High-order cumulants near the critical point from molecular dynamics

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QCD matter

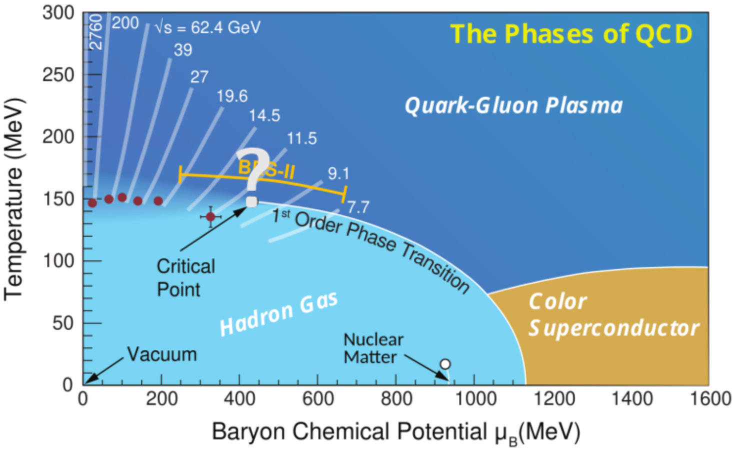


Figure from Bzdak et al., Phys. Rept. 2020 & 2015 Long Range plan

Fluctuations as CP signature

V. A. Kuznietsov et al., Phys. Rev. C 105, 044903 (2022)

In GCE density cumulants shows singularity behavior in the critical point.

$$\ln Z^{\mathrm{gce}}(T, V, \mu)$$

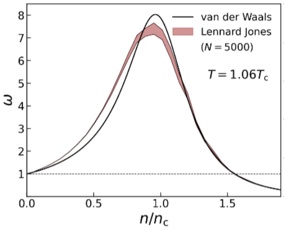
$$= \ln \left[\sum_N e^{\mu N} Z^{\mathrm{ce}}(T, V, N) \right],$$

$$\kappa_n \cong \frac{\partial^n (\ln Z^{\mathrm{gce}})}{\partial (\mu_N)^n}.$$

The real expression for Z^{gce} is unknown in QCD matter.

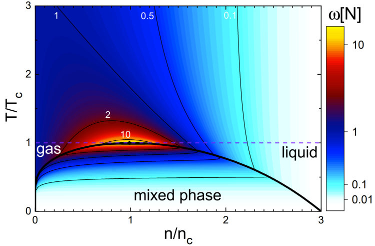
V. Vovchenko, D. V. Anchishkin, M. I. Gorenstein and R. V. Poberezhnyuk, Phys. Rev. C92 054901 (2015)

Scaled variance



$\omega = \kappa_2/\kappa_1$

$\kappa_2 \sim \xi^2$



Fluctuations as CP signature

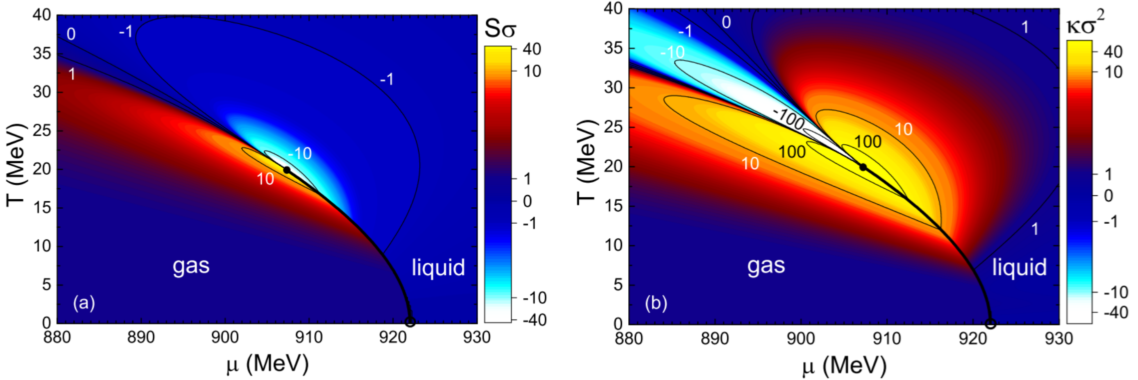
M.A. Stephanov, PRL, 102 (2009), 032301

$\kappa_3 \sim \xi^{9/2}$

Skewness $S\sigma = \kappa_3/\kappa_2$

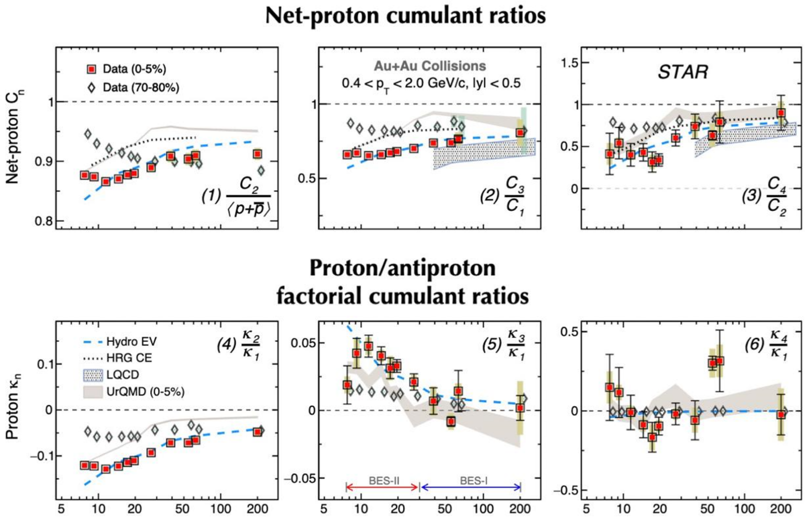
$\kappa_4 \sim \xi^7$

Kurtosis $\kappa\sigma^2 = \kappa_4/\kappa_2$



V. Vovchenko et al, PRC 92 (2015) 5, 054901

STAR measurments



STAR, arXiv:2504.00817

Connection to the experiment

Theory

- Coordinate and/or momentum space
- In contact with the heat bath
- Conserved charges
- Uniform
- Fixed volume
- No CP at the transport models

Experiment

- Momentum space
- Expanding in vacuum
- Non-conserved charges
- Inhomogeneous
- Fluctuating volume
- 3D Izing CP possibility

Need microscopic description of fluctuations

Lennard-Jones potential

The Lennard-Jones potential reads

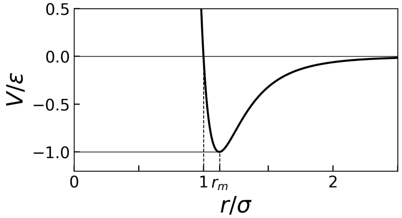
$$V_{\rm LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12}\right],$$

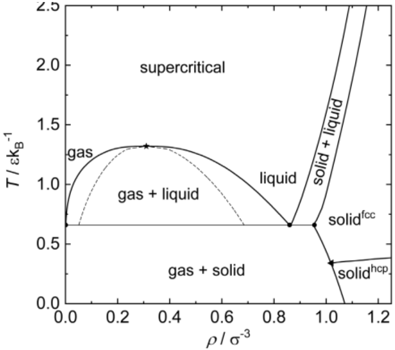
In reduced dimensionless variables it can be rewritten as

$$\tilde{V}_{\rm LJ} = 4[\tilde{r}^{-12} - \tilde{r}^{-6}],$$

where the reduced variables are used: $\tilde{r} = r/\sigma$ and $\tilde{V}_{\rm LJ} = V_{\rm LJ}/\varepsilon$.

The LJ fluid contains a critical point in the 3D Ising universality class.

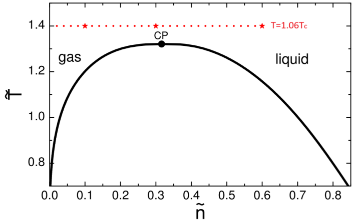


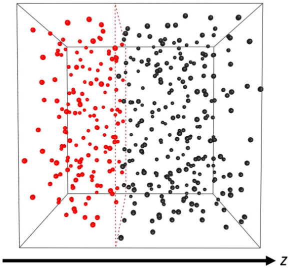


Simulation setup

$$m\frac{d^2\tilde{\mathbf{r}}_{\rm ij}}{d\tilde{t}^2} = -\vec{\nabla}\,\tilde{V}_{\rm LJ}(\tilde{\mathbf{r}}_{\rm ij})$$

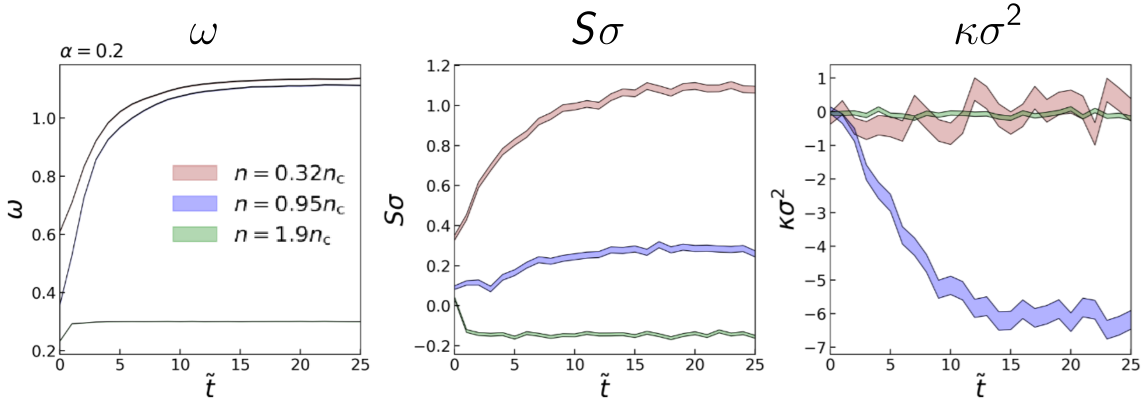
- Three points on the phase diagram, $\tilde{n} = 0.1 \approx 0.3 n_c$, $\tilde{n} = 0.3 \approx 0.95 n_c$, $\tilde{n} = 0.6 \approx 2 n_c$, all for $T = 1.06\, T_c$
- $N_{\rm ev} \simeq 2$ million events at each density.
- Initialize each event with random initial coordinates and momenta
- Run each event for long time ($\tilde{t} = 50$), write snapshots to file at regular time intervals
- Calculate observables as event-by-event (ensemble) average





The simulations are performed on UH PhysGPU cluster.
Code is available at: https://github.com/vlvovch/lennard-jones-cuda

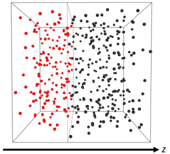
Cumulants equilibration

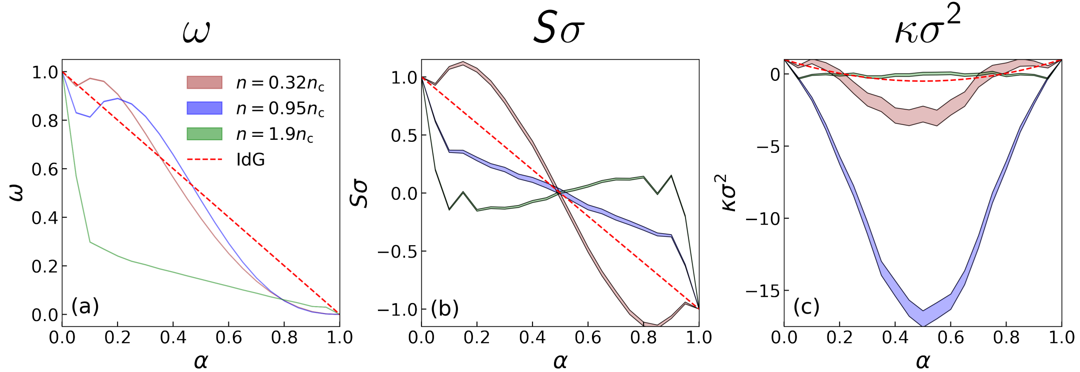


All three cumulant ratios equilibrate at comparable time scales

Acceptance dependence of cumulants

Large CP signal in the coordinate space for all cumulants.

$\alpha \sim$ 



Subensemble method – correction for global conservation

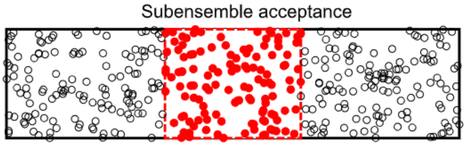
Cumulants, corrected for the baryon conservation reads (**V Vovchenko O. Savchuk, R. Poberezhnyuk, M. Gorenstein, V. Koch, Phys. Let. B, 2020**)

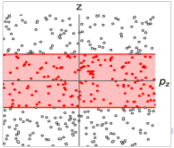
$$\tilde{\omega} \equiv \omega/(1-\alpha),$$

$$\tilde{s\sigma} \equiv s\sigma/(1-2\alpha),$$

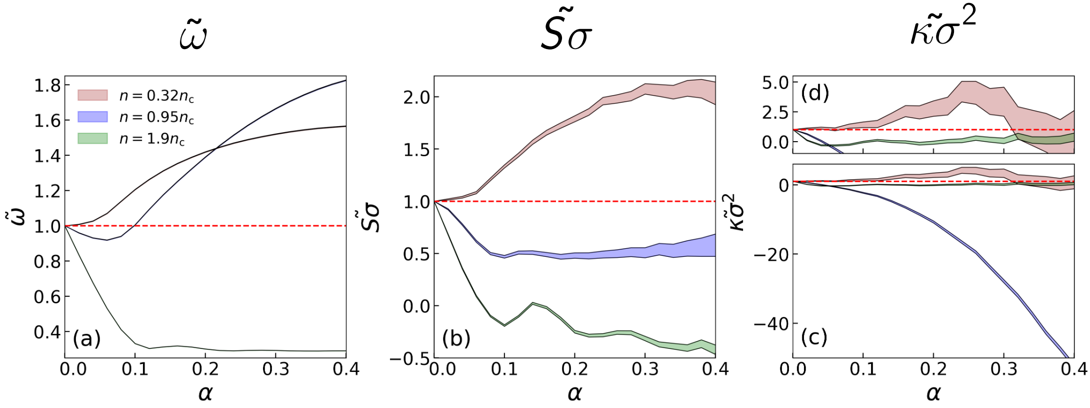
$$\tilde{\kappa\sigma}^2 \equiv \frac{1}{(1-3\alpha(1-\alpha))}\kappa\sigma^2 - \frac{3\alpha(1-\alpha)}{1-3\alpha(1-\alpha)}(\tilde{s\sigma})^2,$$

where $\alpha = \langle N \rangle / N$ - subensemble fraction.
Unfortunately, higher corrected cumulants have pole at $\alpha = 0.5$, which leads to the artificial infinities because we compute the moments values with finite precision.

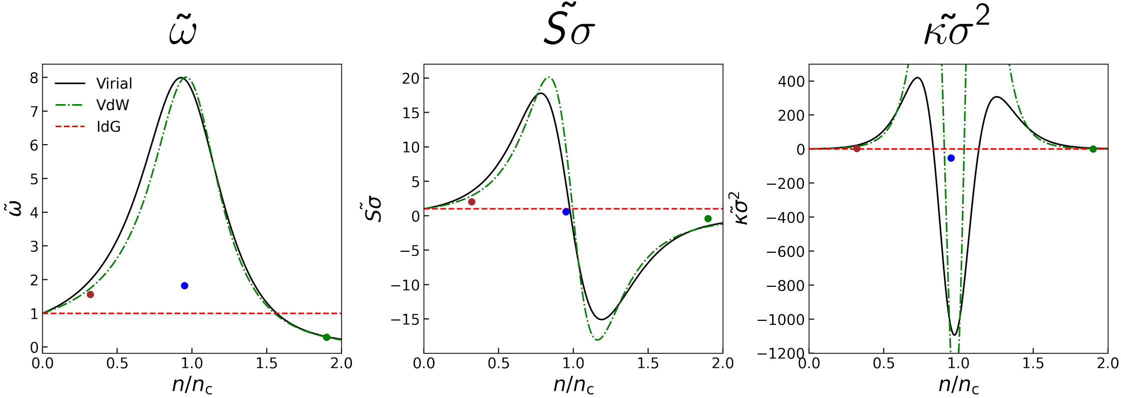




Cumulants with global conservation corrections



Virial estimation of GCE limit

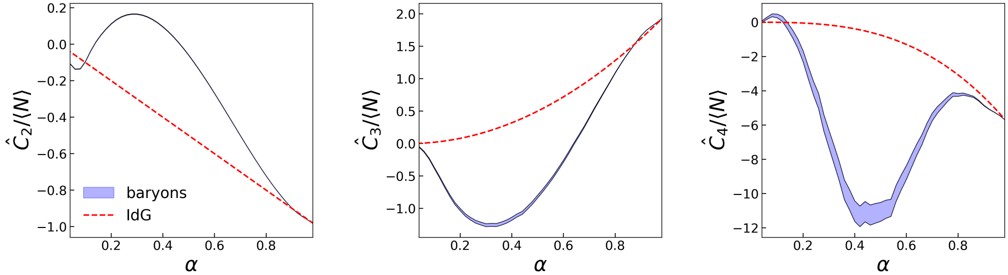


Factorial cumulants ($n = 0.95 n_c$)

One can express the factorial cumulants in terms of the mean density $\langle N \rangle = \kappa_1$ and standard cumulants κ_i

A. Bzdak, V. Koch, and N. Strodthoff, Phys. Rev. C 95, 054906 (2017)

$$\hat{C}_2 = \kappa_2 - \langle N \rangle, \quad \hat{C}_3 = \kappa_3 - 3\kappa_2 + 2\langle N \rangle,$$
$$\hat{C}_4 = -6\langle N \rangle + 11\kappa_2 - 6\kappa_3 + \kappa_4.$$



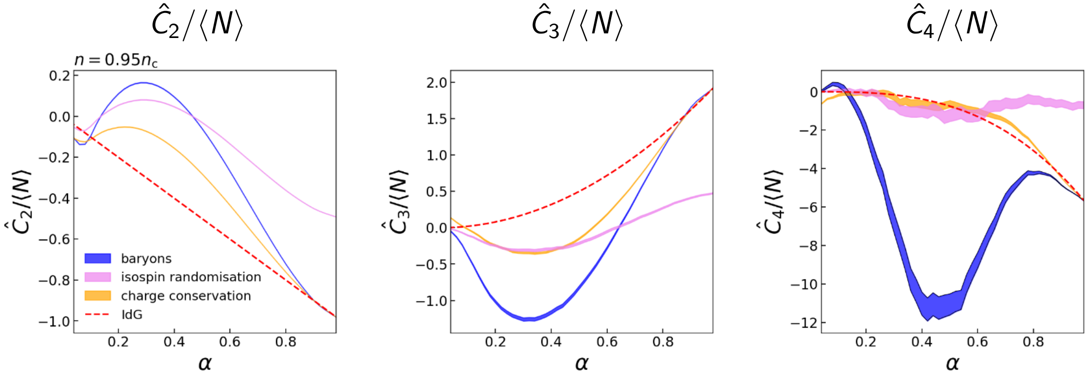
Baryons and protons

Experiments measure protons, rather than not all baryons. There are two ways to incorporate protons:

1. **Isospin randomisation:** Each time, randomly label a baryon as a proton with a probability of 50%. This implies isospin randomization expected to be valid for large collision energies (≥ 10 GeV). In this case, factorial cumulants scale as $F_k^{\mathrm{baryon}} = 2^k F_k^{\mathrm{proton}}$ for a symmetric system.
2. **Charge conservation (conserved proton number):** Neglect the production of pions: charge conservation implies conservation of proton number. Treat the first $N/2$ particles as protons. Expected to be appropriate for smaller energies (< 10 GeV).

M. Kitazawa and M. Asakawa, Phys. Rev. C 86, 024904 (2012)
M. Barej and A. Bzdak, Phys. Rev. C 102, 064908 (2020)

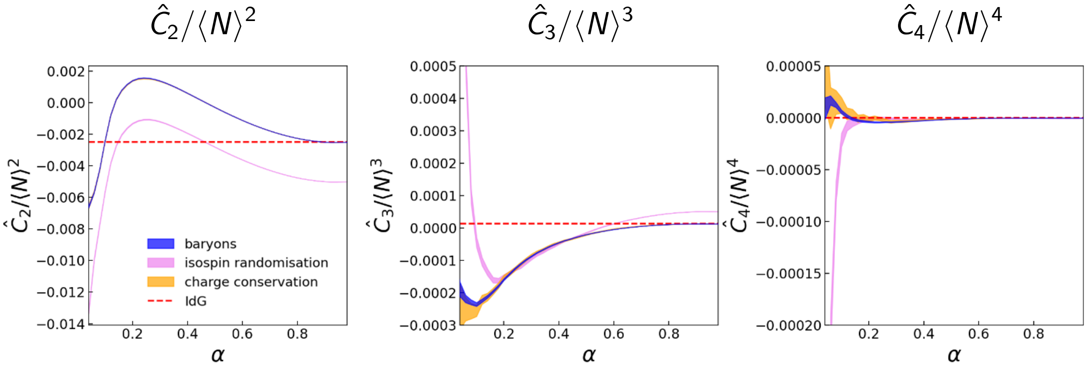
Factorial cumulants ($n = 0.95n_c$)



Taking protons instead of baryons significantly reduces the signal, and no significant deviation from the ideal gas baseline seen for $\hat{C}_4 \implies$ may be relevant for RHIC-BES-II observations?

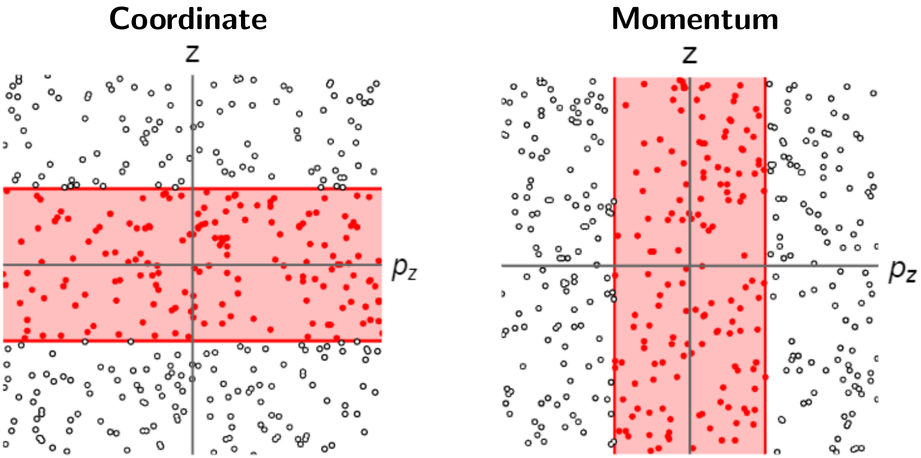
Normalised factorial cumulants ($n = 0.95 n_c$)

Acceptance dependence of normalized FC suggested in **A. Bzdak et al., arXiv:2503.16405**



Normalized factorial cumulants show non-flat acceptance dependence, indicating short-range correlations, the signal is diluted in the case of protons

Momentum vs coordinate cuts



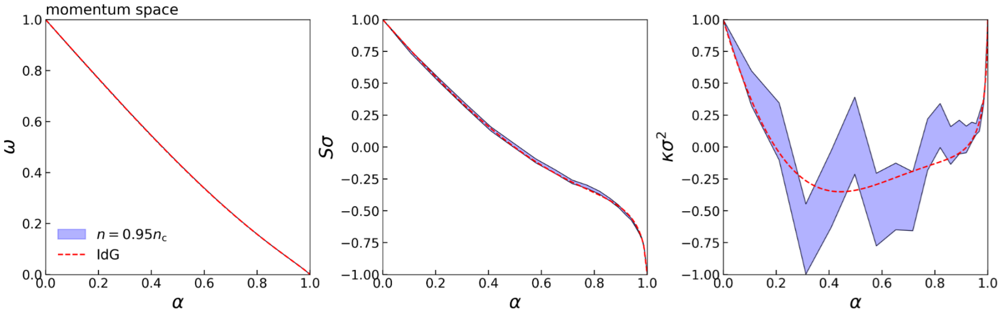
Fluctuations in the momentum space

Red dashed line corresponds to the large N limit formulas for the Ideal gas result with the energy conservation. For scaled variance such formula could be written in a compact form

V. A. Kuznietsov et al., PRC 105, 044903 (2022)

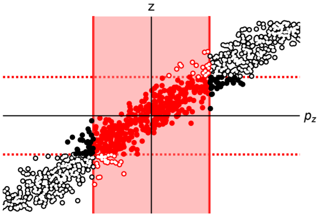
$$\omega_{\rm IdG}^{\rm mom} = 1 - \alpha - \frac{2e^{-2\mathrm{erf}^{-1}(\alpha)^2}\mathrm{erf}^{-1}(\alpha)^2}{3\pi\alpha}.$$

Similar results were found for skewness and kurtosis could, but the analytical form becomes more complicated.



Collective flow

We now add collective flow to the longitudinal velocity (rapidity) as follows



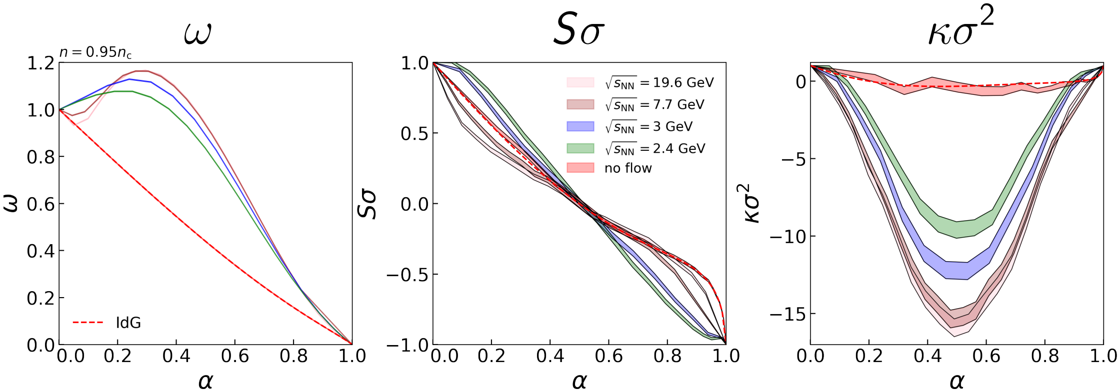
$$\tilde{v}_z = \tilde{v}_z^{\mathrm{LJ}} + \kappa \left(\frac{\tilde{z}}{\tilde{L}} - \frac{1}{2} \right)$$

thermal part collective flow part

$$y(\tilde{z}) = y_{\mathrm{th}} + \sqrt{\frac{T_{\mathrm{frz}}}{m\tilde{T}}} \kappa \left(\frac{\tilde{z}}{\tilde{L}} - \frac{1}{2} \right).$$

We map κ to the collision energies, using the heavy-ion inspired parameters: $T_{\mathrm{frz}} = 150$ MeV, $m = 938$ MeV.

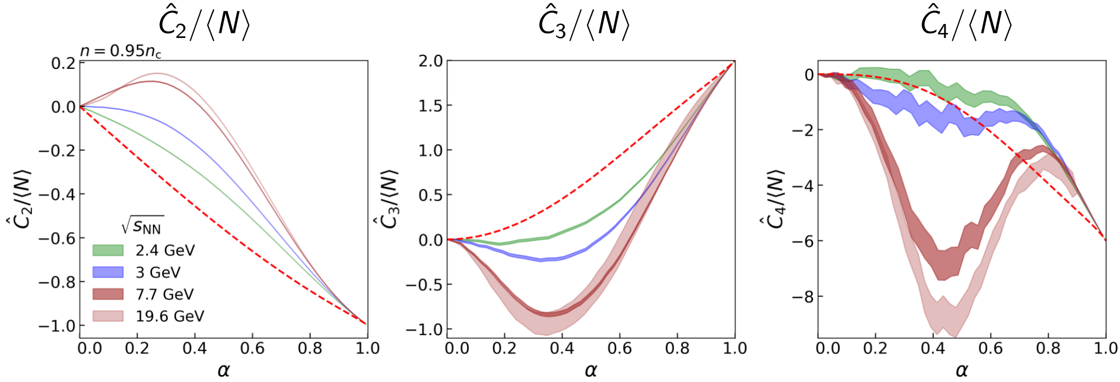
Cumulants at fixed α ($n = 0.95 n_c$)



With correlation cumulants in the momentum space becomes notably non-Gaussian.[1]

[1] NB: This is not a prediction of $\sqrt{s_{NN}}$ dependence but an estimation of the signal for a freeze-out at critical density.

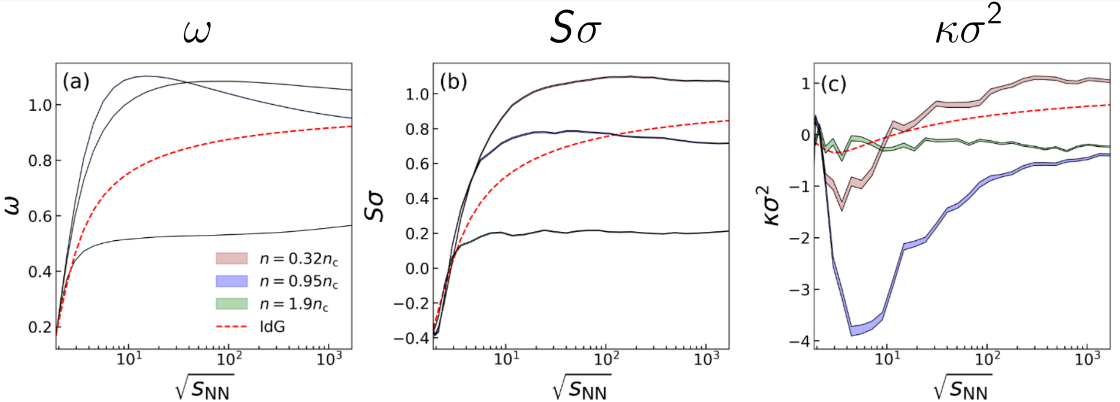
Factorial cumulants at fixed α ($n = 0.95n_c$)



With correlation factorial cumulants in the momentum space becomes notably non-Gaussian.[2]

[2] NB: This is not a prediction of $\sqrt{s_{\rm NN}}$ dependence but an estimation of the signal for a freeze-out at critical density.

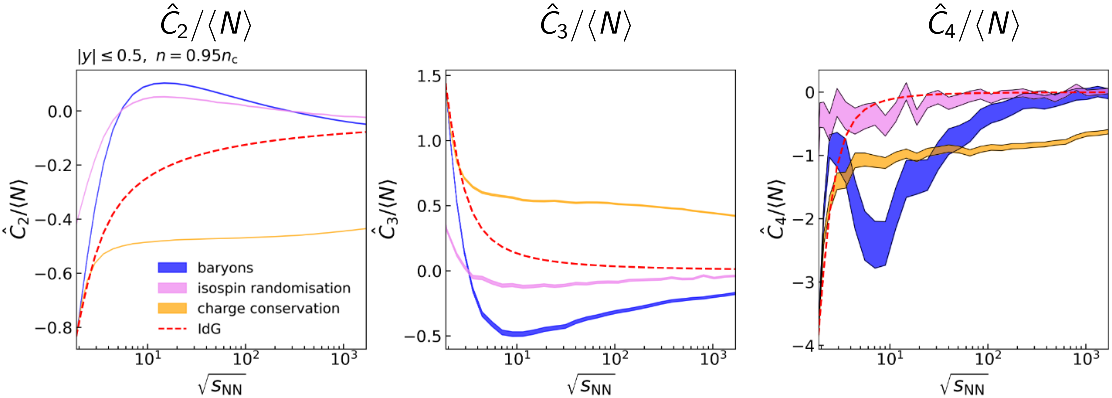
Cumulants at fixed $|y| < 0.5$ acceptance



The interplay between the increasing flow and the decreasing of subsystem fraction α gives a non-trivial dependence on $\sqrt{s_{\mathrm{NN}}}$.[3]

[3] NB: Once again, this is not a prediction of actual $\sqrt{s_{\mathrm{NN}}}$ dependence but an estimation of the signal for a freeze-out at critical density occurring at a given $\sqrt{s_{\mathrm{NN}}}$.

Factorial cumulants at fixed $|y| < 0.5$ acceptance ($n = 0.95n_c$)



Proton factorial cumulants do not show as strong signal as observed for baryons.[4]

[4] NB: Once again, this is not a prediction of actual $\sqrt{s_{\rm NN}}$ dependence but an estimation of the signal for a freeze-out at critical density occurring at a given $\sqrt{s_{\rm NN}}$.

Summary

1. High-statistics (2 million events) simulations of the Lennard-Jones fluid have been performed to compute skewness and kurtosis of particle number for the **first time in a microscopic MD framework**.
2. Scaled variance, skewness, and kurtosis, have same equilibration rates and **show large deviations from Poisson baseline near the CP in coordinate space.** Same is true for the factorial cumulants.
3. Factorial cumulants were counted uncovering the n-particle correlations in the system. High and low energy regime for proton factorial cumulants is studied and signal suppression observed.
4. Momentum-space fluctuations coincide with the analytical expectations for the Ideal gas with the energy conservation $\rightarrow$ *no effects of the CP in momentum space even for the higher cumulants in the system without collective flow.*
5. Implementing the Bjorken-like flow in the system recovers the CP signal in the momentum space. The results confirm the sensitivity of non-Gaussian fluctuations to criticality.

- **Future plans:** Implementation of multiple components (protons, neutrons, ...) and more realistic expansion dynamics, comparison with experimental data, expansions CP studies with LJ virial EOS.

THANK YOU FOR ATTENTION!

Questions?

Cumulants definition

Scaled variance

$$\omega = \frac{\kappa_2}{\kappa_1} = \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle}.$$

Skewness

$$S\sigma = \frac{\kappa_3}{\kappa_2} = \frac{\langle N^3 \rangle - 3\langle N^2 \rangle \langle N \rangle + 2\langle N \rangle^3}{\langle N^2 \rangle - \langle N \rangle^2}.$$

(Excess) kurtosis

$$\kappa\sigma^2 = \frac{\kappa_4}{\kappa_2} = \frac{\langle N^4 \rangle - 4\langle N^3 \rangle \langle N \rangle + 6\langle N^2 \rangle \langle N \rangle^2 - 3\langle N \rangle^4}{\langle N^2 \rangle - \langle N \rangle^2} - 3(\langle N^2 \rangle - \langle N \rangle^2).$$

Collective flow

We can identify the boundary rapidity $y(\tilde{z} = \tilde{L}/2)$ with the center-of-mass rapidity

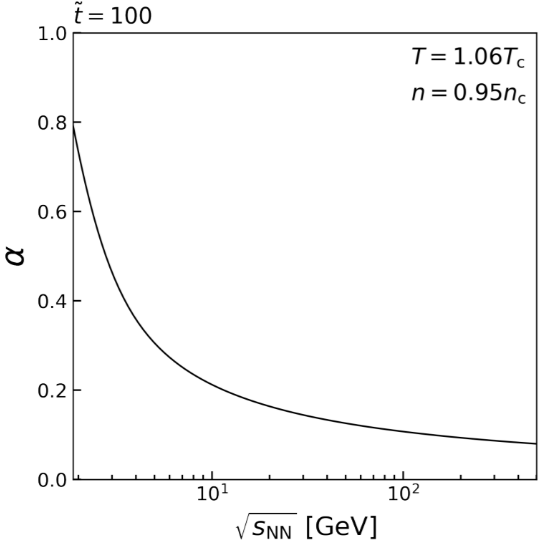
$$y_{\rm cm} = y_{\rm beam}/2 = \ln\left[\frac{\sqrt{s_{\rm NN}} + \sqrt{s_{\rm NN} - 4m_N^2}}{2m_N}\right].$$

$$\langle y(\tilde{z} = \tilde{L}/2)\rangle = \sqrt{\frac{T_{\rm frz}}{m\tilde{T}}}\kappa\frac{1}{2} = y_{\rm cm},$$

therefore

$$\kappa = 2y_{\rm cm}\sqrt{\frac{m\tilde{T}}{T_{\rm frz}}}, \quad \sqrt{s_{\rm NN}} = 2m\,{\rm ch}\left(\frac{\kappa}{2}\sqrt{\frac{T_{\rm fr}}{m\tilde{T}}}\right).$$

α as a function of $\sqrt{s_{\mathrm{NN}}}$ at $y_{\mathrm{cut}} = 0.5$



Flow at fixed $\alpha = 0.2$