Connecting grand-canonical cumulants of conserved charges to experiment

Volodymyr Vovchenko (LBNL)

ALICE *Workshop on event-by-event fluctuations (virtual)*

September 15, 2020

- Subensemble acceptance method (SAM)

  V.V., O. Savchuk, R. Poberezhnyuk, M.I. Gorenstein, V. Koch, arXiv:2003.13905

  V.V., R. Poberezhnyuk, V. Koch, arXiv:2007.03850, JHEP in print

- Particlization routine for event-by-event fluctuations

  V.V., V. Koch, *to appear*

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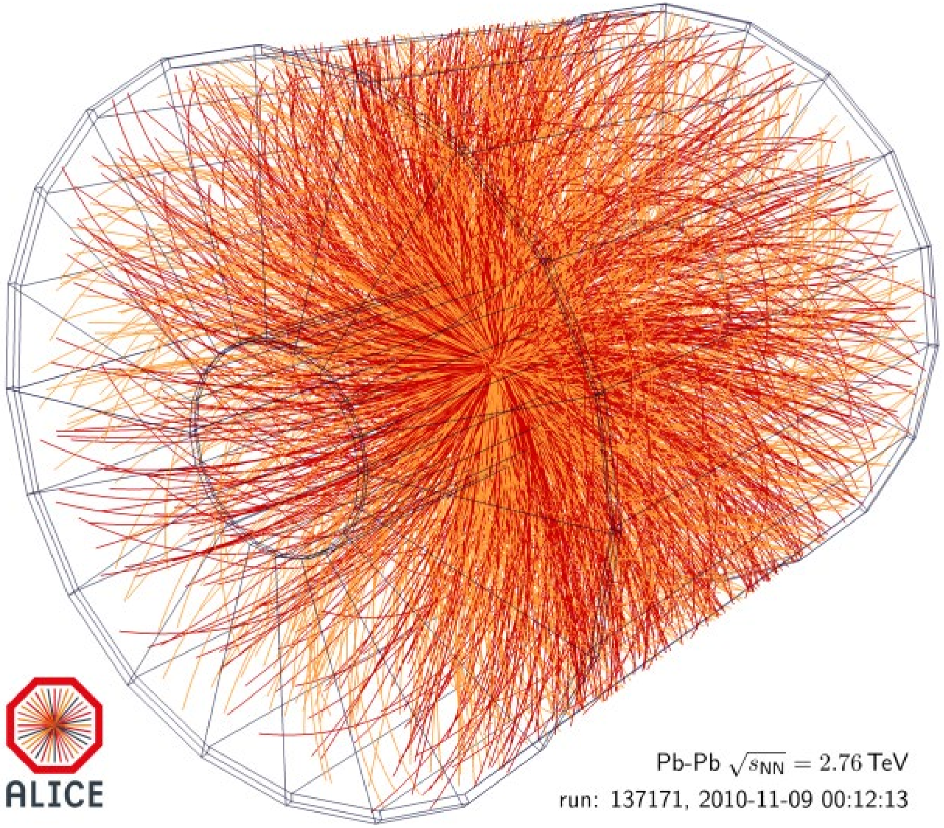
Relativistic heavy-ion collisions



Event display of a Pb-Pb collision in ALICE at the LHC

Thousands of particles created in relativistic heavy-ion collisions

Apply concepts of statistical mechanics

Event-by-event fluctuations: Motivations

Grand-canonical ensemble: $\kappa_n = \frac{1}{VT^3} \chi_B^n(T,\mu)$, $\chi_B^n(T,\mu) = \frac{\partial^n (p/T^4)}{\partial(\mu_B/T)^n}$

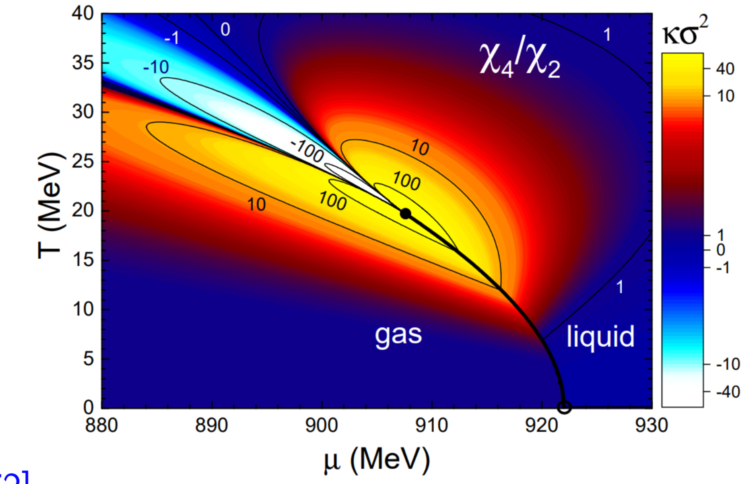
- QCD critical point [M. Stephanov, PRL '09]

  $\kappa_2 \sim \xi^2, \quad \kappa_3 \sim \xi^{4.5}, \quad \kappa_4 \sim \xi^7, \quad \xi \to \infty$

  NA61/SHINE, STAR-BES

- Chiral criticality at $\mu_B = 0$
  - Higher-order baryon number susceptibilties

  LHC Runs 3 & 4 [1812.06772]



[**V.V.** et al, PRC '15]

- Comparisons with first-principle lattice QCD predictions (fluctuations of conserved charges)
  - Direct comparisons of experimental data with grand-canonical fluctuations from different theories is commonplace: lattice QCD (Wuppertal-Budapest; HotQCD), HRG (Houston group; Nahrgang, Bluhm;...), effective QCD approaches (Fischer et al.; Pawlowski et al.),...

Theory vs experiment: Caveats

- proxy observables in experiment (net-proton, net-kaon) vs actual conserved charges in QCD (net-baryon, net-strangeness)

  Asakawa, Kitazawa, PRC '12; **V.V.**, Jiang, Gorenstein, Stoecker, PRC '18

- volume fluctuations

  Gorenstein, Gazdzicki, PRC '11; Skokov, Friman, Redlich, PRC '13; Braun-Munzinger, Rustamov, Stachel, NPA '17

- non-equilibrium (memory) effects

  Mukherjee, Venugopalan, Yin, PRC '15

- final-state interactions in the hadronic phase

  Steinheimer, **V.V.**, Aichelin, Bleicher, Stoecker, PLB '18

- accuracy of the grand-canonical ensemble (global conservation laws)

  Jeon, Koch, PRL '00; Bzdak, Skokov, Koch, PRC '13; Braun-Munzinger, Rustamov, Stachel, NPA '17

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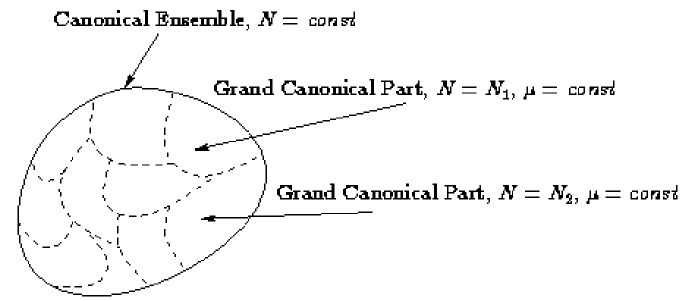
Canonical vs grand-canonical

Grand-canonical ensemble: the system exchanges conserved charges with a heat bath

Canonical ensemble: conserved charges fixed to a same set of values in all microstates



Thermodynamic equivalence: in the limit $V \to \infty$ all statistical ensembles are equivalent wrt to all average quantities, e.g. $\langle N \rangle_{GCE} = N_{CE}$

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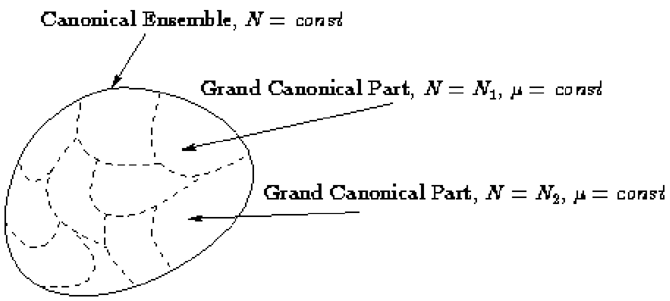

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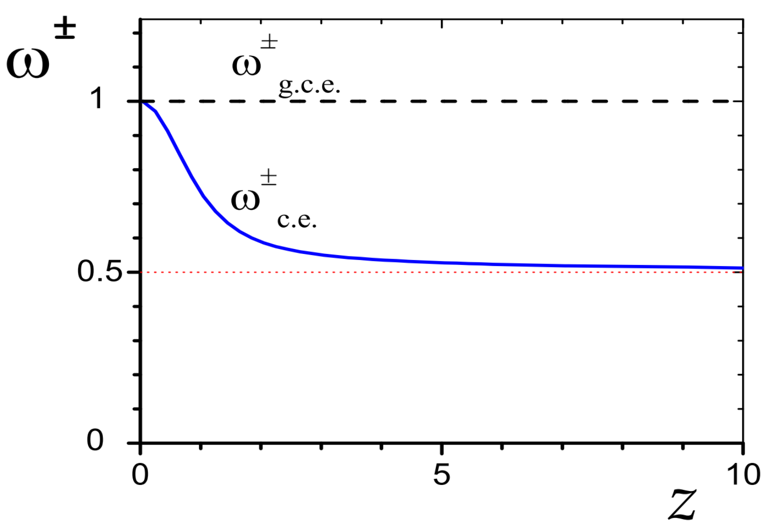


Begun, Gorenstein, Gazdzicki, Zozulya, PRC '04

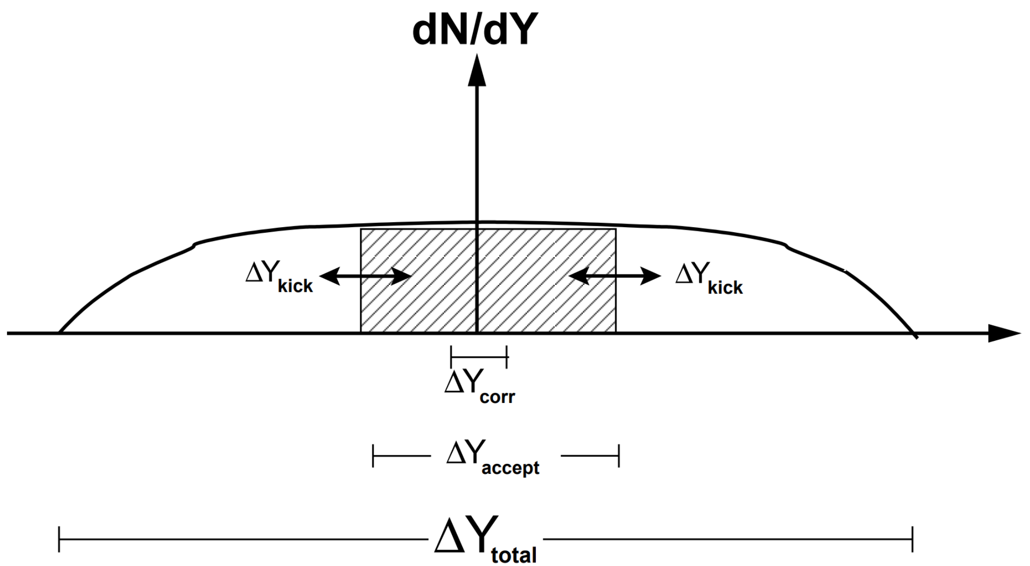
Thermodynamic equivalence does *not* extend to fluctuations. The results are ensemble-dependent in the limit $V \to \infty$

So what ensemble should one use?

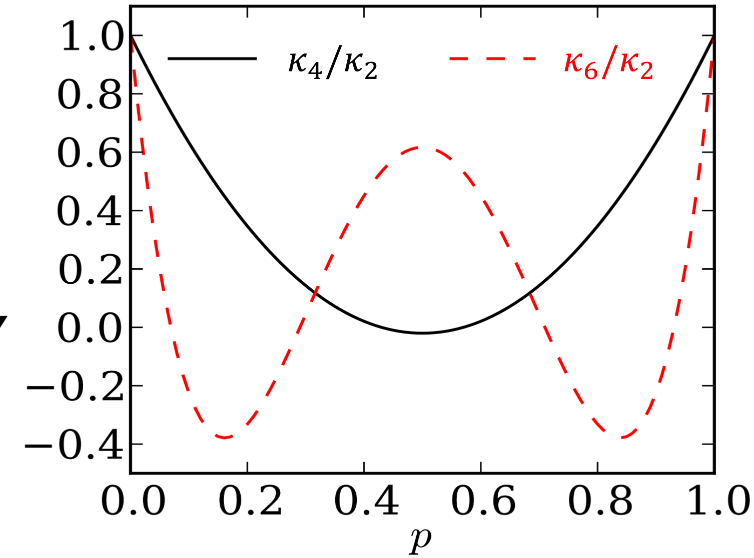
Canonical? Grand-canonical? Something else?

Applicability of the GCE in heavy-ion collisions

Experiments measure fluctuations in a finite momentum acceptance



V. Koch, 0810.2520



Bzdak et al., PRC '13

GCE applies if $\Delta Y_{total} \gg \Delta Y_{accept} \gg \Delta Y_{kick}, \Delta Y_{corr}$ and momentum-space correlation is strong (e.g. Bjorken flow)

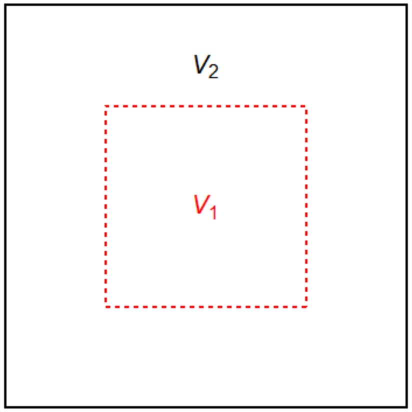
In practice difficult to satisfy all conditions simultaneously

This talk: $\Delta Y_{total} \gg \Delta Y_{accept} \;\; \rightarrow \;\; \Delta Y_{total} > \Delta Y_{accept}$ for *any* equation of state

Subensemble acceptance method (SAM)

Partition a thermal system with a globally conserved charge B *(canonical ensemble)* into two subsystems which can exchange the charge

$V_1 + V_2 = V$



Assume thermodynamic limit:

$$V, V_1, V_2 \to \infty; \quad \frac{V_1}{V} = \alpha = const; \quad \frac{V_2}{V} = (1-\alpha) = const;$$

$$V_1, V_2 \gg \xi^3, \qquad \xi = \text{correlation length}$$

The canonical partition function then reads:

$$Z^{\rm ce}(T,V,B) = \mathrm{Tr}\, e^{-\beta \hat{H}} \approx \sum_{B_1} Z^{\rm ce}(T,V_1,B_1)\, Z^{\rm ce}(T,V-V_1,B-B_1)$$

The probability to have charge B_1 is:

$$P(B_1) \propto Z^{\rm ce}(T,\alpha V,B_1)\, Z^{\rm ce}(T,(1-\alpha)V,B-B_1), \qquad \alpha \equiv V_1/V$$

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

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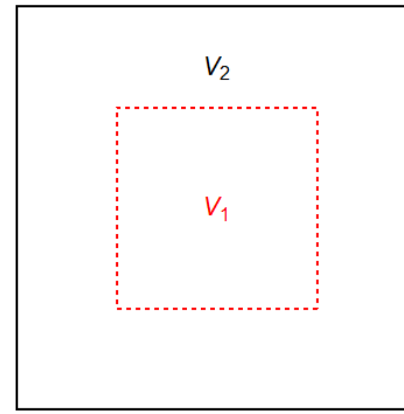

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Textbook: $\alpha \to 0 \implies$ grand-canonical ensemble $\neq$ **SAM:** $0 < \alpha < 1$

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

Subensemble acceptance method (SAM)

In the thermodynamic limit, $V \to \infty$, Z^{ce} expressed through free energy density

$$Z^{\rm ce}(T,V,B) \overset{V\to\infty}{\simeq} \exp\left[-\frac{V}{T} f(T,\rho_B)\right]$$

Cumulant generating function for B_1:

$$G_{B_1}(t) \equiv \ln\langle e^{t\,B_1}\rangle = \ln\left\{\sum_{B_1} e^{t\,B_1}\,\exp\left[-\frac{\alpha V}{T} f(T,\rho_{B_1})\right]\exp\left[-\frac{\beta V}{T} f(T,\rho_{B_2})\right]\right\} + \tilde{C}$$

Cumulants of B_1:

$$\kappa_n[B_1] = \left.\frac{\partial^n G_{B_1}(t)}{\partial t^n}\right|_{t=0} \equiv \tilde{\kappa}_n[B_1(t)]|_{t=0} \qquad \text{or} \qquad \kappa_n[B_1] = \left.\frac{\partial^{n-1}\tilde{\kappa}_1[B_1(t)]}{\partial t^{n-1}}\right|_{t=0}$$

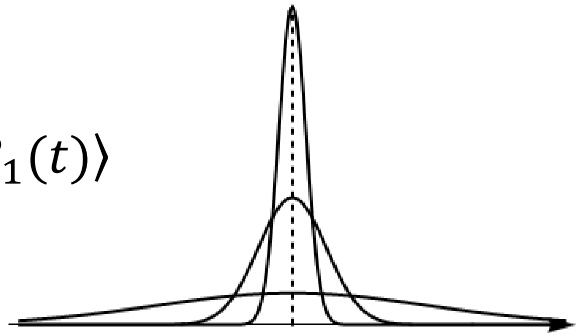
All κ_n can be calculated by determining the t-dependent first cumulant $\tilde{\kappa}_1[B_1(t)]$

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

Subensemble acceptance method (SAM)

$$\tilde{\kappa}_1[B_1(t)] = \frac{\sum_{B_1} B_1 \tilde{P}(B_1;t)}{\sum_{B_1} \tilde{P}(B_1;t)} \equiv \langle B_1(t) \rangle \qquad \text{with} \qquad \tilde{P}(B_1;t) = \exp\left\{ tB_1 - V\,\frac{\alpha f(T,\rho_{B_1}) + \beta f(T,\rho_{B_2})}{T} \right\}.$$

Thermodynamic limit: $\tilde{P}(B_1;t)$ *highly peaked* at $\langle B_1(t) \rangle$



$\langle B_1(t) \rangle$ is a solution to equation $d\tilde{P}/\mathrm{d}B_1 = 0$:

$$t = \hat{\mu}_B[T,\rho_{B_1}(t)] - \hat{\mu}_B[T,\rho_{B_2}(t)]$$

$$\text{where} \quad \hat{\mu}_B \equiv \mu_B/T, \qquad \mu_B(T,\rho_B) = \partial f(T,\rho_B)/\partial \rho_B$$

$t = 0$: $\rho_{B_1} = \rho_{B_2} = B/V$, $B_1 = \alpha B$, i.e. conserved charge uniformly distributed between the two subsystems

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

SAM: Second order cumulant $\kappa_2[B_1]$

$$t = \hat{\mu}_B[T, \rho_{B_1}(t)] - \hat{\mu}_B[T, \rho_{B_2}(t)] \qquad (*)$$

$$\frac{\partial(*)}{\partial t}: \qquad 1 = \left(\frac{\partial \hat{\mu}_B}{\partial \rho_{B1}}\right)_T \left(\frac{\partial \rho_{B1}}{\partial \langle B_1 \rangle}\right)_V \frac{\partial \langle B_1 \rangle}{\partial t} - \left(\frac{\partial \hat{\mu}_B}{\partial \rho_{B2}}\right)_T \left(\frac{\partial \rho_{B2}}{\partial \langle B_2 \rangle}\right)_V \frac{\partial \langle B_2 \rangle}{\partial \langle B_1 \rangle} \frac{\partial \langle B_1 \rangle}{\partial t}$$

$$\left(\frac{\partial \hat{\mu}_B}{\partial \rho_{B1,2}}\right)_T \equiv \left[\chi_2^B\left(T, \rho_{B_{1,2}}\right)\, T^3\right]^{-1}, \qquad \rho_{B_1} \equiv \frac{\langle B_1 \rangle}{\alpha V}, \qquad \rho_{B_2} \equiv \frac{\langle B_2 \rangle}{(1-\alpha) V}, \qquad \langle B_2 \rangle = B - \langle B_1 \rangle, \qquad \frac{\partial \langle B_1 \rangle}{\partial t} \equiv \tilde{\kappa}_2[B_1(t)]$$

Solve the equation for $\tilde{\kappa}_2$:

$$\tilde{\kappa}_2[B_1(t)] = \frac{V\, T^3}{[\alpha\, \chi_2^B(T, \rho_{B_1})]^{-1} + [(1-\alpha)\, \chi_2^B(T, \rho_{B_2})]^{-1}}$$

$t = 0$:

$$\kappa_2[B_1] = \alpha\,(1-\alpha)\, V\, T^3\, \chi_2^B$$

Higher-order cumulants: iteratively differentiate $\tilde{\kappa}_2$ w.r.t. t

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

SAM: Full result up to κ_6

$$\kappa_1[B_1] = \alpha\, VT^3\, \chi_1^B$$

$$\beta = 1 - \alpha$$

$$\kappa_2[B_1] = \alpha\, VT^3\, \beta\, \chi_2^B$$

$$\kappa_3[B_1] = \alpha\, VT^3\, \beta\, (1-2\alpha)\, \chi_3^B$$

$$\kappa_4[B_1] = \alpha\, VT^3\, \beta\, \left[\chi_4^B - 3\alpha\beta \frac{(\chi_3^B)^2 + \chi_2^B\, \chi_4^B}{\chi_2^B}\right]$$

$$\kappa_5[B_1] = \alpha\, VT^3\, \beta\, (1-2\alpha) \left\{[1-2\beta\alpha]\chi_5^B - 10\alpha\beta \frac{\chi_3^B \chi_4^B}{\chi_2^B}\right\}$$

$$\kappa_6[B_1] = \alpha\, VT^3\, \beta\, [1-5\alpha\beta(1-\alpha\beta)]\, \chi_6^B + 5\, VT^3\, \alpha^2\, \beta^2 \left\{9\alpha\beta \frac{(\chi_3^B)^2\, \chi_4^B}{(\chi_2^B)^2} - 3\alpha\beta \frac{(\chi_3^B)^4}{(\chi_2^B)^3} -2(1-2\alpha)^2 \frac{(\chi_4^B)^2}{\chi_2^B} - 3[1-3\beta\alpha] \frac{\chi_3^B\, \chi_5^B}{\chi_2^B}\right\}$$

$$\chi_n^B = \frac{\partial^n (p/T^4)}{\partial(\mu_B/T)^n}$$ – grand-canonical susceptibilities, e.g. from lattice QCD!

Details: **V.V.**, Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

SAM: Cumulant ratios

Some common cumulant ratios:

scaled variance
$$\frac{\kappa_2[B_1]}{\kappa_1[B_1]} = (1-\alpha)\,\frac{\chi_2^B}{\chi_1^B},$$

skewness
$$\frac{\kappa_3[B_1]}{\kappa_2[B_1]} = (1-2\alpha)\,\frac{\chi_3^B}{\chi_2^B},$$

kurtosis
$$\frac{\kappa_4[B_1]}{\kappa_2[B_1]} = (1-3\alpha\beta)\,\frac{\chi_4^B}{\chi_2^B} - 3\alpha\beta\left(\frac{\chi_3^B}{\chi_2^B}\right)^2.$$

- Global conservation (α) and equation of state (χ_n^B) effects factorize in cumulants up to the 3rd order, starting from κ_4 not anymore
- $\alpha \to 0$ – GCE limit*
- $\alpha \to 1$ – CE limit

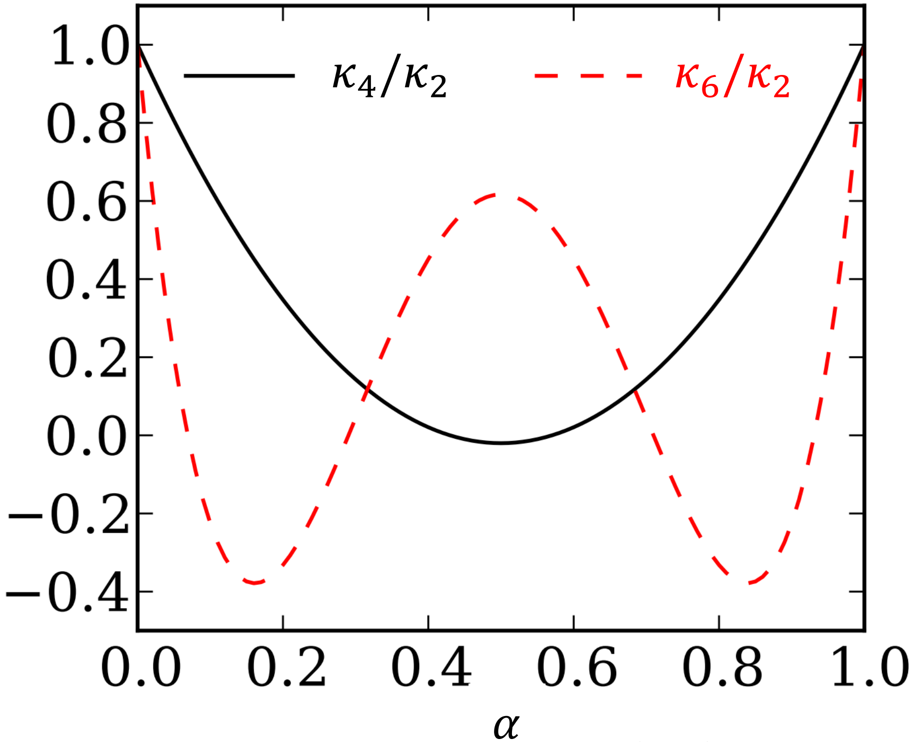
*As long as $V_1 \gg \xi^3$ holds

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

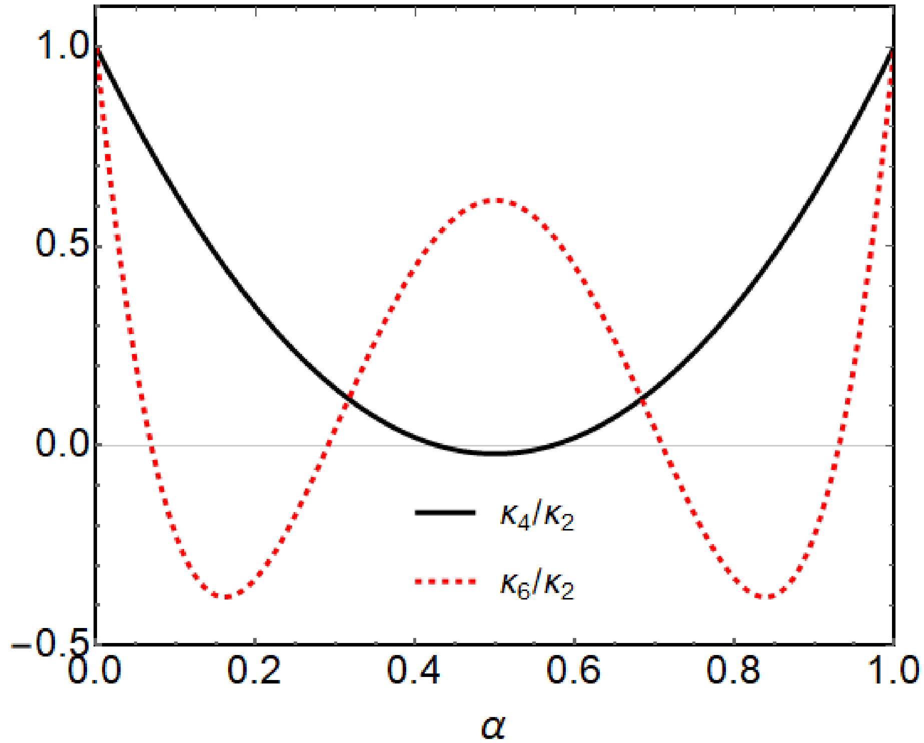
Subensemble acceptance: ideal gas

Ideal gas of baryons and antibaryons: $\chi^B_{2n} \propto \langle N_B \rangle + \langle N_{\bar{B}} \rangle$, $\chi^B_{2n-1} \propto \langle N_B \rangle - \langle N_{\bar{B}} \rangle$

Binomial acceptance [Bzdak et al., PRC '13]



SAM [**V.V.** et al., 2003.13905]

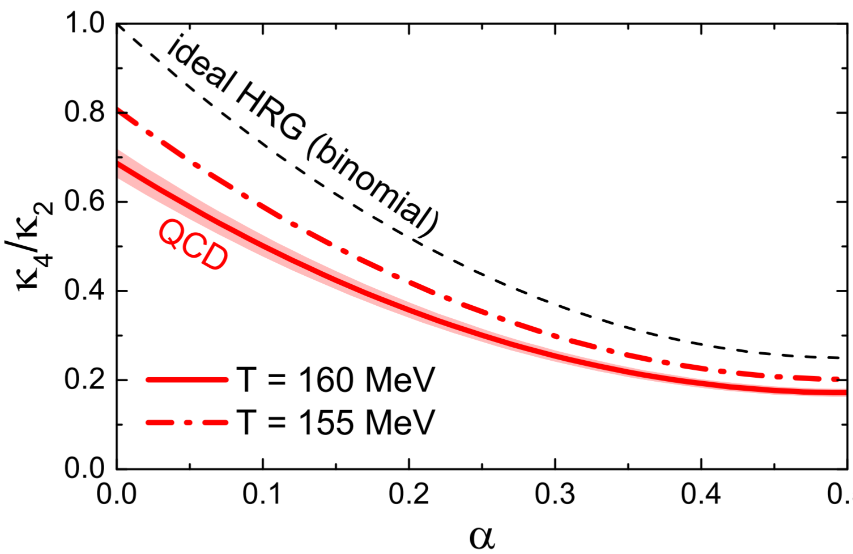


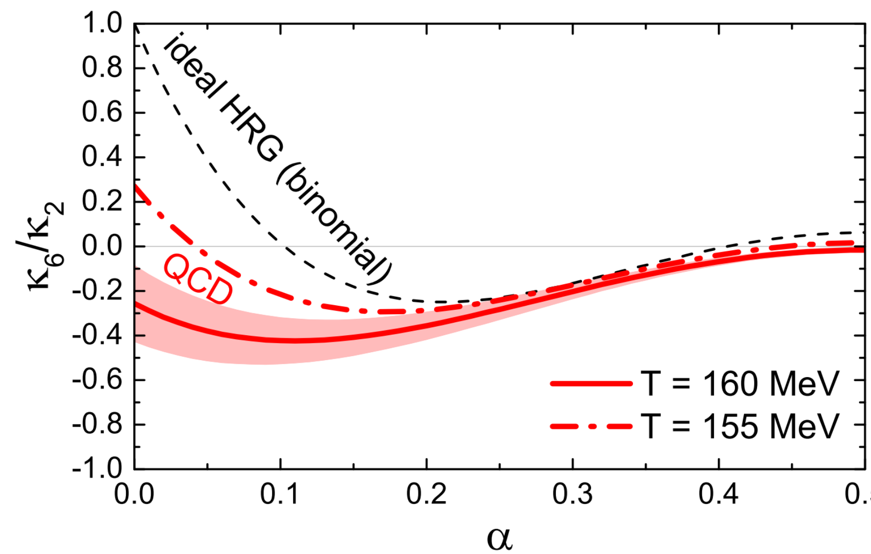
$\langle N_B \rangle = 400, \qquad \langle N_{\bar{B}} \rangle = 100$

For a more involved test (vdW fluid with a CP) see R. Poberezhnyuk, et al., 2004.14358

Net baryon fluctuations at LHC ($\mu_B = 0$)

$$\left(\frac{\kappa_4}{\kappa_2}\right)_{LHC} = (1-3\alpha\beta)\,\frac{\chi_4^B}{\chi_2^B} \qquad \left(\frac{\kappa_6}{\kappa_2}\right)_{LHC} = [1-5\alpha\beta(1-\alpha\beta)]\,\frac{\chi_6^B}{\chi_2^B} - 10\alpha(1-2\alpha)^2\beta\left(\frac{\chi_4^B}{\chi_2^B}\right)^2$$





Lattice data for χ_4^B/χ_2^B and χ_6^B/χ_2^B from Borsanyi et al., 1805.04445

For $\alpha > 0.2$ difficult to distinguish effects of the EoS and baryon conservation in χ_6^B/χ_2^B, $\alpha \leq 0.1$ is a sweet spot where measurements are mainly sensitive to the EoS

Estimates: $\alpha \approx 0.1$ corresponds to $\Delta Y_{acc} \approx 2(1)$ at LHC (RHIC), p_T integrated

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

SAM for multiple conserved charges

$$P(\hat{Q}_1) \propto Z(T, \alpha V, \hat{Q}_1)\, Z(T, \beta V, \hat{Q} - \hat{Q}_1) \qquad \hat{Q} = (B, Q, S, \dots)$$

The result: (see arXiv:2007.03850 for details)

$$\hat{\chi}_{i_1 \dots i_M} = \frac{\partial^M (p/T^4)}{\partial(\mu_{i_1}/T) \dots \partial(\mu_{i_M}/T)}$$

$$\hat{\kappa}_{i_1}[\hat{Q}^1] = \alpha V T^3\, \hat{\chi}_{i_1},$$

$$\hat{\kappa}_{i_1 i_2}[\hat{Q}^1] = \alpha V T^3\, \beta\, \hat{\chi}_{i_1 i_2},$$

$$\hat{\kappa}_{i_1 i_2 i_3}[\hat{Q}^1] = \alpha V T^3\, \beta\, (1 - 2\alpha)\, \hat{\chi}_{i_1 i_2 i_3},$$

$$\hat{\kappa}_{i_1 i_2 i_3 i_4}[\hat{Q}^1] = \alpha V T^3\, \beta \left[(1 - 3\alpha\beta)\, \hat{\chi}_{i_1 i_2 i_3 i_4} - \frac{\alpha\beta}{2!\,2!\,2!} \sum_{\sigma \in S_4} \hat{\chi}^{-1}_{b_1 b_2}\, \hat{\chi}_{i_{\sigma_1} i_{\sigma_2} b_1}\, \hat{\chi}_{i_{\sigma_3} i_{\sigma_4} b_2} \right],$$

...

Results depend on cross-correlators of conserved charges

Mathematica notebook to express any B,Q,S-cumulant of order $n \leq 6$ in terms of grand-canonical susceptibilities available at https://github.com/vlvovch/SAM

V.V., Poberezhnyuk, Koch, 2007.03850, JHEP '20

SAM for multiple conserved charges

Key findings:

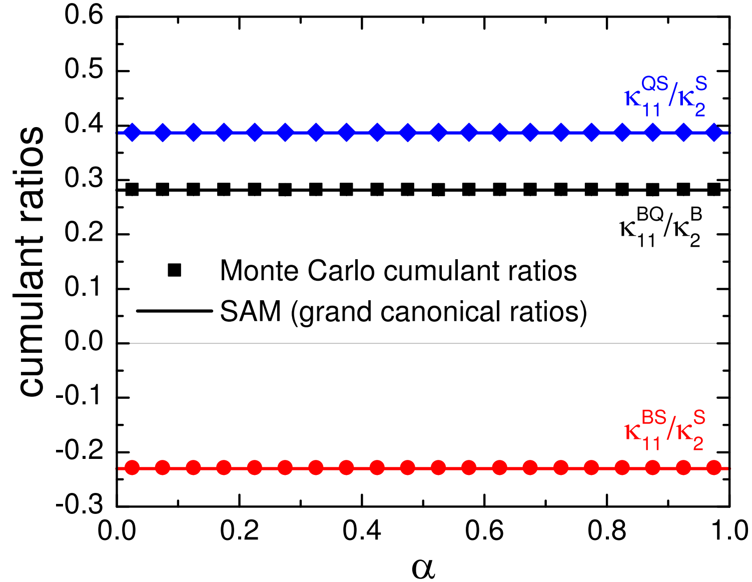
- Cumulants up to 3rd order factorize into product of binomial and grand-canonical cumulants

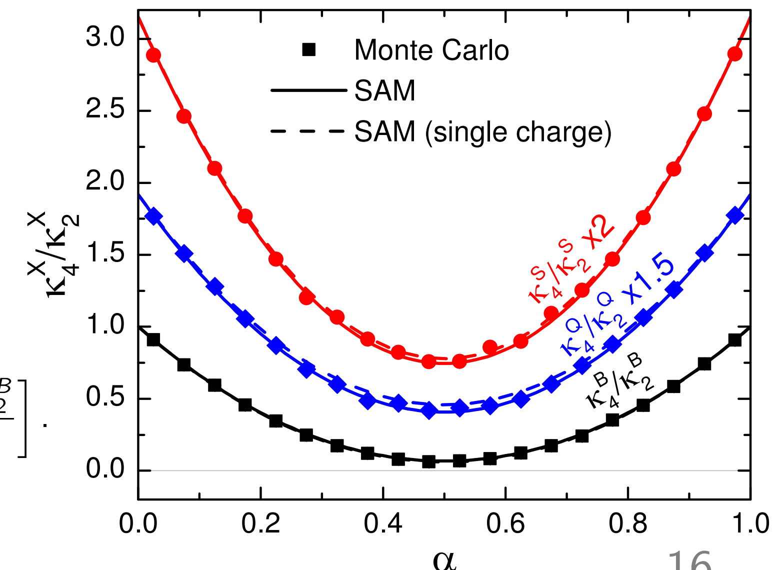
$$\kappa_{l,m,n} = \kappa^{\text{bino}}_{l+m+n}(\alpha) \times \kappa^{\text{gce}}_{l,m,n}\,, \qquad l+m+n \leq 3$$

  - Ratios of second and third order cumulants are NOT sensitive to charge conservation
  - Requires that acceptance fraction α is the same for all particles

- For order $n > 3$ charge cumulants "mix". Effect in HRG is tiny

$$\kappa_4[B^1] = \alpha V T^3 \beta \left[(1-3\alpha\beta)\,\chi_4^B - 3\,\alpha\,\beta\,\frac{(\chi_3^B)^2\chi_2^Q - 2\chi_{21}^{BQ}\chi_{11}^{BQ}\chi_3^B + (\chi_{21}^{BQ})^2\chi_2^B}{\chi_2^B\chi_2^Q - (\chi_{11}^{BQ})^2} \right].$$



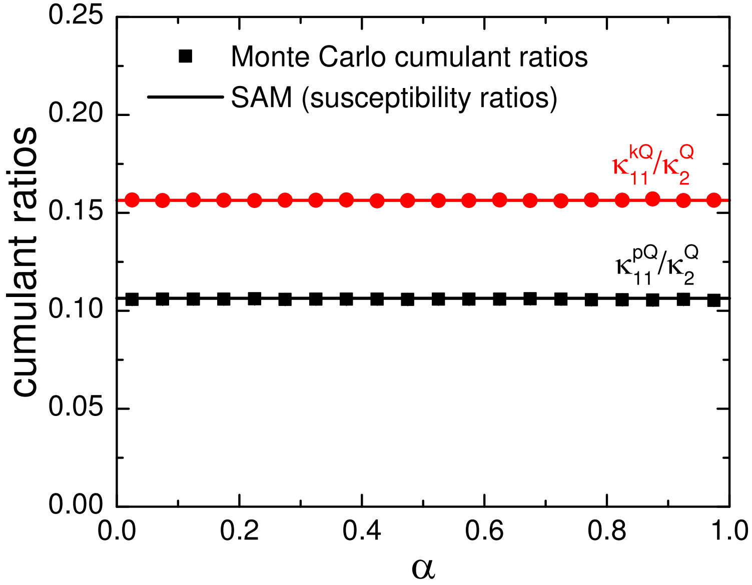


V.V., Poberezhnyuk, Koch, 2007.03850, JHEP '20

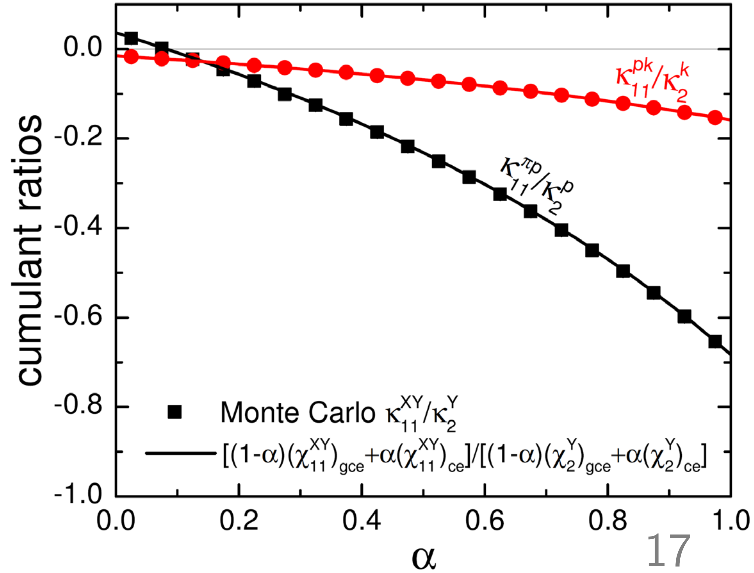
SAM and non-conserved quantities

$$\kappa_{XY} = (1-\alpha)\,\kappa_{XY}^{\mathrm{gce}} + \alpha\,\kappa_{XY}^{\mathrm{ce}}$$

- Mixed cumulants involving one conserved charge e.g. pQ have $\kappa_{pQ}^{ce} = 0$ thus they scale like second order charge cumulants
  - p and Q, again, must have the same a
  - STAR tries to measure these [1903.05370]
  - Can ALICE measure them as well?



- Cancellation does NOT occur for two non-conserved quantities, such as κ_{pK}

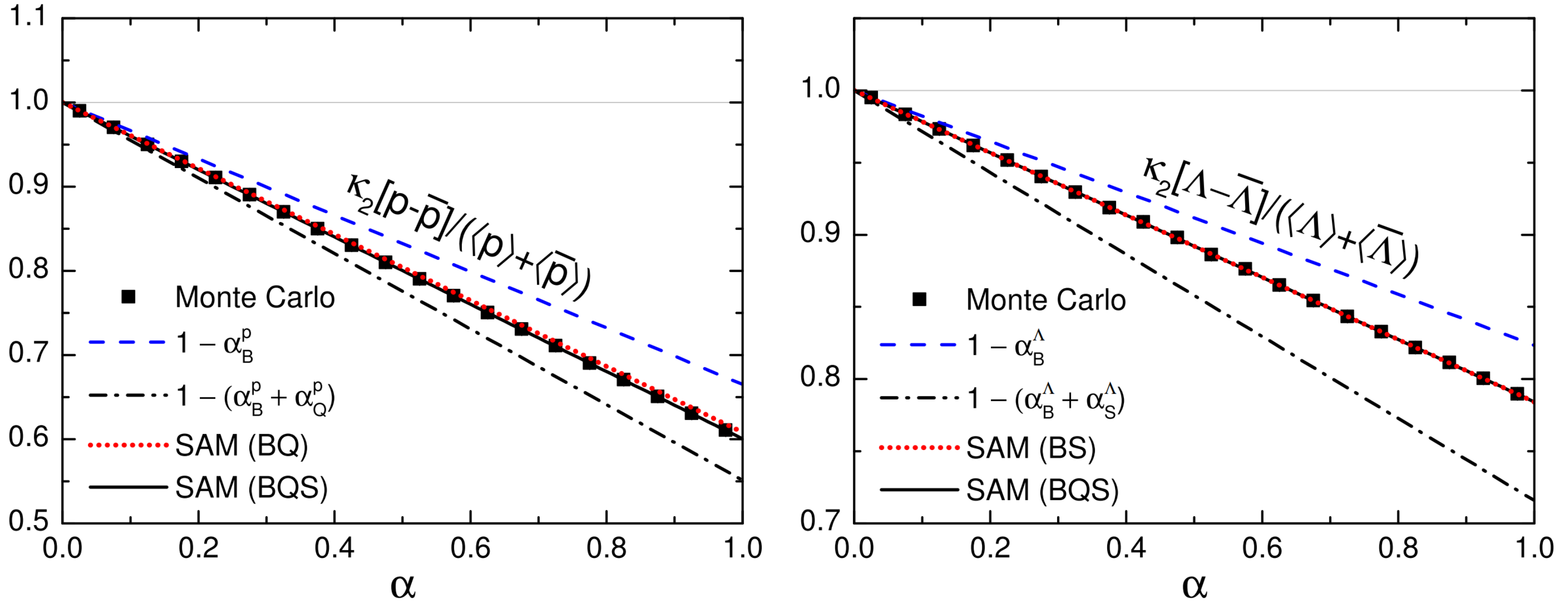


V.V., Poberezhnyuk, Koch, 2007.03850, JHEP '20

Net-proton and net-Λ fluctuations

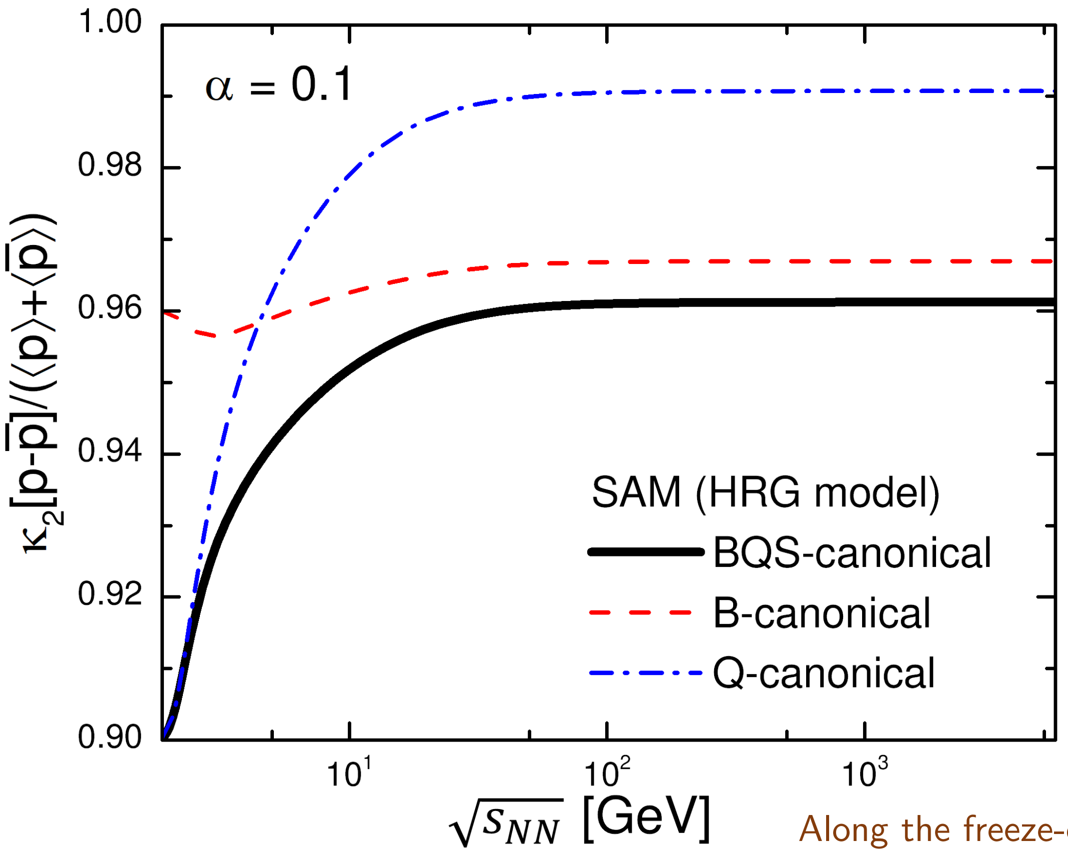
$$\kappa_{pp} = (1-\alpha)\,\kappa_{pp}^{\mathrm{gce}} + \alpha\,\kappa_{pp}^{\mathrm{ce}}$$

- Allows for corrections due to electric charge (protons) or strangeness (Λ) conservation in addition to baryon number conservation.



Truth lies in between the "naïve" corrections
Likely bigger effect for higher orders

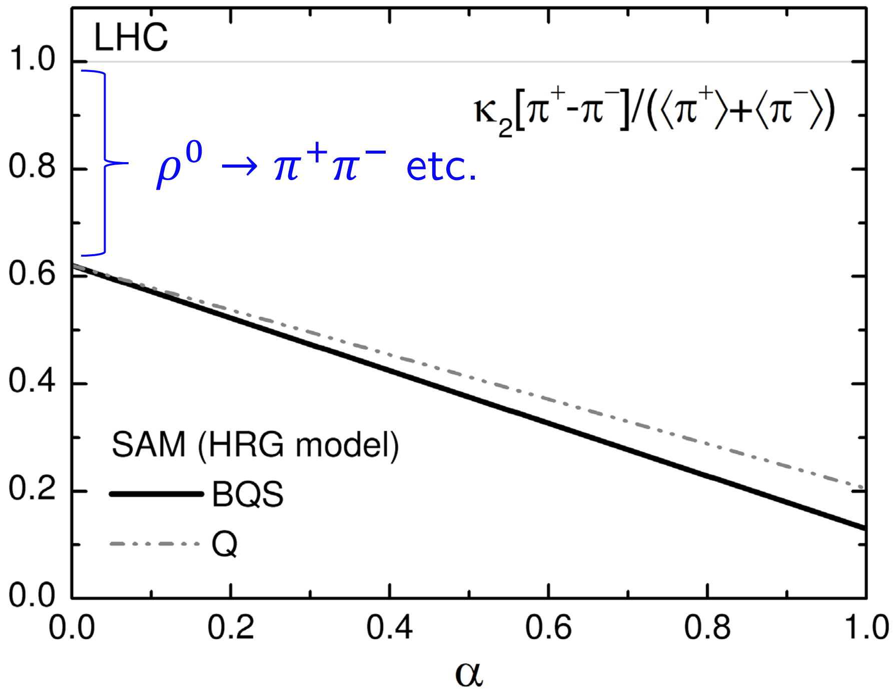
Net-proton fluctuations at various energies

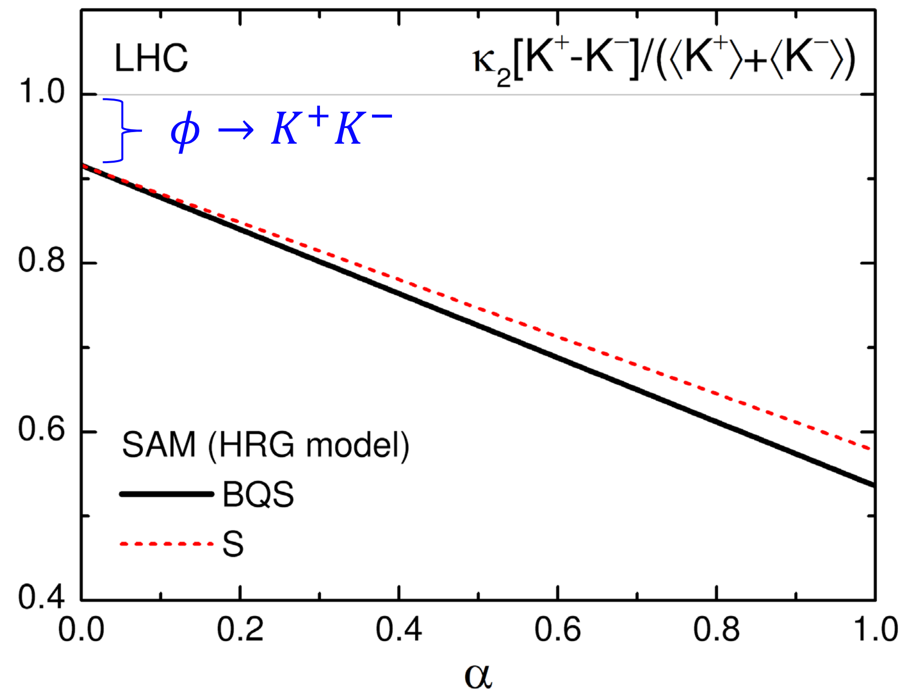


Along the freeze-out curve

- LHC: The most important (but not the only) effect is baryon conservation
- Low energies: net-p ≈ net-Q $\Longrightarrow$ electric charge conservation dominates
- Simultaneous treatment of B and Q conservation is important

Net-pion and net-kaon fluctuations





Global conservation effects for pions (kaons) driven by electric charge (strangeness) conservation. Ratios deviate from unity in $\alpha \to 0$ limit due to resonance decays*

*Argument here is made in coordinate space. In momentum space the ratios do tend to unity in limit $\Delta Y_{acc} \to 0$ due to diffusion of decay products in and out of acceptance

Correlations from resonance decays in HRG model included via [Begun et al., PRC '06]

Applicability and limitations

- Argument is based on partition in ***coordinate*** space but experiments measure in ***momentum*** space
  - OK at high energies where we have **Bjorken flow**
    - For small $\Delta Y_{acc} < 1$: corrections due to thermal smearing and resonance decay kinematics (for Q and S)
  - Limited applicability at lower energies
- **Thermodynamic limit** i.e. $V_1, V_2 \gg \xi^3$:
  - OK at LHC where $\frac{dV}{dy} \sim 4000 - 5000$ fm^3 vs. $V_{lattice} \sim 125$ fm^3
  - Applicability is more limited near the critical point
- Assumes $\boldsymbol{T, \mu_B = const}$ everywhere

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⬇

Address these issues with **Monte Carlo SAM Sampler**

V.V., V. Koch, *to appear*

SAM Sampler

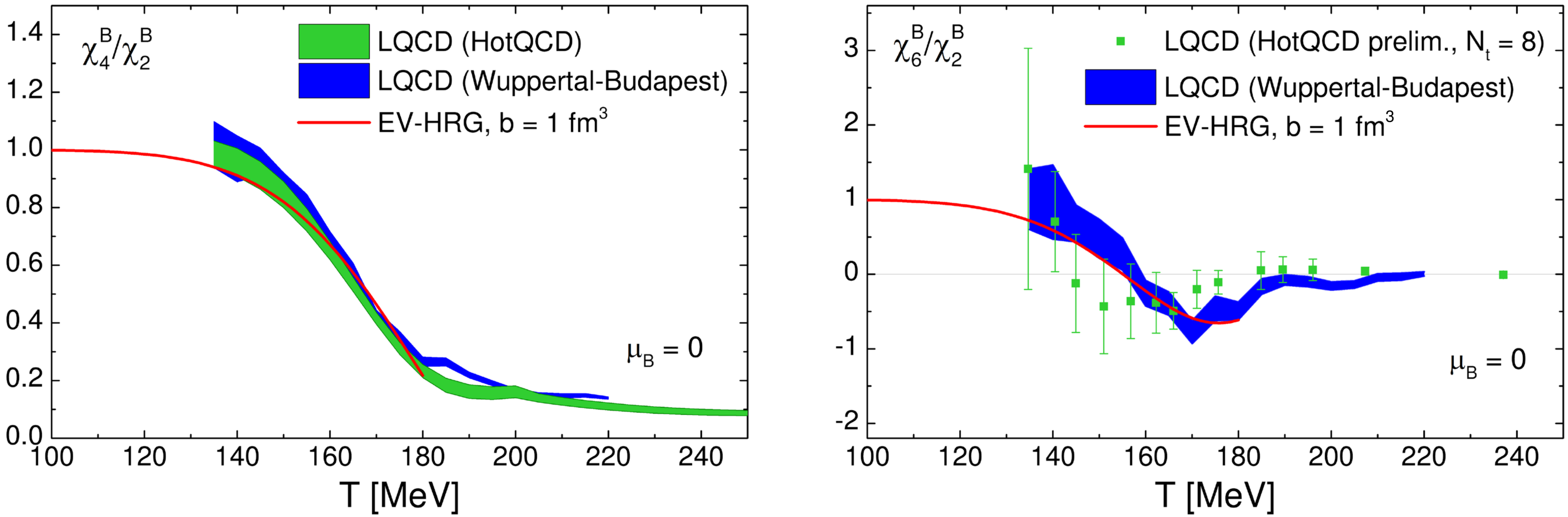
A **particlization** routine that preserves correlations and fluctuations *locally*

1. Partition the hydro (blast-wave) hypersurface into subvolumes along the space-time rapidity axis such that each $V_i \gg \xi^3$ and $\Delta\eta \leq \Delta Y_{\mathrm{acc}}$
2. Sample each subvolume grand-canonically, using the partition function of an *interacting* HRG
3. Reject the event if global conservation is violated
4. Sample the momenta of particles
5. Do resonance decays or plug into hadronic afterburner

✓ **(event-by-event) hydro**
✓ **local correlations**
✓ **global conservation**
✓ **thermal smearing**
✓ **resonance decays**

To be part of **FIST-2.0**

A case study: net baryon fluctuations at $\mu_B = 0$



WB: 1805.04445; HotQCD: 1708.04897

EV-HRG model: V.V., Gorenstein, Stoecker, PRL '17
V.V., Pasztor, Fodor, Katz, Stoecker, PLB '17

Model the deviations of the lattice data from Skellam distribution at T_{pc} with excluded-volume interactions in the baryonic sector (EV-HRG model)

$$P(N) \sim \frac{(V-bN)^N}{N!}\,\theta(V-bN)$$

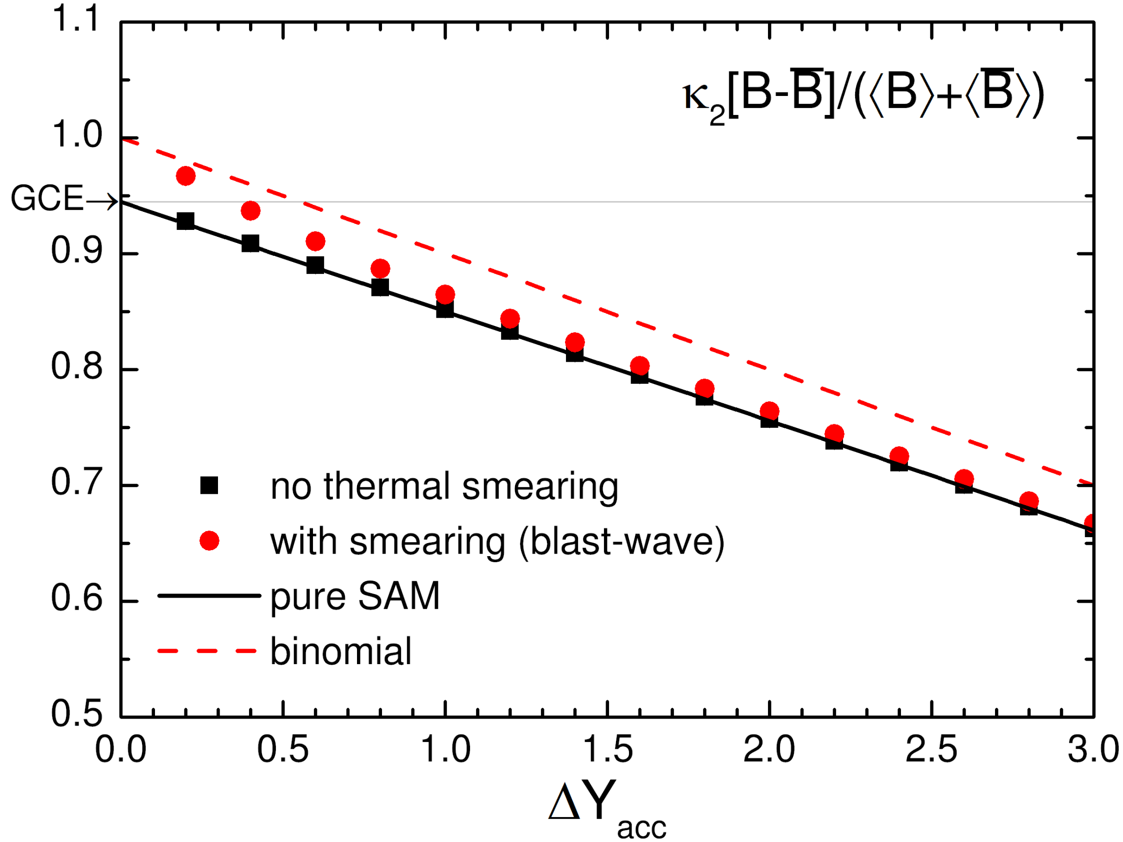
Multiplicity distribution of the EV-HRG model is efficiently sampled with Poisson + rejection sampling

details in V.V., Gorenstein, Stoecker, 1805.01402

A case study: net baryon fluctuations at $\mu_B = 0$

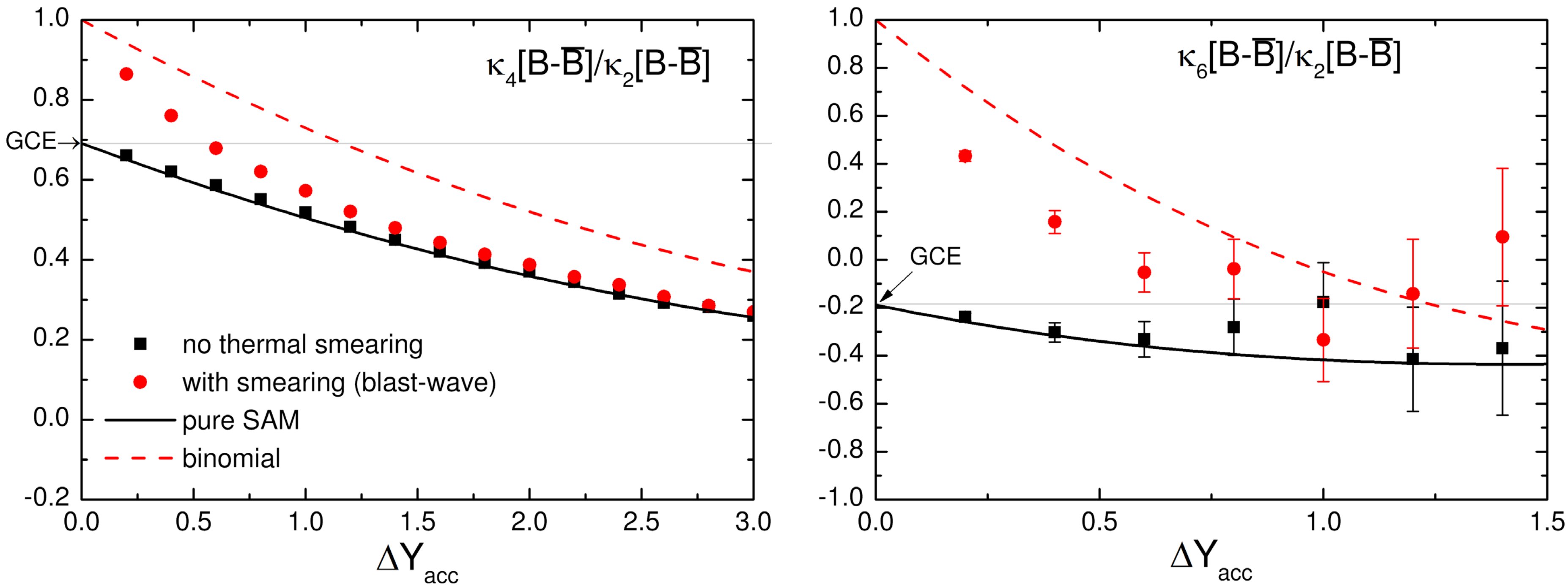
Take only protons and neutrons, T=160 MeV, blast-wave momentum smearing

$$\frac{\chi_2^B}{\chi_{2,Sk}^B} = 0.94, \quad \frac{\chi_4^B}{\chi_2^B} = 0.69, \quad \frac{\chi_6^B}{\chi_2^B} = -0.18 \quad \leftarrow \text{ compatible with lattice}$$



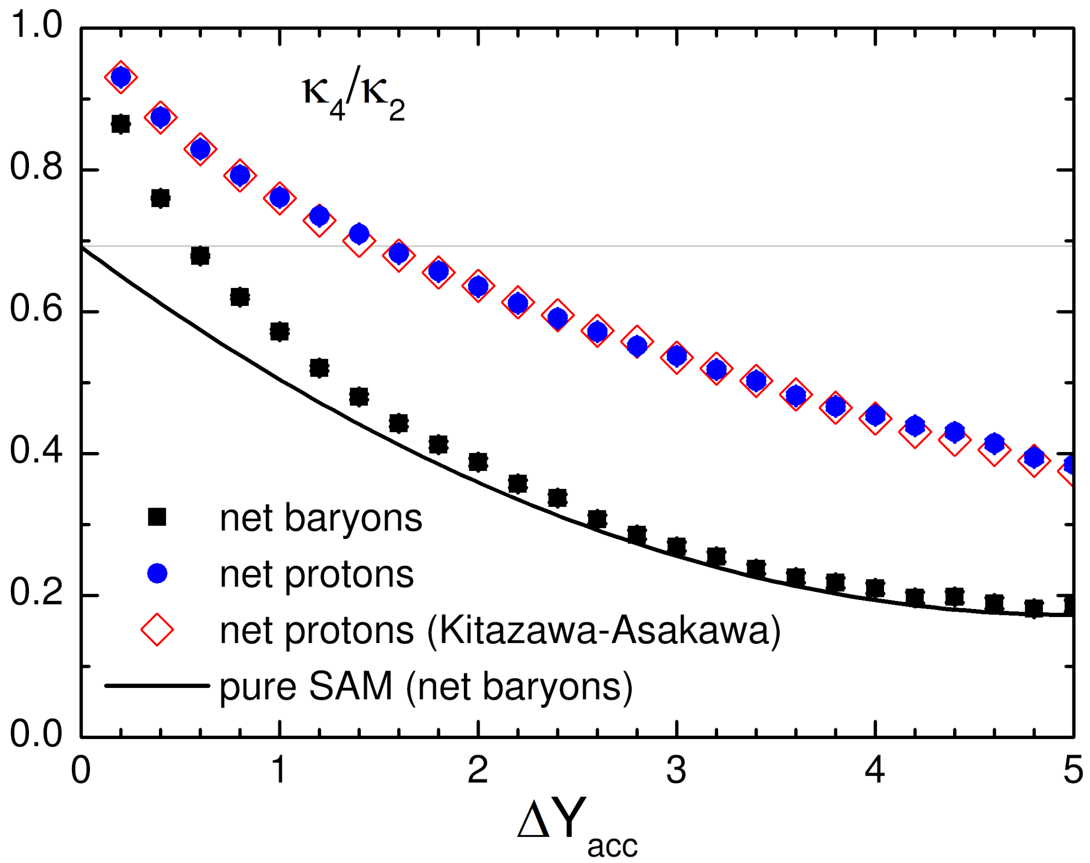
boost-invariant, $\Delta\eta = 0.1$, $\eta_{max} = \pm 5$, $V_i = 20$ fm^3, baryon number conservation only

A case study: net baryon fluctuations at $\mu_B = 0$



- Thermal smearing "poissonizes" fluctuations in small acceptance
- The signal survives for sufficiently large rapidity coverage, $\Delta Y_{acc} \gtrsim 1$

net proton vs net baryon



- **net proton ≠ net baryon**
- net proton kurtosis crosses the GCE/LQCD value of net baryon kurtosis in certain rapidity range ($\Delta Y_{acc} \sim 1-2$) → explanation for apparent agreement between STAR and LQCD reported in [HotQCD, 2001.08530]?

Summary

- SAM is a method to correct cumulants of distributions in heavy-ion collisions for global (multiple) charge conservation for *any* equation of state, not just ideal gas
    - connection to lattice results
    - ratios of second and third order cumulants insensitive to conservation effects as long as acceptance fraction is the same
    - electric charge and strangeness conservations affect net-proton and net-Λ fluctuations in addition to baryon number conservation
- SAM sampler is a particlization routine for quantitative analysis of event-by-event fluctuations

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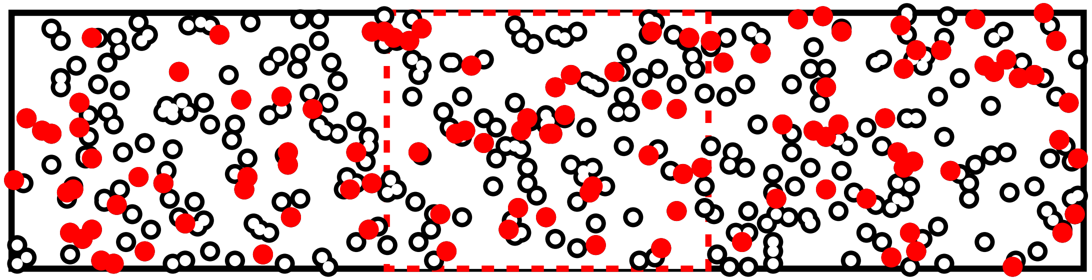
Thanks for your attention!

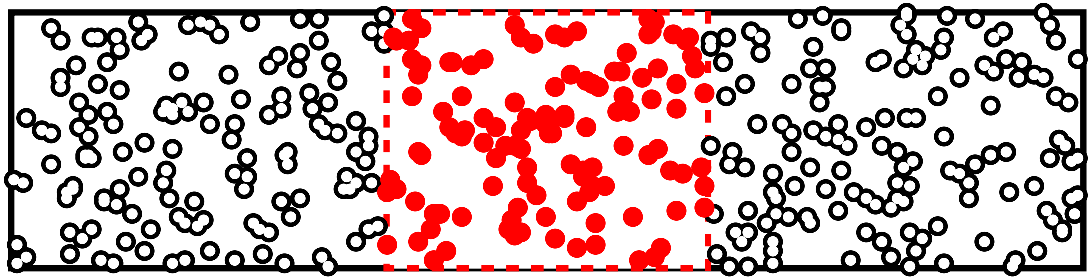
Backup slides

Binomial acceptance vs actual acceptance

Binomial acceptance: accept each particle (charge) with a probability α independently from all other particles



SAM:

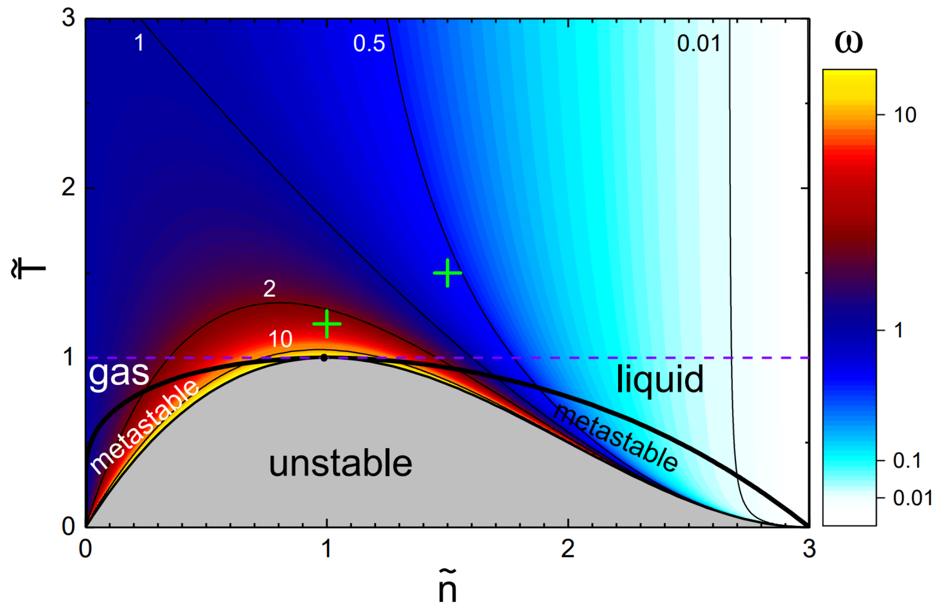


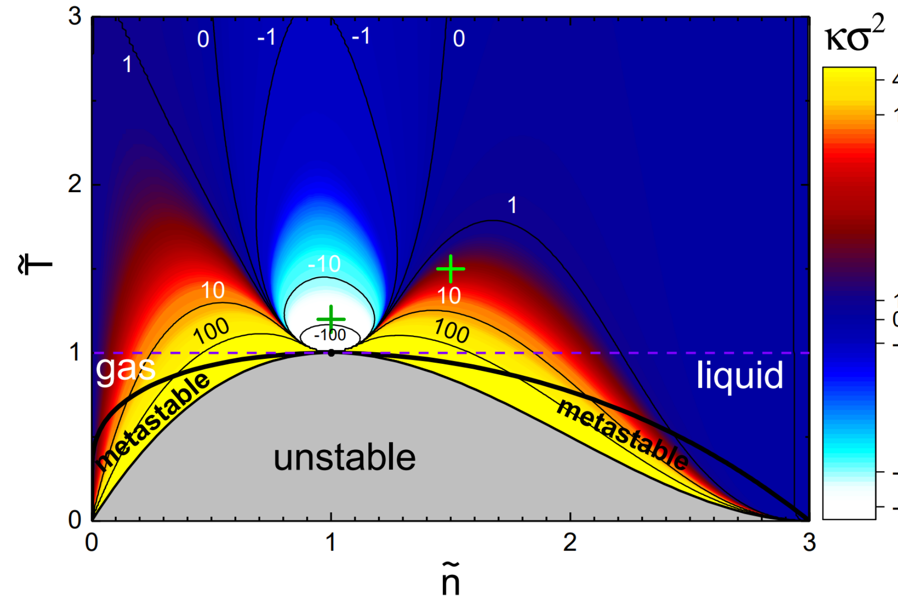
Subensemble acceptance: van der Waals fluid

van der Waals equation of state: first-order phase transition and a critical point

$$Z^{\rm ce}_{\rm vdW}(T,V,N) = Z^{\rm ce}_{\rm id}(T,V-bN,N)\,\exp\left(\frac{aN^2}{VT}\right)\,\theta(V-bN)$$

Rich structures in cumulant ratios close to the CP





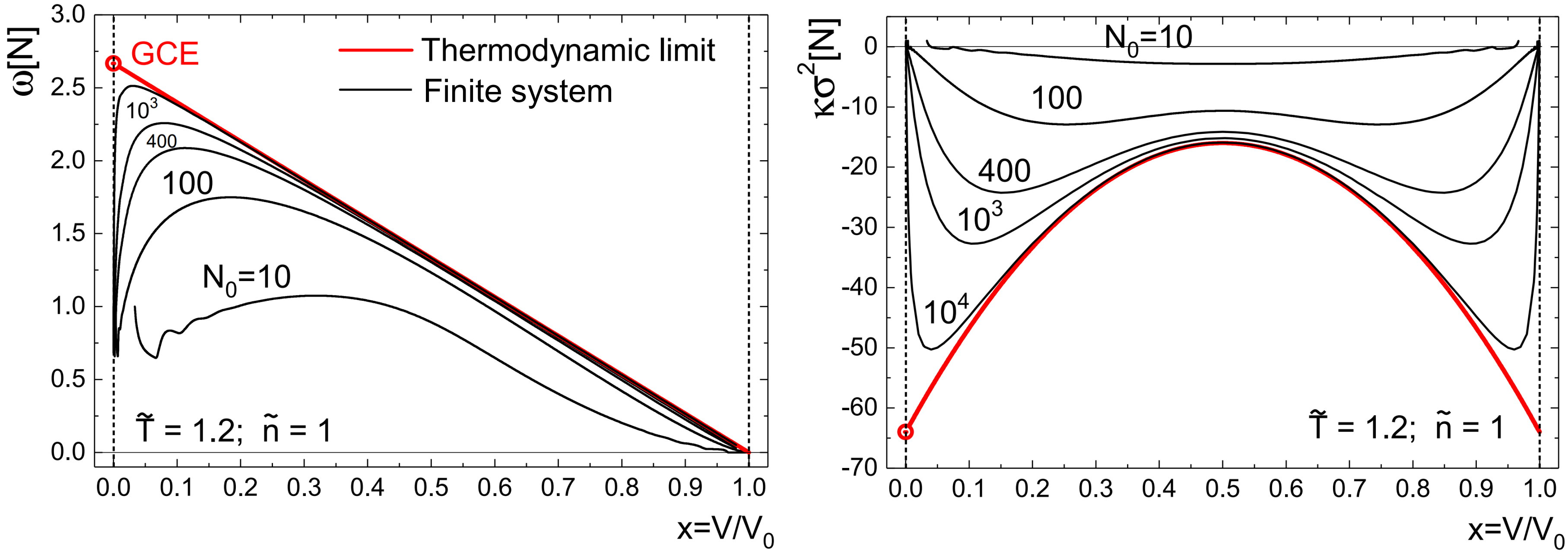
V.V., Poberezhnyuk, Anchishkin, Gorenstein, 1507.06537

Subensemble acceptance: van der Waals fluid

Calculate cumulants $\kappa_n[N]$ in a subvolume directly from the partition function

$$P(N) \propto Z^{\rm ce}_{\rm vdW}(T, xV_0, N)\, Z^{\rm ce}_{\rm vdW}(T, (1-x)V_0, N_0 - N)$$

and compare with the subensemble acceptance results



Results agree with subsensemble acceptance in thermodynamic limit ($N_0 \to \infty$)

Finite size effects are strong near the critical point: a consequence of large correlation length ξ

R. Poberezhnyuk, O. Savchuk, et al., 2004.14358