Equation of State of (2+1)-flavor QCD: An update based on high precision Taylor expansion results

D. Bollweg\textsuperscript{1}, F. Karsch\textsuperscript{2}, A. Lahiri\textsuperscript{2}, S. Mukherjee\textsuperscript{3}, P. Petreczky\textsuperscript{3}

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\textsuperscript{1}Columbia University

\textsuperscript{2}Bielefeld University

\textsuperscript{3}Brookhaven National Lab

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Based on [arXiv:2202.09184] and forthcoming
1 Motivation

2 Computational approach

3 Equation of state at $\mu_Q = \mu_S = 0$ and $n_Q/n_B = 0.4, n_S = 0$

4 Outlook
Bulk thermodynamic properties (Energy density $\epsilon$, Pressure $p$, Entropy density $s$, number densities $n$, ...) of QCD are fundamental inputs for wide range of phenomena (HIC, early universe, compact stars, ...)

Perturbative approaches face challenges.

Widely used Hadron Resonance Gas shows deviations from QCD even below $T_{pc}$ already in second order susceptibilities. [arxiv: 2107.10011]

Non-perturbative, first-principle determination of QCD Equation of State necessary.
Equation of State at $\mu = 0$

- EoS at $\bar{\mu} = 0$ is accessed via trace anomaly $\Theta^{\mu\mu}$:

$$\frac{\Theta^{\mu\mu}(T)}{T^4} = -\frac{1}{VT^3} \frac{d \ln Z}{d \ln a} = \frac{\epsilon - 3p}{T^4} = T \frac{d}{dT} \left( \frac{p}{T^4} \right).$$

- Integral method yields pressure:

$$\frac{p(T)}{T^4} = \frac{p_0}{T^4} + \int_{T_0}^T dT' \frac{\Theta^{\mu\mu}(T')}{T^5}.$$

- “Solved” problem for (2+1)-flavor lattice QCD.

**Figure:** EoS calculated by WB (grey) and HotQCD (color) [arxiv:1407.6387]
Finite Density sign problem prevents direct simulations.

“Production ready” approaches to reach $\mu > 0$:

- Analytical continuation from $\mu^2 < 0$ (see talk by Jana Günther).
- Taylor expansion around $\mu = 0$:

\[
\frac{p(T, \mu)}{T^4} = \sum_{i,j,k=0}^{i,j,k} \frac{\chi_{ijk}^{BQS}(T)}{i!j!k!} \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k, \quad \hat{x} = \frac{\mu_x}{T},
\]

\[
\chi_{ijk}^{BQS}(T) = \frac{1}{VT^3} \left. \frac{\partial^{i+j+k} \ln Z}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k} \right|_{\vec{\mu} = 0}.
\]
μ dependence of ϵ and s are extracted from expansion of trace anomaly:

\[
\frac{\epsilon - 3p}{T^4} = T \frac{\partial p/T^4}{\partial T} = \sum_{i,j,k=0}^{\Xi_{BQS}(T)} \frac{\Xi_{BQS}(T)}{i!j!k!} \hat{\mu}_B \hat{\mu}_Q \hat{\mu}_S, \quad \Xi_{BQS}(T) = T \frac{\partial \chi_{i,j,k}^{BQS}(T)}{\partial T},
\]

\[
\frac{\epsilon}{T^3} = \sum_{i,j,k=0}^{\Xi_{BQS}(T)} \frac{\Xi_{BQS}(T)}{i!j!k!} \hat{\mu}_B \hat{\mu}_Q \hat{\mu}_S;
\]

\[
\frac{s}{T^3} = \sum_{i,j,k=0}^{\Xi_{BQS}(T)} \frac{\Xi_{BQS}(T) + (4 - i - j - k)\chi_{i,j,k}^{BQS}(T)}{i!j!k!} \hat{\mu}_B \hat{\mu}_Q \hat{\mu}_S.
\]
Equation of State at $\mu > 0$

Constrain Taylor expansion to lines parameterized by $\mu_B$:

\[
\frac{\Delta p}{T^4} = \sum_n P_{2n}\hat{\mu}_B^{2n}, \quad \frac{n_B}{T^3} = \sum_n N_{2n-1}\hat{\mu}_B^{2n-1},
\]

\[
\frac{\Delta \epsilon}{T^3} = \sum_n \epsilon_{2n}\hat{\mu}_B^{2n}, \quad \frac{\Delta \sigma}{T^3} = \sum_n \sigma_{2n}\hat{\mu}_B^{2n}.
\]

- Simplest case: $\mu_Q = \mu_S = 0 \rightarrow$ EoS can be calculated from diagonal $\chi_{2n}^B$'s alone ($P_{2n} \sim N_{2n-1} \sim \chi_{2n}^B$).
- Heavy Ion Collision case: $n_Q/n_B = 0.4$, $n_S = 0 \rightarrow$ express $\mu_Q$ and $\mu_S$ via baryon chemical potential $\mu_B$ and fulfill constraints order by order.

\[
\hat{\mu}_Q = q_1(T)\hat{\mu}_B + q_3(T)\hat{\mu}_B^3 + q_5(T)\hat{\mu}_B^5 + \cdots,
\]

\[
\hat{\mu}_S = s_1(T)\hat{\mu}_B + s_3(T)\hat{\mu}_B^3 + s_5(T)\hat{\mu}_B^5 + \cdots,
\]

EoS then involves off-diagonal $\chi_{ijk}^{BQS}$'s as well.
Generalized Susceptibilities via lattice QCD

\[ \chi_{ijk}^{BQS} \equiv \frac{1}{VT^3} \frac{\partial^i + j + k}{\partial \hat{\mu}_B \partial \hat{\mu}_Q \partial \hat{\mu}_S} \log Z \quad \hat{\mu}_X \equiv \frac{\mu_X}{T} \]

To compute \( \chi_{ijk}^{BQS} \), we need to solve integrals of the form

\[
\frac{1}{Z} \int \prod_{x,\nu} dU_{x,\nu} \text{Tr} \left( M_f^{-1} M'_f \cdots \right) e^{-S_{\text{eff}}}.
\]

These are calculated via Markov-Chain Monte-Carlo:

1. Generate \( \{U_{x,\nu}\} \)-ensembles via RHMC algorithm\(^1\).

2. Evaluate \( \text{Tr} \left( M_f^{-1} M'_f \cdots \right) \) on \( \{U_{x,\nu}\} \)-ensembles using random noise method:

   \[
   \text{Tr} \left( \hat{M}_f \right) \sim \frac{1}{N} \sum_{i=0}^{N} \eta_i^* \hat{M}_f \eta_i. \quad \rightarrow \text{Sparse matrix inversions with 500-2000 right-hand sides } \eta_i \text{ for each trace. (Optimizations: Multi-RHS CG + TR-Lanczos with spectrum filter)}
   \]

\(^1\)https://github.com/LatticeQCD/SIMULATeQCD
Dynamical Fermions (HISQ) with $N_f = 2 + 1$, physical quark masses ($\frac{m_s}{m_l} = 27$), $T \in [135, 175]$ MeV and lattice sizes $N_\tau = 6, 8, 12, 16, N_\sigma = 4N_\tau$.

For Temperatures $T > 180$ MeV: $\frac{m_s}{m_l} = 20$ and $N_\tau = 6, 8, 12^2$.


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$^2$Only lowest orders available for $N_\tau = 12$ at $T > 180$ MeV
Continuum extrapolation strategy

- For $\mu_Q = \mu_S = 0$ and isospin symmetric data analysis details: Talk by Jishnu Goswami & [arxiv:2202.09184].
- For $n_Q/n_B = 0.4$: need continuum extrapolations of $P_{2n}(T)$, $N_{2n-1}(T)$, $q_{2n-1}(T)$ and their $T$-derivatives.
- Errors in data points at individual $T$ and $N_\tau$ are normally distributed and independent.
- Fit $P_{2n}(T)$, $N_{2n-1}(T)$, $q_{2n-1}(T)$ on each bootstrap sample generated from joint $N_\tau = 6, 8, 12, 16^3$ data set using $1/N_\tau^2$ corrections.
- Error bands are given by $1\sigma$ spread of bootstrap values at given $T$.

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3rd order: $N_\tau = 6, 8, 12$, 6th order: $N_\tau = 8$ fit, 8th order $N_\tau = 8$ spline
Continuum extrapolations: $P_{2n}$ for $n_Q/n_B = 0.4$, $n_S = 0$ (preliminary)
Equation of State for $\mu_Q = \mu_S = 0$

- Better control over $O(\mu_B^6)$ significantly reduces spurious “wiggles” at high $\mu_B/T$.

EoS 2017 (top) vs 2022 (bottom)
Equation of State for $n_Q/n_B = 0.4, n_S = 0$ (preliminary)

Better control over $O(\mu_B^6)$ significantly reduces spurious “wiggles” at high $\mu_B/T$.

EoS 2017 (top) vs 2022 (bottom)
Equation of State for $n_Q/n_B = 0.4, n_S = 0$ (preliminary)

$O(\mu_B^6)$ coefficients that contain derivatives ($\epsilon_6, \sigma_6$) remain hard to compute!

Smaller range of reliability compared to $P$ and $n_B$ at $O(\mu_B^6)$.
Summary & Outlook

- Multi-year computation campaign generating high statistics data set of (2+1)-flavor HISQ configurations.
- Extension of Equation of State Taylor expansion coefficients up to 8th order.
- Significantly improved control over 6th order coefficients removes spurious “wiggles” of earlier study.
- No evidence for a breakdown of convergence of the Taylor Series for $\mu_B/T < 2.5$ in the entire temperature range explored in this study.

Upcoming:

- Taylor series resummation using Pade method (see talk by Jishnu Goswami).
- Updated parametrization of Equation of State for strangeness neutral systems.
- Updated calculations of isothermal & isoentropic speed-of-sound.