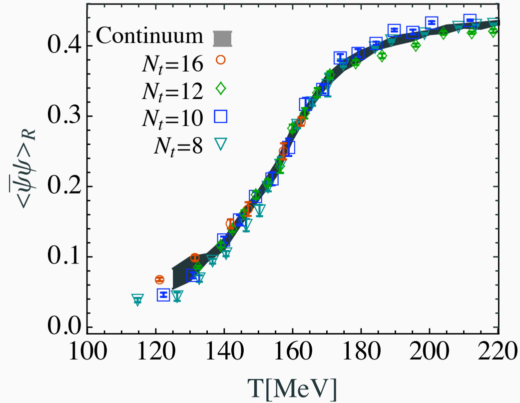
Different phases of QCD matter (in equilibrium) are depicted in (temperature vs baryo-chemical potential) phase diagram

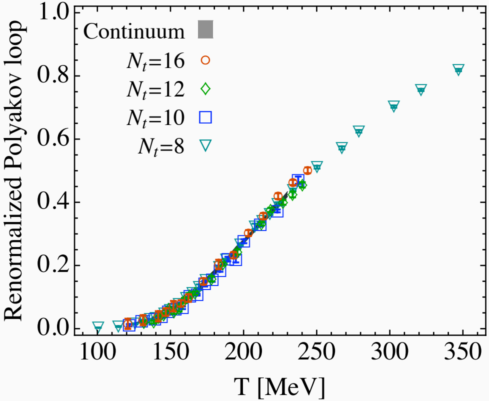
- **Hadron gas** at low-T and/or low-μ_B
- **Quark Gluon Plasma (QGP)** at large T and (possibly) at large μ_B
- **More exotic phases** proposed at low-T and high-μ_B (color superconductivity, etc...)



The QCD transition: observables

Both observables are able to distinguish between the two phases:





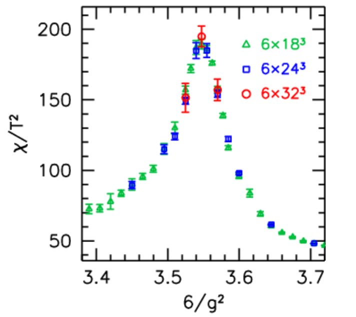
Borsanyi et al. JHEP 1009:073 (2010)

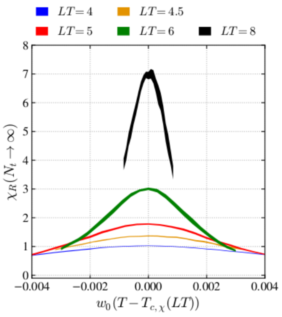
The QCD transition: crossover vs. first order

On the lattice we study the volume scaling of certain quantities to determine the order of the transition

Left: physical masses

Right: infinite masses (pure gauge)





- For a crossover (left), **the peak height is independent of the volume**
- For a first order transition, **it scales linearly with the volume**

Aoki *et al.* Nature 443 (2006), Borsányi, PP *et al.*, PRD 105 (2022)

Finite density: the sign/complex action problem

Euclidean path integrals are calculated with MC methods using importance sampling, interpreting the factor $\det M[U]\, e^{-S_G[U]}$ as the Boltzmann weight for the configuration U

$$
\begin{aligned}
Z(V,T,\mu) &= \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi}\; e^{-S_F(U,\psi,\bar{\psi})-S_G(U)} \\
&= \int \mathcal{D}U\; \det M(U) e^{-S_G(U)}
\end{aligned}
$$

- If there is particle-antiparticle-symmetry ($\mu = 0$) $\det M(U)$ is real
- For real chemical potential ($\mu^2 > 0$) $\rightarrow$ $\det M(U)$ is complex (**complex action problem**) and has wildly oscillating phase (**sign problem**)
  $\Rightarrow$ It cannot serve as a statistical weight
- For *purely imaginary* chemical potential ($\mu^2 < 0$) $\rightarrow$ $\det M(U)$ is real again, simulations can be made!

Lattice QCD at finite μ_B

Lattice QCD can take advantage of a number of methods to work around the sign problem at finite chemical potential:

- **Taylor expansion** around $\mu_B = 0$, e.g.:

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

- **Analytical continuation from imaginary μ_B**
- More methods to work around the sign problem $\rightarrow$ still in more exploratory stages
  - Reweighting techniques
  - Complex Langevin
  - Lifshitz thimbles
  - ...

Lattice QCD for heavy-ion physics

i. **Transition line** (**location**, **curvature**, **“hyper-curvature”**, ...) in the QCD phase diagram

$$\frac{T_c(\mu_B)}{\mathbf{T_c(\mu_B = 0)}} = 1 + \kappa_2 \left(\frac{\mu_B}{T_c(\mu_B)}\right)^2 + \kappa_4 \left(\frac{\mu_B}{T_c(\mu_B)}\right)^4 + \mathcal{O}(\mu_B^6)$$

ii. **Equation of state** (EoS) at $\mu_B = 0$ and finite chemical potential: p, s, n_i, ϵ, etc.. (crucial for hydro simulations)

iii. **Fluctuation of conserved charges** (bridge to experiment, expansion of EoS, signatures for critical point)

$$\chi_{ijk}^{BQS}(T) = \left.\frac{\partial^{i+j+k}\left(p/T^4\right)}{\partial\left(\mu_B/T\right)^i \partial\left(\mu_Q/T\right)^j \partial\left(\mu_S/T\right)^k}\right|_{\mu=0}$$

iv. Hadron spectroscopy at $T = 0$ and finite T

v. ... and more ..

I. Transition line

II.

III.

The QCD transition at finite chemical potential

One defines the transition line $T_c(\mu_B)$ as:

$$\frac{T_c(\mu_B)}{T_c(\mu_B=0)} = 1 + \kappa_2 \left(\frac{\mu_B}{T_c(\mu_B)}\right)^2 + \kappa_4 \left(\frac{\mu_B}{T_c(\mu_B)}\right)^4$$

Observables that probe the chiral transition:

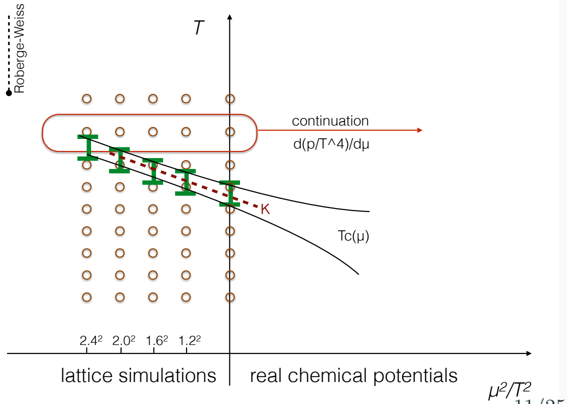
Chiral condensate

$$\langle \bar{\psi}\psi \rangle = \frac{T}{V}\frac{\partial \ln Z}{\partial m_{ud}}$$

Chiral susceptibility

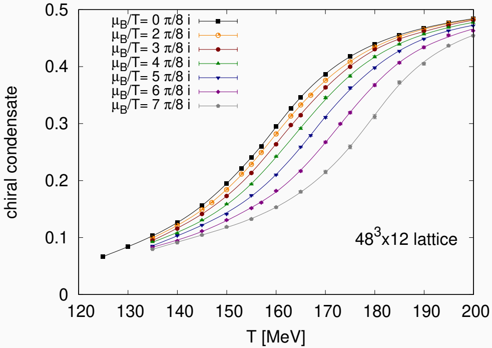
$$\chi = \frac{T}{V}\frac{\partial^2 \ln Z}{\partial m_{ud}^2}$$

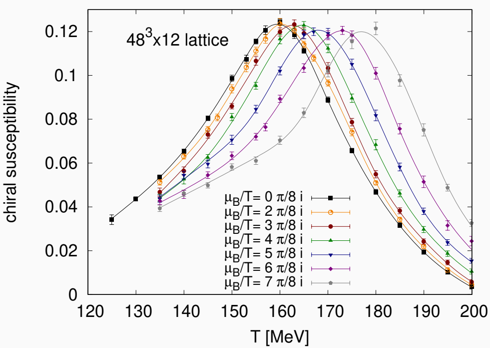
At the transition temperature T_C, the chiral condensate has an inflection point, and the chiral susceptibility has a peak.



Chiral observables at imaginary μ_B

Chiral condensate and chiral susceptibility at imaginary chemical potential

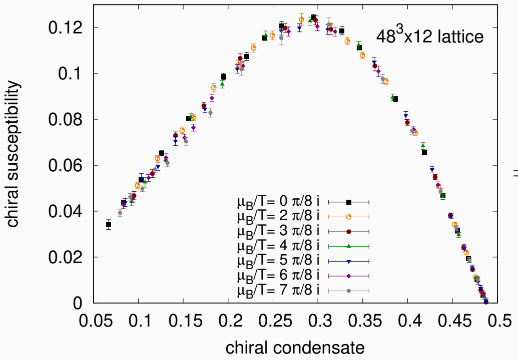




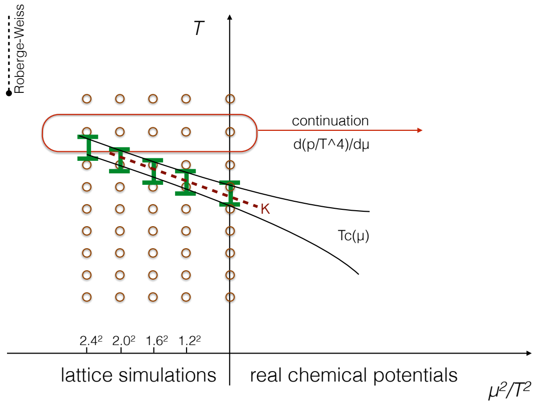
Borsányi, PP *et al.* PRL 125 (2020), 052001

Chiral observables at imaginary μ_B

Plot $\chi(\langle\bar{\psi}\psi\rangle)$, whose form is extremely simple



$\Rightarrow$



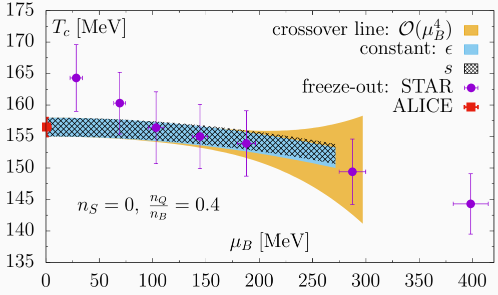
Extract the peak at each μ_B, for every N_τ, and find the transition line

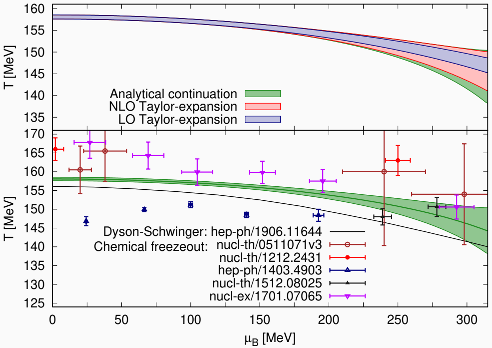
Borsányi, PP *et al.* PRL 125 (2020), 052001

The transition at finite chemical potential

Current results (different collaborations agree within errors):

$$T_c(\mu_B = 0) = 158.0 \pm 0.6 \text{ MeV} \qquad \kappa_2 = 0.0153 \pm 0.0018 \qquad \kappa_4 = 0.00032 \pm 0.00067$$





Bazavov *et al.* PLB 795 (2019) 15-21; Borsányi, PP *et al.* PRL 125 (2020), 052001

I.

II. **Equation of state**

III.

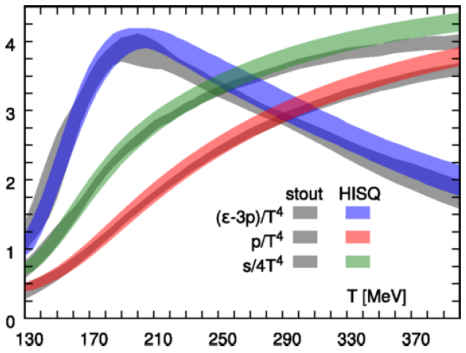
Lattice QCD: equation of state (EoS)

★ A crucial input to hydrodynamic simulations of e.g., heavy-ion collisions

★ 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 - Taylor coefficients

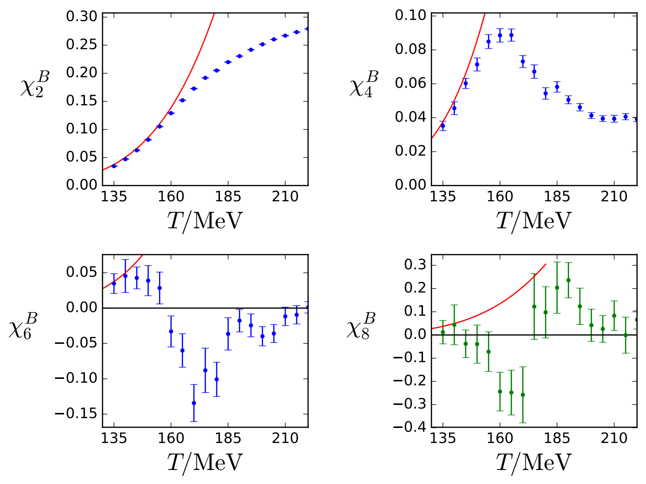
Results for the Taylor coefficients are currently available up to $\mathcal{O}(\hat{\mu}_B^8)$, but the reach of the equations of state is still limited to $\hat{\mu}_B \lesssim 2 - 2.5$ despite great computational effort

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

$$\frac{p(T,\mu_B)}{T^4} = \sum_{n=0}^{\infty} c_{2n}(T) \left(\frac{\mu_B}{T}\right)^{2n} ,$$

$$\text{with } c_n(T) = \frac{1}{n!}\chi_n^B(T, \mu_B = 0)$$

- Very computationally demanding
- Signal extraction is increasingly difficult with higher orders



Borsányi *et al.* JHEP 10 (2018) 205

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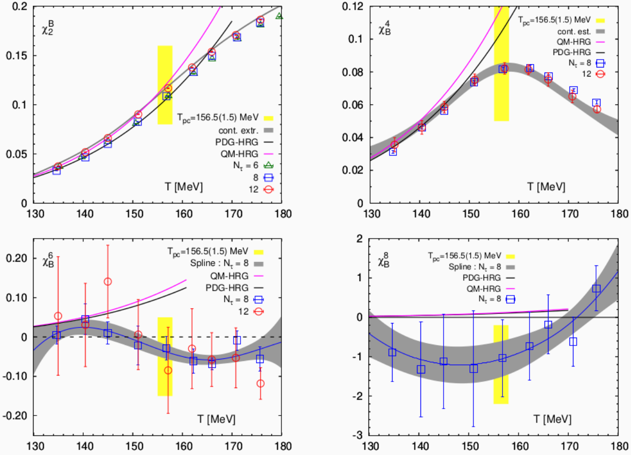
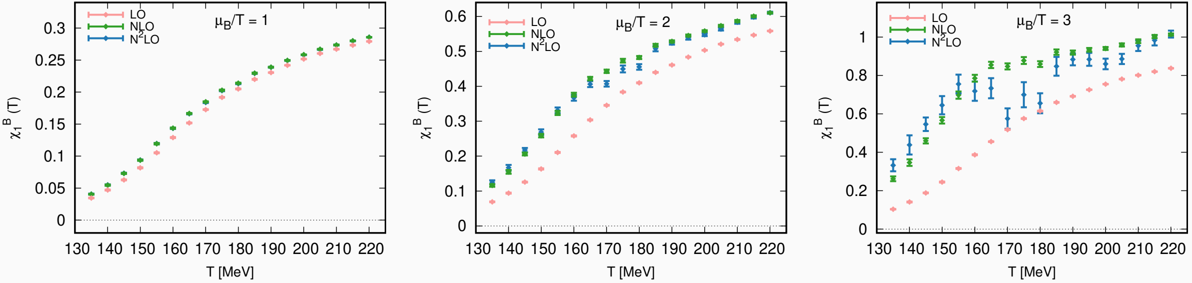


Bazavov *et al.* PRD101 (2020), 074502

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



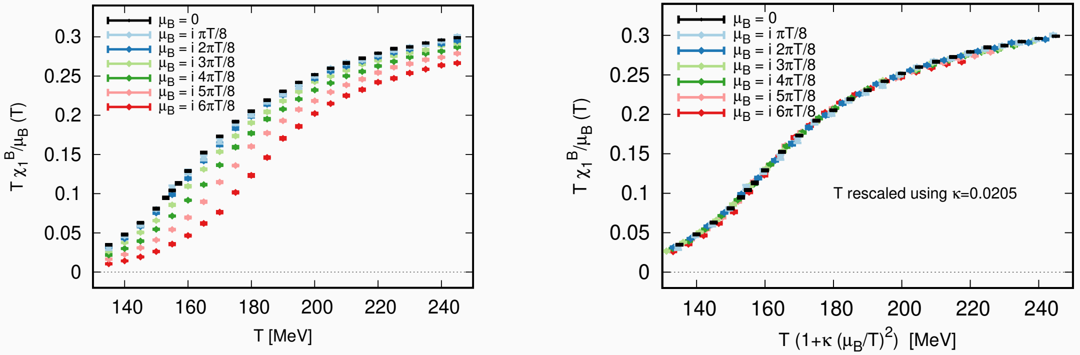
- Inherent problem with Taylor expansion: carried out at $T = \text{const}$. This doesn't cope well with $\hat{\mu}_B-$dependent transition temperature
- Alternative approach to improve finite-$\hat{\mu}_B$ behavior?

Borsányi, PP *et al.* PRL 126 (2021), 232001

An alternative approach

In simulations at imaginary μ_B one sees 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:

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



Borsányi, PP *et al.* PRL 126 (2021), 232001

Rigorous formulation

- 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

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

- We exploit imaginary-$\hat{\mu}_B$ simulations to calculate:

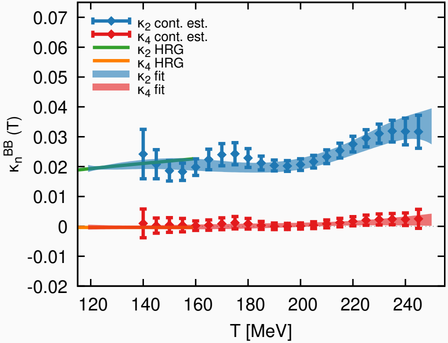
$$\frac{T'-T}{T\,\hat{\mu}_B^2} = \kappa_2(T)+\kappa_4(T)\,\hat{\mu}_B^2+\mathcal{O}(\hat{\mu}_B^4)$$

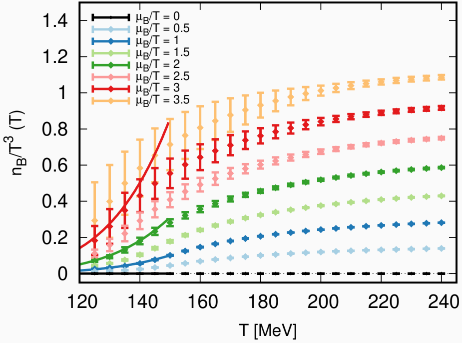
  fit $\frac{T'-T}{T\,\hat{\mu}_B^2}$ at different $\hat{\mu}_B^2$ and $1/N_\tau^2$ at each temperature, obtaining a continuum estimate for $\kappa_2(T)$ and $\kappa_4(T)$

Thermodynamics at finite (real) μ_B

Thermodynamics at (real) μ_B is reconstruted from the same ansatz:

$$\frac{\chi_1^B(T,\hat\mu_B)}{T^3} = \hat\mu_B \chi_2^B(T',0) \qquad T' = T(1+\kappa_2(T)\,\hat\mu_B^2 + \kappa_4(T)\,\hat\mu_B^4)$$



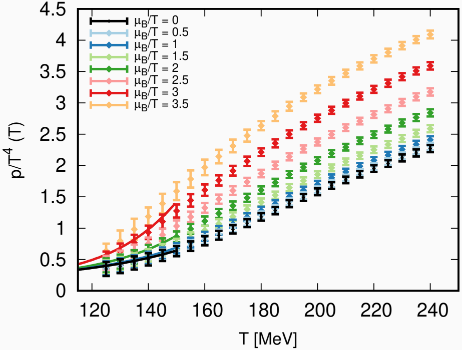


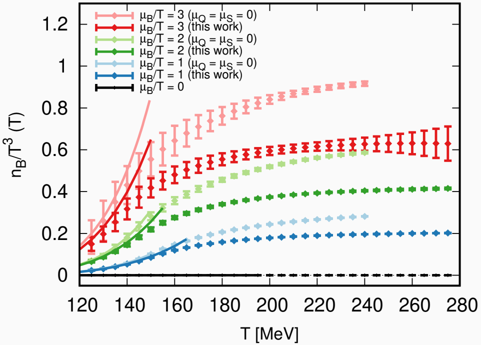
Borsányi, PP *et al.* PRL 126 (2021), 232001

Thermodynamics at finite (real) μ_B

The pressure is just the integral:

$$\frac{p(T,\,\hat\mu_B)}{T^4} = \frac{p(T,0)}{T^4} + \int_0^{\hat\mu_B} \mathrm{d}\hat\mu'_B \, \frac{\chi_1^B(T,\,\hat\mu'_B)}{T^3}$$





Borsányi, PP *et al.* PRL 126 (2021), 232001

I.

II.

III. Fluctuations

Fluctuations of conserved charges

- **Theory**

  Fluctuations are defined as the susceptibilities of the QCD pressure:

  $$\chi_{ijk}^{BQS}(T,\mu_B,\mu_Q,\mu_S) = \frac{\partial^{i+j+k} P\left(T,\mu_B,\mu_Q,\mu_S\right)/T^4}{\partial\left(\mu_B/T\right)^i \partial\left(\mu_Q/T\right)^j \partial\left(\mu_S/T\right)^k}$$

  Have been calculated extensively on the lattice for different conserved charges B, Q, S

- **Experiment**

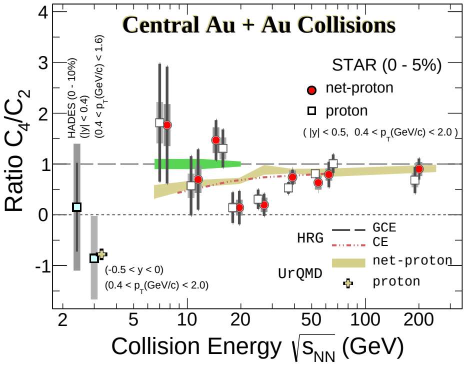
  We can measure the moments/cumulants of net-particle distributions:

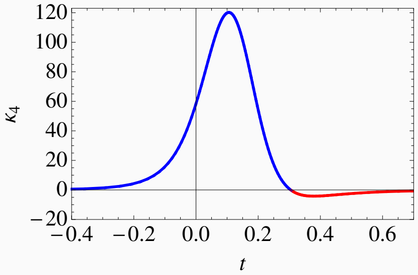
mean:	$M = \chi_1$	variance:	$\sigma^2 = \chi_2$
skewness:	$S = \chi_3/\left(\chi_2\right)^{3/2}$	kurtosis:	$\kappa = \chi_4/\left(\chi_2\right)^2$

  Most common measurements are fluctuations of net-proton and net charge distributions. More recently, net-strangeness has been investigated through net-K and net-Λ fluctuations

Example: looking for critical behavior

- The most promising signatures for the critical point are (higher order) baryon fluctuations → **net-proton cumulants**
- Famous results at different energies (latest from HADES) of net-proton χ_4^B/χ_2^B. Expectation is a peak followed by a dip at decreasing energy



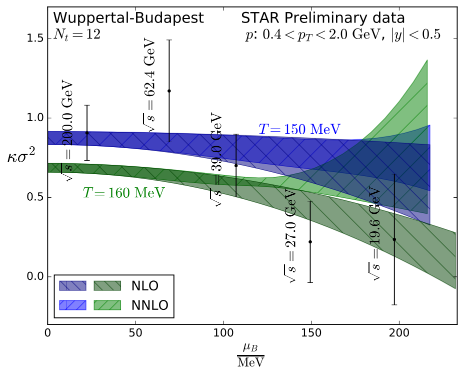


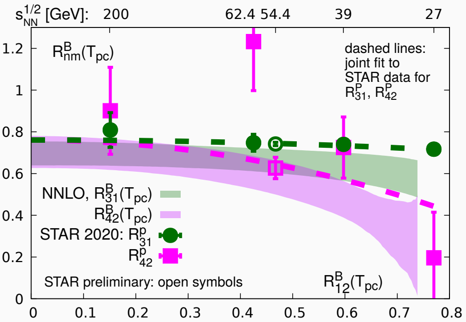
STAR: PRL 128 (2022), 202303; Stephanov, PRL 107 (2011) 052301

Example: looking for critical behavior

- Net-baryon fluctuations χ_n^B are the same used for Taylor expansion of the pressure
- One can Taylor expand net-baryon fluctuations too, then, e.g.:

$$\chi_2^B(T,\mu_B) = \chi_2^B(T) + \frac{1}{2}\chi_4^B(T) + \frac{1}{24}\chi_6^B(T) + \cdots$$





Borsányi *et al.*, JHEP 10 (2018) 205; Bazavov *et al.* PRD101 (2020), 074502

Summary

- ⋆ Lattice QCD is a staple in our understanding of QCD thermodynamics at both finite temperature and density
- ⋆ The sign problem remains a tough obstacle, yet recent results from lattice simulations keep pushing forward our knowledge of the phase diagram
- ⋆ Much more precise determinations of the transition line, equation of state at finite density are emerging from improved techniques (and many more results than I could cover)
- ⋆ Fluctuations calculations allow us to test against experiment, but reaching further out is a struggle

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Thank you!