Cluster expansion model for QCD baryon number fluctuations

Volodymyr Vovchenko


Thanks to: Z. Fodor, S.D. Katz, A. Pásztor, O. Philipsen, J. Steinheimer, H. Stoecker

Palaver WS 2017/18

ITP, Frankfurt
November 27, 2017
Outline

1. Motivation: QCD equation of state at finite $\mu_B$

2. Lattice QCD data at imaginary $\mu_B$
   - Fourier coefficients of fugacity expansion
   - Interpretation in terms of baryonic excluded volume

3. Cluster expansion model
   - Fourier coefficients
   - Taylor expansion coefficients (baryon susceptibilities)
   - Radius of convergence

4. Summary and outlook
Strongly interacting matter

- Theory of strong interactions: Quantum Chromodynamics (QCD)
- Basic degrees of freedom: quarks and gluons
- At smaller energies confined into hadrons: baryons ($qqq$) and mesons ($q\bar{q}$)

Sketch of the QCD Phase Diagram

Lattice QCD EoS at $\mu_B = 0$

Relevant for heavy-ion collisions, neutron stars, early universe

First-principle tool: Lattice QCD. Direct simulations restricted to $\mu_B = 0$.

What can we learn about EoS at finite $\mu_B$ from lattice and effective models?
Lattice-based methods for equation of state at finite $\mu_B$

- Taylor expansion [Allton et al.; Gavai, Gupta; HotQCD Collaboration]

\[
\frac{p(T, \mu_B)}{T^4} = \frac{p(T, 0)}{T^4} + \frac{\chi^B_2(T, 0)}{2!} (\mu_B / T)^2 + \frac{\chi^B_4(T, 0)}{4!} (\mu_B / T)^4 + \ldots
\]

$\chi^B_k$ – cumulants (susceptibilities) of net baryon distribution
Can be computed in Lattice QCD at $\mu_B = 0$

- Analytic continuation from imaginary $\mu_B$ [de Forcrand, Philipsen; D’Elia, Lombardo]
No sign problem at $\mu_B = i\tilde{\mu}_B$: Observables can be computed at $\mu^2_B < 0$
Then analytically continued to $\mu^2_B > 0$

- Other methods: Reweighting, complex Langevin, etc.
QCD observables at imaginary $\mu_B$

QCD thermodynamics with relativistic fugacity expansion:

Pressure: \[ \frac{p(T, \mu_B)}{T^4} = \sum_{k=0}^{\infty} p_k(T) \cosh \left( \frac{k \mu_B}{T} \right), \]

Net baryon density: \[ \frac{\rho_B(T, \mu_B)}{T^3} = \sum_{k=1}^{\infty} b_k(T) \sinh \left( \frac{k \mu_B}{T} \right), \quad b_k(T) \equiv k p_k(T) \]

Lattice QCD is problematic at real $\mu$ but tractable at imaginary $\mu$

$\mu_B \rightarrow i\tilde{\mu}_B \quad \Rightarrow \quad$ QCD observables obtain trigonometric Fourier series form

Pressure: \[ \frac{p(T, i\tilde{\mu}_B)}{T^4} = \sum_{k=0}^{\infty} p_k(T) \cos \left( \frac{k \tilde{\mu}_B}{T} \right), \]

Net baryon density: \[ \frac{\rho_B(T, i\tilde{\mu}_B)}{T^3} = i \sum_{k=1}^{\infty} b_k(T) \sin \left( \frac{k \tilde{\mu}_B}{T} \right), \quad b_k(T) \equiv k p_k(T) \]

Coefficients $b_k(T)$ can and are now being calculated in LQCD
Expected asymptotics

- **At low T/densities** QCD $\simeq$ ideal hadron resonance gas

$$\frac{p_{\text{hrg}}(T, \mu_B)}{T^4} = \frac{\phi_M(T)}{T^3} + 2 \frac{\phi_B(T)}{T^3} \cosh \left(\frac{\mu_B}{T}\right),$$

$$\phi_B(T) = \sum_{i \in B} \int dm \rho_i(m) \frac{d_i m^2 T}{2\pi^2} K_2 \left(\frac{m}{T}\right),$$

$$p_{\text{hrg}}^0(T) = \frac{\phi_M(T)}{T^3}, \quad p_{\text{hrg}}^1(T) = \frac{2 \phi_B(T)}{T^3}, \quad p_{\text{hrg}}^k(T) \equiv 0, \quad k = 2, 3, \ldots$$

- **At high T** QCD $\simeq$ ideal gas of massless quarks and gluons

$$\frac{p_{\text{SB}}(T, \mu_B)}{T^4} = \frac{8\pi^2}{45} + \sum_{f=u,d,s} \left[ \frac{7\pi^2}{60} + \frac{1}{2} \left(\frac{\mu_f}{T}\right)^2 + \frac{1}{4\pi^2} \left(\frac{\mu_f}{T}\right)^4 \right], \quad \mu_f = \frac{\mu_B}{3} \text{ *},$$

$$p_{\text{SB}}^0 = \frac{64\pi^2}{135}, \quad p_{\text{SB}}^k = \frac{(-1)^{k+1}}{k^2} \frac{4\left[3 + 4(\pi k)^2\right]}{27(\pi k)^2}, \quad b_{\text{SB}}^k = k p_{\text{SB}}^k.$$

This work explores intermediate, transition region $130 < T < 230$ MeV

*In this study we assume that $\mu_S = \mu_Q = 0$*
Lattice QCD results on imaginary $\mu_B$ observables

Coefficients $b_k(T)$ of net-baryon expansion are now calculated on the lattice

$$\frac{\rho_B(T, i\tilde{\mu}_B)}{T^3} = i \sum_{j=1}^{\infty} b_j(T) \sin \left( j \frac{\mu_B}{T} \right)$$

- Ideal HRG describes well $b_1(T)$ at small temperatures
- All four coefficients appear to converge slowly to Stefan-Boltzmann limit
- What is the mechanism of appearance of non-zero $b_k$ for $k > 1$?

V.V., A. Pásztor, Z. Fodor, S.D. Katz, H. Stoecker, 1708.02852; S. Borsányi, QM2017
Imaginary $\mu_B$ and repulsive baryonic interactions

Repulsive baryonic interactions with excluded-volume [Rischke et al., Z. Phys. C '91]

$$V \rightarrow V - bN \quad \Rightarrow \quad p_B(T, \mu_B) = p_B^{id}(T, \mu_B - bp)$$

HRG with baryonic EV repulsion:

$$b_{1}^{ev}(T) = 2 \frac{\phi_B(T)}{T^3}$$

$$b_{2}^{ev}(T) = -4 [b \phi_B(T)] \frac{\phi_B(T)}{T^3}$$

$$b_{3}^{ev}(T) = 9 [b \phi_B(T)]^2 \frac{\phi_B(T)}{T^3}$$

$$b_{4}^{ev}(T) = -\frac{64}{3} [b \phi_B(T)]^3 \frac{\phi_B(T)}{T^3}$$

- Ideal HRG describes well $b_{1}(T)$ at small temperatures
- Non-zero $b_{j}(T)$ for $j \geq 2$ signal deviations from ideal HRG
- Addition of EV interactions between baryons reproduces lattice trend

V.V., A. Pásztor, Z. Fodor, S. Katz, H. Stoecker, 1708.02852; S. Borsányi, QM2017
“Excluded volume” parameter of $BB$ interactions can be estimated from lattice

$$b(T) = -\frac{b_2(T)}{[b_1(T)]^2 T^3}$$

$b(T)$ mostly consistent with $1 \text{ fm}^3$ at $T < 190 \text{ MeV}$

V.V., A. Pásztor, Z. Fodor, S.D. Katz, H. Stoecker, 1708.02852
Relation between leading and higher order coefficients

EV-HRG describes similarly well leading four coefficients

A particular feature of the model: temperature-independent ratios

\[ \alpha_3 = \frac{b_1(T)}{[b_2(T)]^2} b_3(T), \quad \alpha_4 = \frac{[b_1(T)]^2}{[b_2(T)]^3} b_4(T), \ldots \]

Also hold true for many other models with short-range interaction

Excluded volume model:

\[ \alpha_3^{EV} = 1.125, \quad \alpha_4^{EV} = 1.333 \]

\( \alpha_3 \) and \( \alpha_4 \) are approximately \( T \)-independent on the lattice, EV somewhat off
Relation between leading and higher order coefficients

EV-HRG describes similarly well leading four coefficients

A particular feature of the model: temperature-independent ratios

\[ \alpha_3 = \frac{b_1(T)}{[b_2(T)]^2} b_3(T), \quad \alpha_4 = \frac{[b_1(T)]^2}{[b_2(T)]^3} b_4(T), \quad \ldots \]

Also hold true for many other models with short-range interaction

Excluded volume model:

\[ \alpha_3^{EV} = 1.125, \quad \alpha_4^{EV} = 1.333 \]

Stefan-Boltzmann limit:

\[ \alpha_3^{SB} \approx 1.394, \quad \alpha_4^{SB} \approx 2.198 \]

\( \alpha_3 \) and \( \alpha_4 \) are approximately \( T \)-independent on the lattice, EV somewhat off

Ratios are consistent with the Stefan-Boltzmann limit of massless quarks
Cluster Expansion Model (CEM)

\( \alpha_3 \) and \( \alpha_4 \) are consistent with SB limit. Now assume the same for all higher-order coefficients

**CEM formulation:**

- \( b_1(T) \) and \( b_2(T) \) are model input
- All higher order coefficients are then predicted

\[
  b_k(T) = \alpha_k^{SB} \frac{[b_2(T)]^{k-1}}{[b_1(T)]^{k-2}}
\]

- All observables are calculated from fugacity expansion for baryon density

\[
  \frac{\rho_B(T)}{T^3} = \chi_1^B(T) = \sum_{k=1}^{\infty} b_k(T) \sinh(k \mu_B/T)
\]

Fugacity expansion convergence criterion is given by the ratio test:

\[
  \lim_{k \to \infty} \left| \frac{b_{k+1}(T) \sinh \left[ \frac{(k+1) \mu_B}{T} \right]}{b_k(T) \sinh \left[ \frac{k \mu_B}{T} \right]} \right| = \left| \frac{b_2(T) b_1^{SB}}{b_1(T) b_2^{SB}} \right| e^{\frac{|\mu_B|}{T}} < 1.
\]
Baryon number susceptibilities at $\mu_B = 0$:

$$\chi^B_{2n}(T) \equiv \left. \frac{\partial^{2n}(p/T^4)}{\partial (\mu_B/T)^{2n}} \right|_{\mu_B=0} = \sum_{k=1}^{\infty} k^{2n-1} b_k(T).$$

**CEM-LQCD:** $b_1(T)$ and $b_2(T)$ taken from LQCD simulations at imaginary $\mu_B$

**CEM-HRG:** $b_1(T)$ and $b_2(T)$ from EV-HRG model with $b = 1$ fm$^3$
CEM: 4th and 6th order ratios

\[
\chi_B^{2n}(T) \equiv \left. \frac{\partial^{2n}(p/T^4)}{\partial (\mu_B/T)^{2n}} \right|_{\mu_B=0} = \sum_{k=1}^{\infty} k^{2n-1} b_k(T).
\]

\[
\chi_B^{4}/\chi_B^{2}
\]

\[
\chi_B^{6}/\chi_B^{2}
\]

Consistency with available LQCD data

Hadronic description with interactions (CEM-HRG) works up to \( T \simeq 185 \text{ MeV} \)

V.V., J. Steinheimer, O. Philipsen, H. Stoecker, 1711.01261

LQCD data from 1507.04627 (Wuppertal-Budapest), 1701.04325 & 1708.04897 (HotQCD)
CEM: predictions for high orders

\[ \chi^B_{2n}(T) \equiv \frac{\partial^{2n}(p/T^4)}{\partial(\mu_B/T)^{2n}} \bigg|_{\mu_B=0} = \sum_{k=1}^{\infty} k^{2n-1} b_k(T). \]

To be verified on the lattice

V.V., J. Steinheimer, O. Philipsen, H. Stoecker, 1711.01261
Radius of convergence

Taylor expansion of QCD pressure:

\[
\frac{p(T, \mu_B)}{T^4} = \frac{p(T, 0)}{T^4} + \frac{\chi^B_2(T)}{2!} \left(\frac{\mu_B}{T}\right)^2 + \frac{\chi^B_4(T)}{4!} \left(\frac{\mu_B}{T}\right)^4 + \ldots
\]

Radius of convergence \( r_{\mu/T} \) of the expansion is the distance to the nearest singularity of \( p/T^4 \) in the complex \( \mu_B/T \) plane at a given temperature \( T \).

If the nearest singularity is at a real \( \mu_B/T \) value, this could point to the QCD critical point.

Lattice QCD strategy: Estimate \( r_{\mu/T} \) from few leading terms

M. D'Elia et al., 1611.08285; S. Datta et al., 1612.06673; A. Bazavov et al., 1701.04325

Ratio estimator:

\[
\left| \frac{(2n + 2)(2n + 1)\chi^B_{2n}}{\chi^B_{2n+2}} \right|^{1/2}, \quad r_{\mu/T} = \lim_{n \to \infty} r_n
\]

CEM allows to analyze \( r_n \) to very high order.
Domb-Sykes plot: $1/r_n^2$ vs $1/n$, linear extrapolation to $1/n = 0$ yields $r_\mu/T$

CEM-LQCD @ $T = 160$ MeV

$\lim_{n \to \infty} r_n$ does not exist!
Radius of convergence: Structure of Taylor coefficients

Ratio estimator works only when coefficients have \textit{regular asymptotic structure}: they either share the \textit{same sign} or they \textit{alternate in sign}.
Ratio estimator works only when coefficients have **regular asymptotic structure**: they either share the same sign or they alternate in sign.

Negative coefficients appear from $\chi^B_8$ on.

They never settle into a regular pattern.

This means that limiting singularity lies in the *complex* $\mu_B/T$ plane.
Radius of convergence: Mercer-Roberts estimator

A more involved Mercer-Roberts estimator:

\[ r_n = \left| \frac{c_{n+1} c_{n-1} - c_n^2}{c_{n+2} c_n - c_{n+1}^2} \right|^{1/4}, \quad c_n = \frac{\chi_{2n}^B}{(2n)!}. \]

Taylor expansions for \( p/T^4 \), \( \chi_2^B \), and \( \chi_4^B \) all point to the same

\[ \lim_{n \to \infty} r_n^{-2} \approx 0.064 \quad \Rightarrow \quad r_{\mu/T} \approx 3.95 \text{ at } T = 160 \text{ MeV} \]
Radius of convergence: Temperature dependence

Applying the same procedure at other temperatures

Radius of convergence of Taylor expansion sees Roberge-Weiss transition? R-W transition expected at \( T > T_{RW} \) and \( \text{Im}[\mu_B/T] = \pi \) [Roberge, Weiss, NPB '86]

Lattice estimate: \( T_{RW} \sim 200 \text{ MeV} \) [C. Bonati et al., 1602.01426]
Padé approximant for $\chi_2^B$:

$$\chi_2^B(T, \mu_B/T) \approx \frac{\sum_{j=0}^{m} a_j (\mu_B/T)^j}{1 + \sum_{k=1}^{n} b_k (\mu_B/T)^k}$$

$a_j$ and $b_k$ constructed from $\chi_{2n}^B$ to match Taylor expansion

Poles of Padé approximants often point to true singularities of the function

$\text{Im}[\mu_B/T]_c = \pi$, while $\text{Re}[\mu_B/T]_c$ decreases towards zero with temperature
Going beyond the radius of convergence

Padé approximants allow to go beyond the radius for convergence

Example: $\chi^B_4 / \chi^B_2$ at finite $\mu_B / T$

CEM-LQCD, $T = 150$ MeV

- Taylor expansion
- Pade approximants
Summary

- LQCD data at imaginary $\mu_B$ suggests presence of repulsive baryonic interactions with 2nd virial coefficient $b \sim 1 \text{ fm}^3$ in the crossover region

- It provides a first-principle evidence for the baryonic “excluded-volume”

- CEM describes all available lattice data on net baryon susceptibilities

- Radius of convergence of Taylor expansion sees a Roberge-Weiss like transition

- No evidence for QCD phase transition at $\mu_B/T < \pi$

Outlook

- QCD equation of state at finite $\mu_B/T$ within CEM

- Isospin and strangeness chemical potentials
Summary

• LQCD data at imaginary $\mu_B$ suggests presence of repulsive baryonic interactions with 2nd virial coefficient $b \sim 1 \text{ fm}^3$ in the crossover region

• It provides a first-principle evidence for the baryonic “excluded-volume”

• CEM describes all available lattice data on net baryon susceptibilities

• Radius of convergence of Taylor expansion sees a Roberge-Weiss like transition

• No evidence for QCD phase transition at $\mu_B/T < \pi$

Outlook

• QCD equation of state at finite $\mu_B/T$ within CEM

• Isospin and strangeness chemical potentials

Thanks for your attention!
Backup slides
Baryonic excluded volume

Baryon-baryon interactions seem to exhibit a repulsive core – excluded volume

EV model: a simple approach for repulsive interactions [Rischke et al., Z. Phys. C '91]

\[ V \to V - bN \quad \Rightarrow \quad p(T, \mu) = p_{id}(T, \mu - bp) \]

EV-HRG model

- Identical EV interactions for all baryon-baryon and antibaryon-antibaryon pairs
- Baryon-antibaryon, meson-meson, meson-baryon EV terms neglected
- A single parameter \( b \) characterizing interactions

Three independent subsystems: mesons + baryons + antibaryons

\[ p(T, \mu) = p_M(T, \mu) + p_B(T, \mu) + p_{\bar{B}}(T, \mu), \]

\[ p_M(T, \mu) = \sum_{j \in M} p_{id}^{j}(T, \mu_j) \quad \text{and} \quad p_B(T, \mu) = \sum_{j \in B} p_{id}^{j}(T, \mu_j - b p_B) \]

Total density of baryons: \( n_B^{ev} = (1 - b n_B^{ev}) e^{\mu_B/T} \phi_B(T) \exp \left( - \frac{b n_B^{ev}}{1 - b n_B^{ev}} \right) \).