




Role of van der Waals interactions in hadron systems: from nuclear matter to lattice QCD

Volodymyr Vovchenko^{a,b,c}

^aFrankfurt Institute for Advanced Studies 

^bInstitute for Theoretical Physics, University of Frankfurt 

^cTaras Shevchenko National University of Kiev 

Collaborators: Paolo Alba, Dmitry Anchishkin, Mark Gorenstein, and
Horst Stoecker

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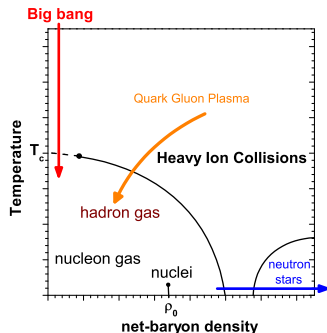
FIAS Frankfurt Institute
for Advanced Studies 

GOETHE
UNIVERSITÄT
FRANKFURT AM MAIN 

HGS-HiRe for FAIR
Helmholtz Graduate School for Hadron and Ion Research

Strongly interacting matter

- Theory of strong interactions: **Quantum Chromodynamics** (QCD)
- Basic degrees of freedom: quarks and gluons
- At smaller energies confined into hadrons (baryons and mesons)



Where is it relevant?

- Early universe
- Neutron stars
- Heavy-ion collisions

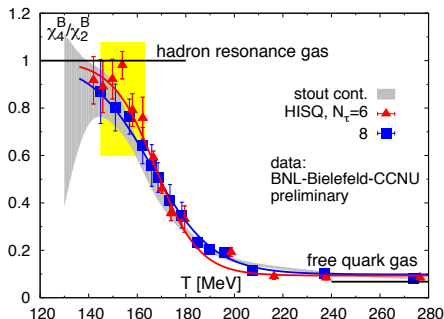
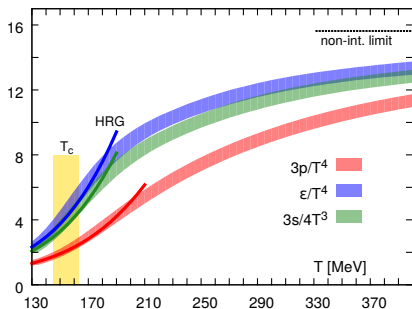
First principles of QCD are rather established,
but direct calculations are problematic

Phenomenological tools are very useful

Experiment: **heavy-ion collisions**

QCD equation of state at $\mu = 0$

Lattice simulations provide EoS at $\mu = 0^1$



Common model for confined phase is ideal **HRG**: non-interacting gas of known hadrons and resonances

- Good description of thermodynamic functions up to 180 MeV
- Rapid breakdown in crossover region for description of susceptibilities²
- Often interpreted as clear signal of deconfinement...
- But what is the role of hadronic interactions beyond normal HRG?

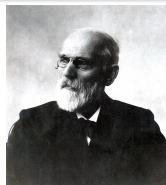
¹Bazavov et al., PRD 90, 094503 (2014); Borsanyi et al., PLB 730, 99 (2014)

²Ding, Karsch, Mukherjee, IJMPE 24, 1530007 (2015)

Van der Waals equation

Van der Waals equation

$$P(T, V, N) = \frac{NT}{V - bN} - a\frac{N^2}{V^2}$$



Formulated in
1873.

Simplest model which contains
attractive and **repulsive** interactions

Contains **1st order phase transition**
and **critical point**

Can elucidate role of fluctuations in
phase transitions



Nobel Prize in
1910.

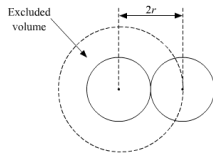
Two ingredients:

1) Short-range **repulsion**: particles are hard spheres,

$$V \rightarrow V - bN, \quad b = 4\frac{4\pi r^3}{3}$$

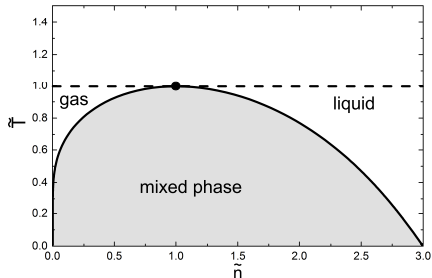
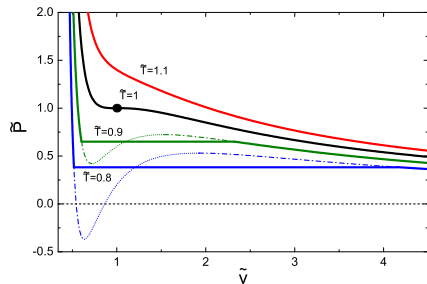
2) **Attractive** interactions in mean-field approximation,

$$P \rightarrow P - an^2$$



Van der Waals equation

- VDW isotherms show irregular behavior below certain temperature T_C
- Below T_C isotherms are corrected by **Maxwell's rule of equal areas**
- Results in appearance of **mixed phase**



Critical point

$$\frac{\partial p}{\partial v} = 0, \quad \frac{\partial^2 p}{\partial v^2} = 0, \quad v = V/N$$

$$p_C = \frac{a}{27b^2}, \quad n_C = \frac{1}{3b}, \quad T_C = \frac{8a}{27b}$$

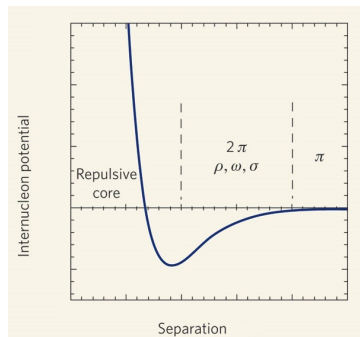
Reduced variables

$$\tilde{p} = \frac{p}{p_C}, \quad \tilde{n} = \frac{n}{n_C}, \quad \tilde{T} = \frac{T}{T_C}$$

Nucleon-nucleon interaction

Nucleon-nucleon potential:

- Repulsive core at small distances
- Attraction at intermediate distances
- Suggestive similarity to VDW interactions
- Could nuclear matter described by VDW equation?



Standard VDW equation is for **canonical ensemble** and **Boltzmann** statistics

Nucleons are fermions, obey Pauli exclusion principle

Unlike for classical fluids, **quantum statistics** is important

VDW equation originally formulated in **canonical ensemble**

How to transform **CE** pressure $P(T, n)$ into **GCE** pressure $P(T, \mu)$?

- Calculate $\mu(T, V, N)$ from standard TD relations
- Invert the relation to get $N(T, V, \mu)$ and put it back into $P(T, V, N)$
- Consistency due to thermodynamic equivalence of ensembles

Result: transcendental equation for $n(T, \mu)$

$$\frac{N}{V} \equiv n(T, \mu) = \frac{n_{\text{id}}(T, \mu^*)}{1 + b n_{\text{id}}(T, \mu^*)}, \quad \mu^* = \mu - b \frac{nT}{1 - bn} + 2an$$

- Implicit equation in GCE, in CE it was explicit
- May have multiple solutions below T_C
- Choose one with largest pressure – equivalent to Maxwell rule in CE

Advantages of the GCE formulation

- 1) **Hadronic** physics applications: number of hadrons usually **not conserved**.
- 2) **CE** cannot describe particle number **fluctuations**. N-fluctuations in a **small** ($V \ll V_0$) subsystem follow **GCE** results.
- 3) Good starting point to include effects of **quantum statistics**.

Scaled variance in VDW equation

New application from GCE formulation: **particle number fluctuations**

Scaled variance is an **intensive** measure of N-fluctuations

$$\frac{\sigma^2}{N} = \omega[N] \equiv \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle} = \frac{T}{n} \left(\frac{\partial n}{\partial \mu} \right)_T = \frac{T}{n} \left(\frac{\partial^2 P}{\partial \mu^2} \right)_T$$

In **ideal** Boltzmann gas fluctuations are Poissonian and $\omega_{id}[N] = 1$.

$\omega[N]$ in VDW gas (pure phases)

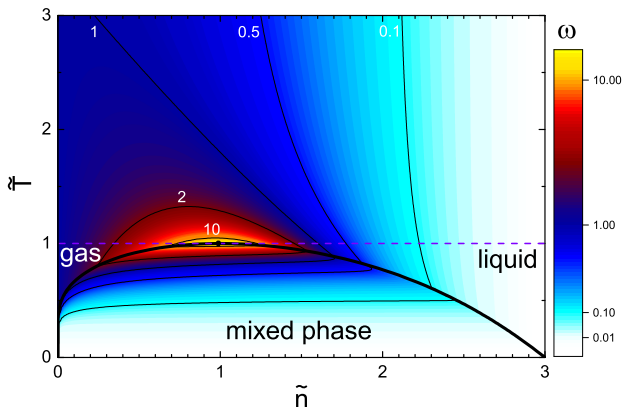
$$\omega[N] = \left[\frac{1}{(1 - bn)^2} - \frac{2an}{T} \right]^{-1}$$

- **Repulsive** interactions **suppress** N-fluctuations
- **Attractive** interactions **enhance** N-fluctuations

N-fluctuations are useful because they

- Carry information about finer details of EoS, e.g. **phase transitions**
- Measurable **experimentally**

$$\omega[N] = \frac{1}{9} \left[\frac{1}{(3 - \tilde{n})^2} - \frac{\tilde{n}}{4\tilde{T}} \right]^{-1}$$



- Deviations from unity signal effects of interaction
- Fluctuations grow rapidly near critical point

V. Vovchenko et al., J. Phys. A 305001, 48 (2015)

VDW equation with quantum statistics in GCE

Requirements for VDW equation with quantum statistics

- 1) Reduce to **ideal quantum gas** at $a = 0$ and $b = 0$
- 2) Reduce to **classical VDW** when quantum statistics are negligible
- 3) $s \geq 0$ and $s \rightarrow 0$ as $T \rightarrow 0$

Ansatz: Take pressure in the following form^{1,2}

$$p(T, \mu) = p^{\text{id}}(T, \mu^*) - an^2, \quad \mu^* = \mu - bp - abn^2 + 2an$$

where $p^{\text{id}}(T, \mu^*)$ is pressure of ideal **quantum** gas.

$$n(T, \mu) = \left(\frac{\partial p}{\partial \mu} \right)_T = \frac{n^{\text{id}}(T, \mu^*)}{1 + bn^{\text{id}}(T, \mu^*)}$$

Algorithm for GCE

- 1) Solve system of eqs. for p and n at given (T, μ)
- 2) Choose the solution with **largest** pressure

¹V. Vovchenko, D. Anchishkin, M. Gorenstein, Phys. Rev. C 91, 064314 (2015)

²**Alternative derivation:** K. Redlich, K. Zalewski, arXiv:1605.09686 (2016)

³ $a=0 \Rightarrow$ **excluded-volume** model, D. Rischke et al., Z.Phys. C51, 485 (1991)

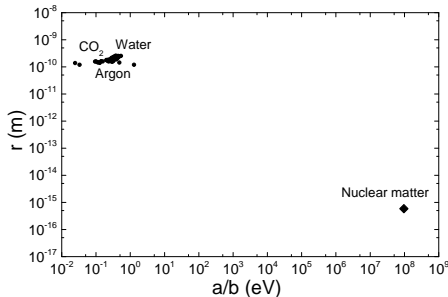
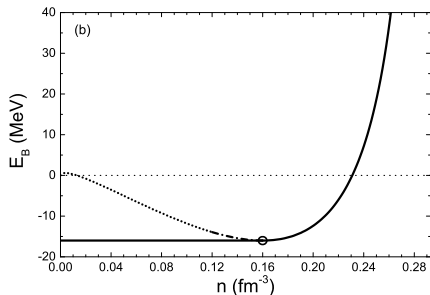
VDW gas of nucleons: zero temperature

How to fix a and b ? For classical fluid usually tied to CP location.

Different approach: Reproduce **saturation density** and **binding energy**

From $E_B \cong -16$ MeV and $n = n_0 \cong 0.16 \text{ fm}^{-3}$ at $T = p = 0$ we obtain:

$$a \cong 329 \text{ MeV fm}^3 \text{ and } b \cong 3.42 \text{ fm}^3$$

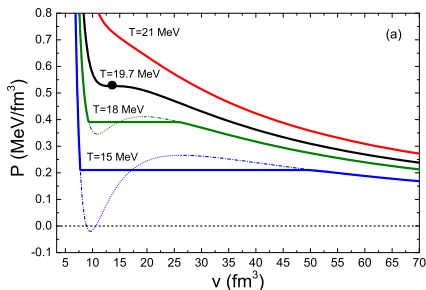
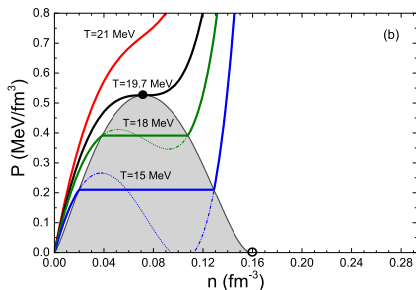


Mixed phase at $T = 0$ is specific:
A mix of vacuum ($n = 0$) and liquid
at $n = n_0$

VDW eq. now at very different scale!

CE pressure

$$p = p^{\text{id}} \left[T, \mu^{\text{id}} \left(\frac{n}{1 - bn}, T \right) \right] - an^2$$



Behavior qualitatively **same** as for Boltzmann case

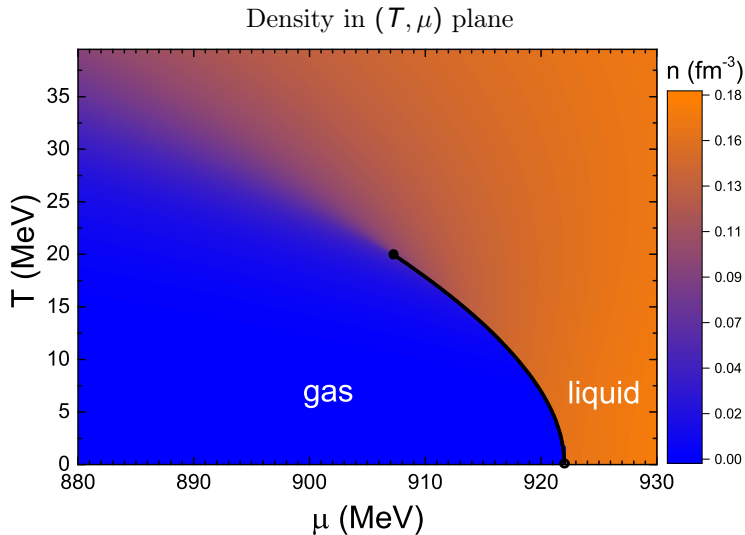
Mixed phase results from **Maxwell construction**

Critical point at $T_c \cong 19.7$ MeV and $n_c \cong 0.07$ fm⁻³

Experimental estimate¹: $T_c = 17.9 \pm 0.4$ MeV, $n_c = 0.06 \pm 0.01$ fm⁻³

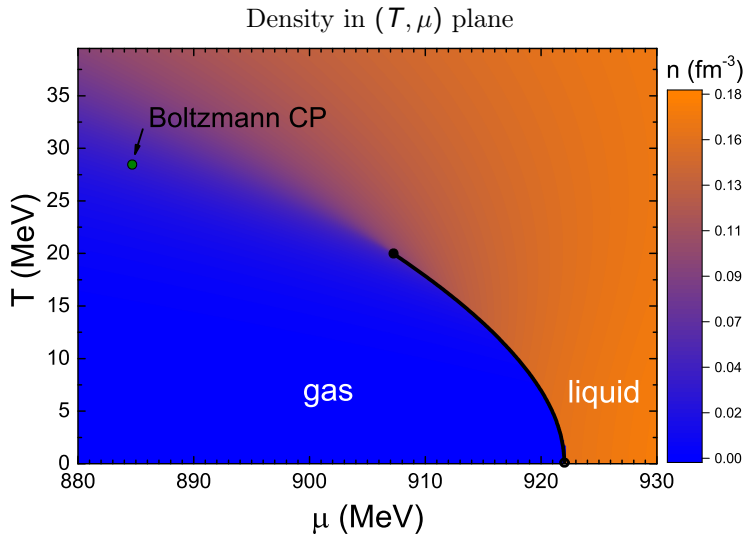
¹J.B. Elliot, P.T. Lake, L.G. Moretto, L. Phair, Phys. Rev. C 87, 054622 (2013)

VDW gas of nucleons: (T, μ) plane



Crossover region at $\mu < \mu_C \cong 908$ MeV is clearly seen

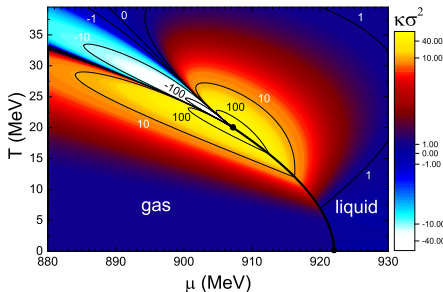
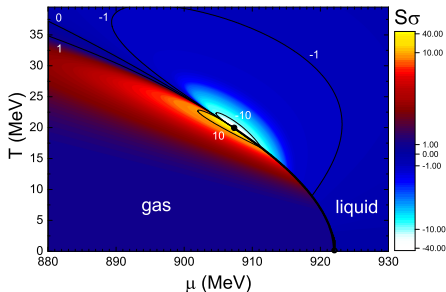
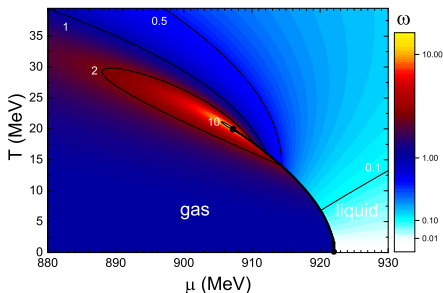
VDW gas of nucleons: (T, μ) plane



Boltzmann: $T_C = 28.5$ MeV. Classical VDW does not work!

VDW-HRG gas of nucleons: fluctuations

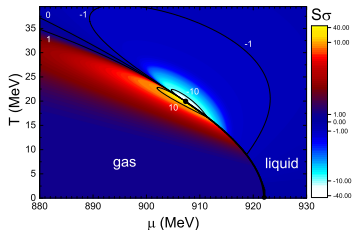
- Results for $\sigma^2/\langle N \rangle$, $S\sigma$, and $\kappa\sigma^2$
- Fluctuations diverge at CP (as expected)
- For higher moments singularity is specific: sign depends on path of approach



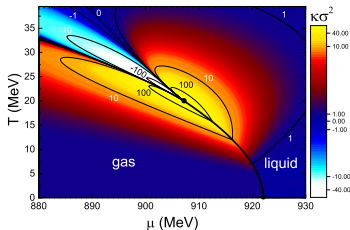
Vovchenko, Anichishkin, Gorenstein, Poberezhnyuk, PRC 91, 064314 (2015)

VDW gas of nucleons: skewness and kurtosis

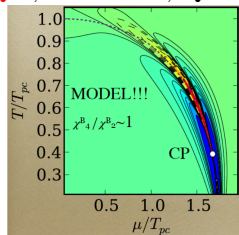
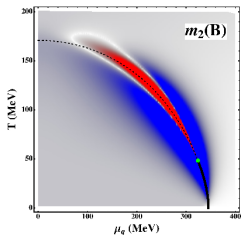
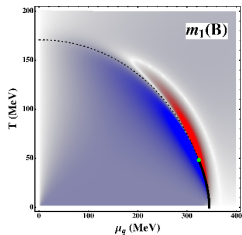
VDW Skewness



VDW Kurtosis



NJL, J.W. Chen et al., PRD 93, 034037 (2016) PQM, V. Skokov, QM2012

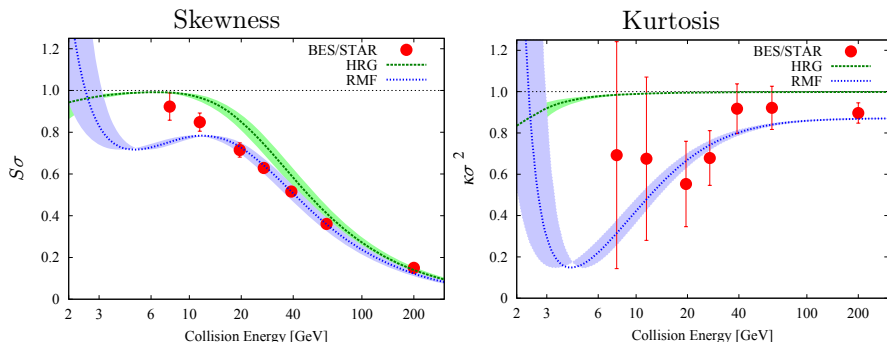


Fluctuation patterns in VDW very similar to effective QCD models

Net-baryon fluctuations and nuclear matter

Are NN interactions relevant for observables in HIC region?

Net-nucleon fluctuations within RMF (σ - ω model) of nuclear matter
along line of “chemical freeze-out”



K. Fukushima, PRC 91, 044910 (2015)

A notable effect in fluctuations even at $\mu \simeq 0$

Reconciliation of HRG with nuclear matter can be interesting

Simplest generalization of VDW nuclear matter model to full HRG:

- Similar VDW interactions between baryons and baryons
- The baryon-antibaryon, meson-meson, and meson-baryon VDW interactions are neglected
- Baryon VDW parameters extracted from ground state of nuclear matter ($a = 329 \text{ MeV fm}^3$, $b = 3.42 \text{ fm}^3$)

Three independent subsystems: mesons + baryons + antibaryons

$$P(T, \mu) = P_M(T, \mu) + P_B(T, \mu) + P_{\bar{B}}(T, \mu),$$

$$P_M(T, \mu) = \sum_{j \in M} p_j^{\text{id}}(T, \mu_j) \quad \text{and} \quad P_B(T, \mu) = \sum_{j \in B} p_j^{\text{id}}(T, \mu_j^{B*}) - a n_B^2$$

$$n_B(T, \mu) = (1 - b n_B) \sum_{j \in B} n_j^{\text{id}}(T, \mu_j^{B*}).$$

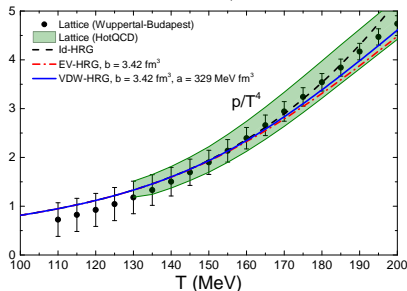
In this simplest setup model is essentially “parameter-free”

Transcendental equations for P_B and n_B

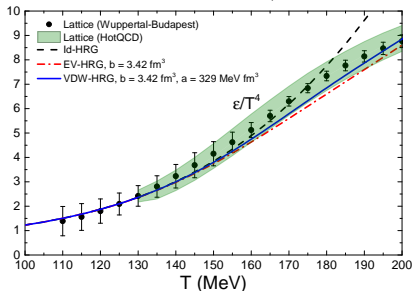
VDW-HRG at $\mu = 0$: thermodynamic functions

Comparison of VDW-HRG with lattice QCD at $\mu = 0$

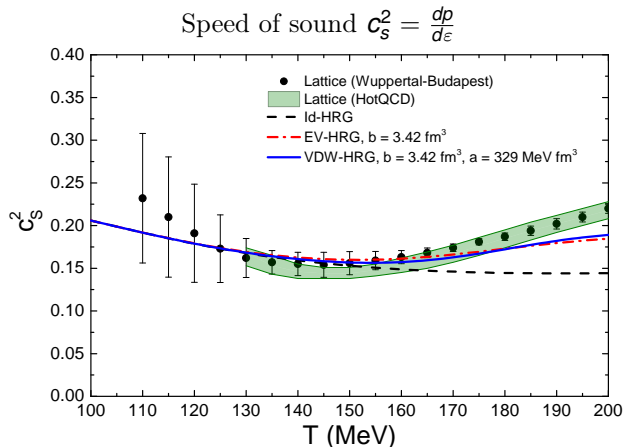
Pressure p/T^4



Energy density ε/T^4



- VDW-HRG **does not spoil** existing agreement of Id-HRG with lQCD despite significant EV interactions between baryons
- Not surprising: matter **meson-dominated** at $\mu = 0$

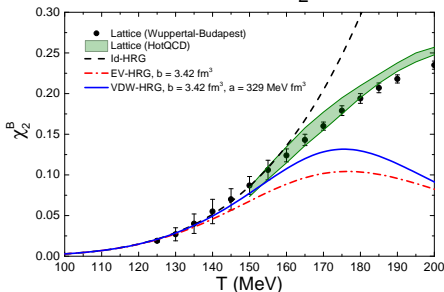


- Monotonic decrease in Id-HRG, at odds with lattice
- **Minimum** for EV-HRG/VDW-HRG at 150-160 MeV
- **No acausal** behavior, often an issue in models with eigenvolumes

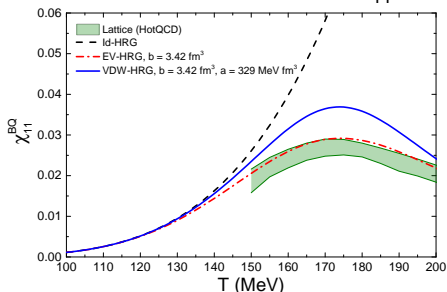
VDW-HRG at $\mu = 0$: baryon number fluctuations

$$\text{Susceptibilities: } \chi_{lmn}^{BSQ} = \frac{\partial^{l+m+n} \rho / T^4}{\partial(\mu_B/T)^l \partial(\mu_S/T)^m \partial(\mu_Q/T)^n}$$

Net-baryon χ_2^B



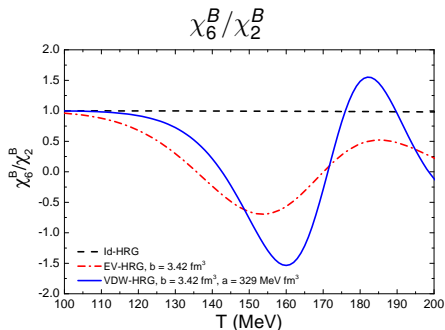
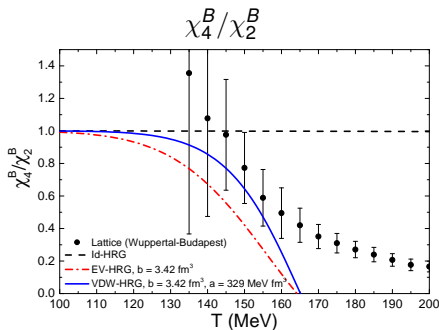
Baryon-charge correlator χ_{11}^{BQ}



- Very different qualitative behavior between Id-HRG and VDW-HRG
- For χ_2^B lattice data is between Id-HRG and VDW-HRG at high T
- For χ_{11}^{BQ} lattice data is below all models, closer to EV-HRG

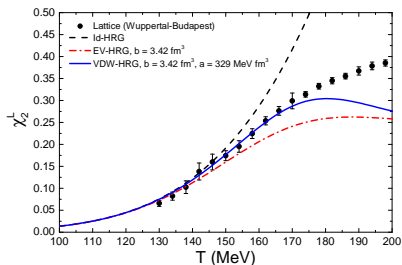
VDW-HRG at $\mu = 0$: baryon number fluctuations

Higher-order of fluctuations are expected to be even more sensitive



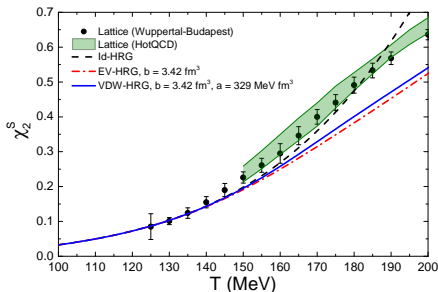
- χ_4^B deviates from χ_2^B at high enough T , stays equal in Id-HRG
- Cannot be related only to onset of deconfinement
- VDW-HRG predicts strong non-monotonic behavior for χ_6^B / χ_2^B

VDW-HRG at $\mu = 0$: net-light and net-strangeness



- Net number of light quarks χ_2^L
- $L = (u + d)/2 = (3B + S)/2$
- Improved description in VDW-HRG

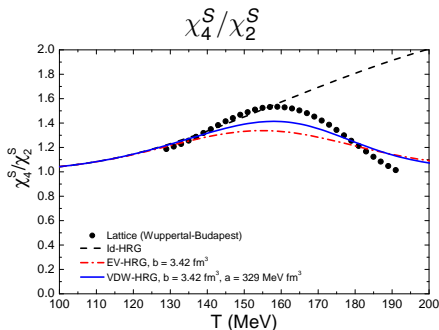
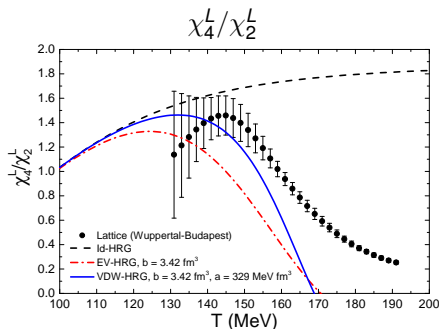
- Net-strangeness χ_2^S
- Underestimated by HRG models, similar for χ_{11}^{BS}
- Extra strange states?¹
- Weaker VDW interactions for strange baryons?²



¹Bazavov et al., PRL 113, 072001 (2014)

²Alba et al., arXiv:1606.06542 and **P. Alba's talk**

VDW-HRG at $\mu = 0$: net-light and net-strangeness



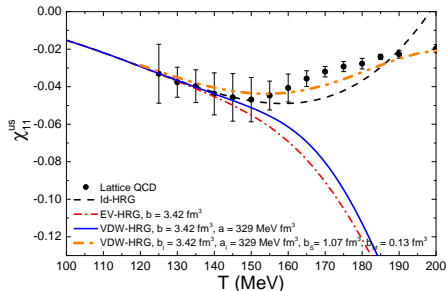
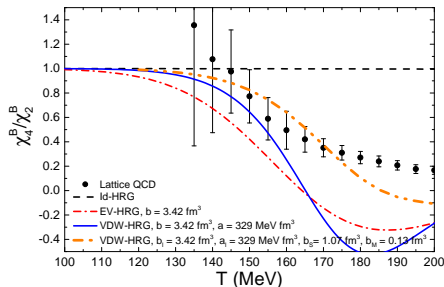
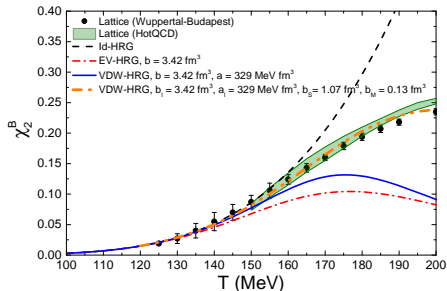
- Lattice shows peaked structures in crossover regions
- Not at all reproduced by Id-HRG, signal for deconfinement?¹
- Peaks at different T for net-L and net-S \Rightarrow flavor hierarchy?²
- VDW-HRG also shows peaks and flavor hierarchy \Rightarrow cannot be traced back directly to deconfinement

¹S. Ejiri, F. Karsch, K. Redlich, PLB 633, 275 (2006)

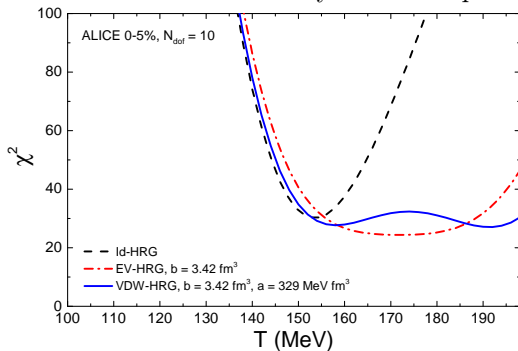
²Bellwied et al., PRL 111, 202302 (2013)

Effect of reducing VDW interactions involving strange hadrons

- 3 times smaller EV for strange baryons
- Small EV for mesons
- Illustrative calculation (preliminary!)
- Most observables improved



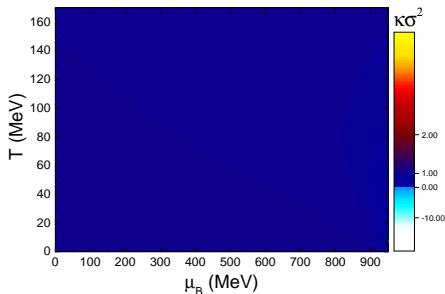
VDW interactions change relative hadron yields
Thermal fit to ALICE hadron yields: from pions to Ω



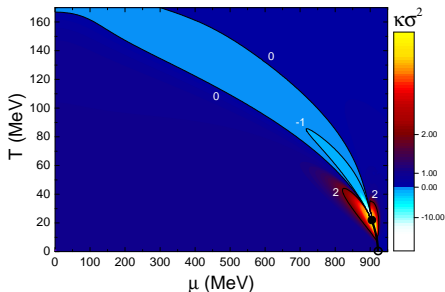
- Fit quality slightly better in EV-HRG/VDW-HRG vs Id-HRG but very different picture!
- All temperatures between 150 and 200 MeV yield similarly fair data description in VDW-HRG
- Results likely to be sensitive to further modifications, e.g for strangeness

Net-baryon fluctuations in T - μ plane: χ_4^B/χ_2^B

Id-HRG



VDW-HRG



- Almost no effect in Id-HRG, only Fermi statistics
- Rather rich structure for VDW-HRG
- Likely relevant for net-baryon fluctuations in HIC

- VDW equation provides **simple insight** on fluctuations near CP
- **Nuclear matter** can be described as VDW equation with Fermi statistics
- VDW interactions between baryons have strong influence on **fluctuations of conserved charges** in the crossover region within HRG
- VDW-HRG captures **basic features** of both lattice results at $\mu = 0$ and nuclear matter properties
- Freeze-out parameters extracted from thermal fits within ideal HRG are **not unique**, procedure sensitive to modeling of VDW interactions
- Interpretation of results obtained within standard **ideal HRG** should be done with extreme care

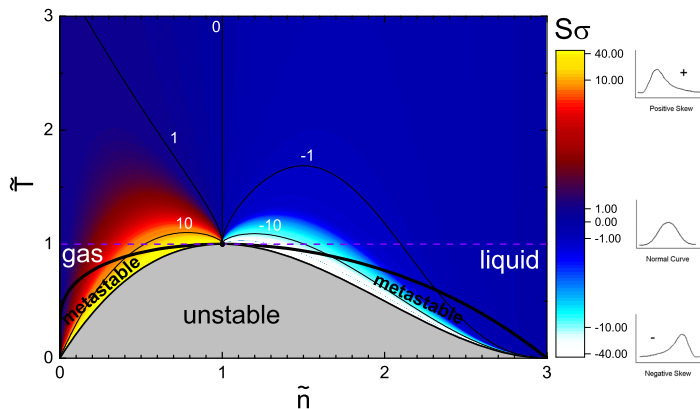
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Thanks for your attention!

Backup slides

Higher-order (non-gaussian) fluctuations are even more sensitive

Skewness:
$$S\sigma = \frac{\langle(\Delta N)^3\rangle}{\sigma^2} = \omega[N] + \frac{T}{\omega[N]} \left(\frac{\partial\omega[N]}{\partial\mu} \right)_T$$
 asymmetry

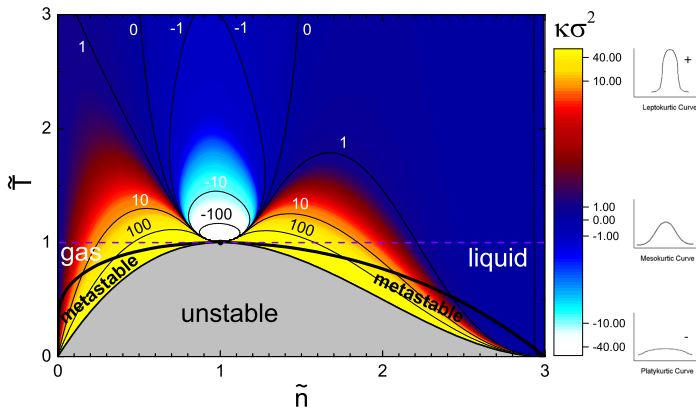


Skewness is

- **Positive** (right-tailed) in **gaseous** phase
- **Negative** (left-tailed) in **liquid** phase

Kurtosis: $\kappa\sigma^2 = \frac{\langle(\Delta N)^4\rangle - 3\langle(\Delta N)^2\rangle^2}{\sigma^2}$

peakedness

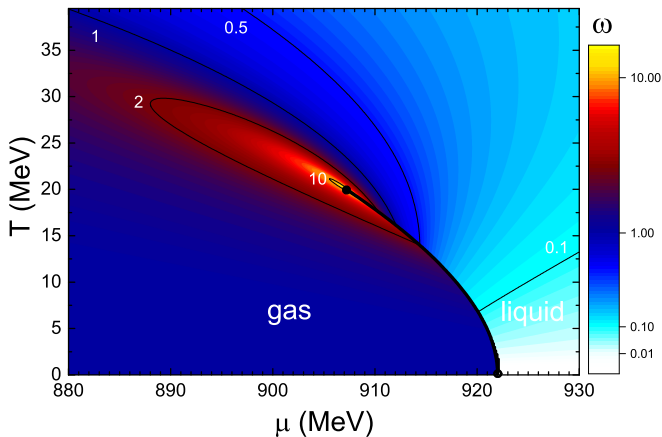


Kurtosis is **negative** (flat) above critical point (crossover), **positive** (peaked) elsewhere and very **sensitive** to the **proximity** of the critical point

V. Vovchenko et al., J. Phys. A 015003, 49 (2016)

Scaled variance in quantum VDW:

$$\omega[N] = \omega_{\text{id}}(T, \mu^*) \left[\frac{1}{(1 - bn)^2} - \frac{2an}{T} \omega_{\text{id}}(T, \mu^*) \right]^{-1}$$



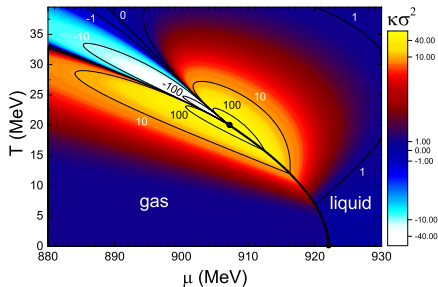
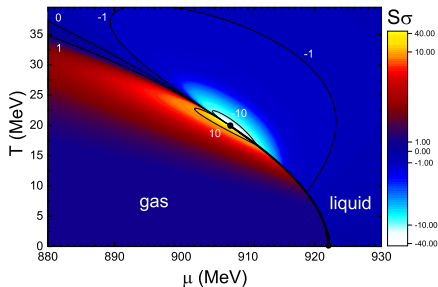
VDW gas of nucleons: skewness and kurtosis

Skewness

$$S\sigma = \omega[N] + \frac{T}{\omega[N]} \left(\frac{\partial \omega[N]}{\partial \mu} \right)_T$$

Kurtosis

$$\kappa\sigma^2 = (S\sigma)^2 + T \left(\frac{\partial [S\sigma]}{\partial \mu} \right)_T$$



For skewness and kurtosis singularity is rather specific: sign depends on the path of approach

V. Vovchenko et al., Phys. Rev. C 92, 054901 (2015)

VDW-HRG at $\mu = 0$: baryon number fluctuations

$$\chi_6^B / \chi_2^B$$

