Quantum statistical van der Waals equation and its QCD applications

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PhD Defense

\[ p(T, n) = p_{q}^{\text{id}} \left( T, \frac{n}{1 - b n} \right) - a n^2 \]

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Strongly interacting matter

- Theory of strong interactions: *Quantum Chromodynamics* (QCD)
  \[
  \mathcal{L} = \sum_{q=u,d,s,\ldots} \bar{q}[i\gamma^\mu (\partial_\mu - igA_\mu^a \lambda_a) - m_q]q - \frac{1}{4} G^a_{\mu\nu} G^{a\mu\nu}
  \]
- Basic degrees of freedom: quarks and gluons
- At smaller energies confined into baryons (qqq) and mesons (q\bar{q})

Where is it relevant?
- Early universe
- Neutron star (mergers)
- Heavy-ion collisions (lab!)

Length scale: 1 fm = 10^{-15} m 
Energy scale: 100 MeV = 10^{12} K 
\[ \hbar = c = k_B = 1 \]
QCD equation of state at $\mu = 0$

Lattice QCD simulations provide the equation of state at $\mu_B = 0$

- A crossover-type transition
- Common model for confined phase is ideal HRG: non-interacting gas of known hadrons and resonances, clearly breaks down as $T$ increases
- What is the role of hadronic interactions beyond those in ideal HRG?

HotQCD Collaboration: 1407.6387, 1701.04325, 1708.04897
Wuppertal-Budapest Collaboration: 1112.4416, 1309.5258, 1507.04627
van der Waals equation

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

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

Contains 1st order phase transition and critical point

Formulated in 1873.

Nobel Prize in 1910.

1. Short-range repulsion: excluded volume (EV) procedure
   \[ V \rightarrow V - bN, \quad b = 4\frac{4\pi r_c^3}{3} \]

2. Intermediate range attraction in mean-field approx.
   \[ P \rightarrow P - a n^2, \quad a = \pi \int_{2r_c}^{\infty} |U_{12}(r)| r^2 dr \]

A fairly generic extension of ideal gas for interactions
Excluded volume effects on thermal fits

Ideal HRG: \[ N_i \propto \exp\left(-\frac{m_i}{T}\right) \exp\left(\frac{b_i \mu_B}{T}\right) + \text{feeddown} \]

\[
\begin{array}{cccccccc}
\pi & K^\pm & K^0 & K^* & \phi & p & \Lambda & \Xi & \Omega & d & \Lambda H & He \\
\end{array}
\]

ALICE Collaboration, SQM2015, QM2015

How robust are conclusions based on ideal gas?
Excluded volume effects on thermal fits

Excluded-volume: 
\[ N_i \propto \exp \left( -v_i \frac{p}{T} \right) \leftarrow \text{larger hadrons suppressed} \]

- **Bag model:** 
  \[ v_i \propto m_i \]  
  [Chodos et al., PRD '74; Kapusta, et al., NPA '83, PRC '15]
- **Two-component model:** 
  \[ r_M = 0, \ r_B = 0.3 \ \text{fm} \]  
  [Andronic et al., 1201.0693]

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**Graph:**

ALICE, Pb+Pb, \( s_{NN}^{1/2} = 2.76 \ \text{TeV}, \ 0-5\% \text{centrality} \)

\[ \chi^2 / N_{\text{dof}} \]

- \( r = 0.0 \ \text{fm} \)
- \( r_M = 0.0 \ \text{fm}, \ r_B = 0.3 \ \text{fm} \)
- \( r_i \sim m_i^{1/3}, \ r_p = 0.5 \ \text{fm} \)

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**Excluded-volume model:**

Rischke, Gorenstein, Stoecker, Greiner, Z. Phys. C (1991)
D. Anchishkin, Sov. JETP (1992)
Excluded volume effects on thermal fits: finite $\mu_B$

Fits to NA49 and STAR data

"Crossterms" EV, $r_p = 0.5$ fm
Contours show valleys of $\chi^2$ minima

V.V., H. Stoecker, Phys. Rev. C 95, 044904 (2017)

Entropy per baryon, $S/A$, is a robust observable
Full van der Waals equation: GCE formulation

Full vdW equation opens new applications, such as criticality

\[ p = \frac{Tn}{1 - bn} - an^2 \]

First step: transform the CE pressure \( p(T, V, N) \) into the GCE

**Result:** van der Waals equation in the grand canonical ensemble

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

*Never published in 100+ years!

- Implicit equation in the GCE, now depends on mass and degeneracy
- May have multiple solutions below \( T_C \)
- Choose one with largest pressure – equivalent to the Maxwell rule in CE

Scaled variance for classical VDW equation

Particle number fluctuations in a classical vdW gas within the GCE

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

- Repulsive interactions suppress \( N \)-fluctuations
- Attractive interactions enhance \( N \)-fluctuations

Nucleon-nucleon interaction

Nuclear liquid-gas transition appears due to the vdW type structure of the nucleon-nucleon interaction

Nucleon-nucleon potential:

- Repulsive core at small distances
- Attraction at intermediate distances
- Suggestive similarity to vdW interactions

Could nuclear matter be described by the van der Waals equation?

*Yes! But we need Fermi statistics...*
Quantum statistical van der Waals fluid

Free energy of classical vdW fluid:

\[ F(T, V, N) = F^{id}(T, V - bN, N) - a \frac{N^2}{V} \]

Ansatz: \( F^{id} \Rightarrow F^{id}_q(T, V - bN, N) \) is free energy of ideal quantum gas

Quantum van der Waals equation:

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

\( p^{id}_q(T, n) \) corresponds to Fermi-Dirac or Bose-Einstein distribution

Model properties:

- Reduces to the classical vdW equation when quantum statistics are negligible
- Reduces to ideal quantum gas for \( a = 0 \) and \( b = 0 \)
- Entropy density non-negative and \( s \to 0 \) with \( T \to 0 \)

QvdW gas of nucleons: pressure isotherms

\( a \) and \( b \) fixed to reproduce saturation density and binding energy:

\[ n_0 = 0.16 \text{ fm}^{-3}, \quad E/A = -16 \text{ MeV} \Rightarrow a \approx 329 \text{ MeV fm}^3 \text{ and } b \approx 3.42 \text{ fm}^3 \]

Behavior qualitatively same as for Boltzmann case

Mixed phase results from Maxwell construction

Critical point at \( T_c \approx 19.7 \text{ MeV} \) and \( n_c \approx 0.07 \text{ fm}^{-3} \)

Experimental estimate\(^1\): \( T_c = 17.9 \pm 0.4 \text{ MeV}, \ n_c = 0.06 \pm 0.01 \text{ fm}^{-3} \)

Pioneering measurements: J. Pochodzalla et al. [ALADIN collaboration], PRL '95
QvdW-HRG model

We are now ready to include QvdW interactions into HRG model

QvdW-HRG model [V.V., M.I. Gorenstein, H. Stoecker, PRL 118, 182301 (2017)]

- Hadron Resonance Gas (HRG) with attractive and repulsive vdw interactions between baryons
- vdw parameters $a = 329$ MeV fm$^3$ and $b = 3.42$ fm$^3$ tuned to nuclear ground state properties
- Critical point of nuclear matter at $T_c \approx 19.7$ MeV, $\mu_c \approx 908$ MeV

3 subsystems: non-int. mesons + QvdW baryons + QvdW antibaryons

$$p(T, \mu) = P_M(T, \mu) + P_B(T, \mu) + P_{\overline{B}}(T, \mu),$$

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

A “parameter-free” minimal-interaction extension
QvdW-HRG at $\mu_B = 0$: thermodynamics

Comparison of QvdW-HRG with lattice QCD at $\mu_B = 0$

Pressure $p/T^4$

Speed of sound $c_s^2 \equiv \frac{dp}{d\varepsilon}$

- QvdW-HRG does not spoil existing agreement of Id-HRG with LQCD despite significant excluded-volume interactions between baryons
- No acausal behavior
**QvdW-HRG at $\mu_B = 0$: susceptibilities**

- **$\chi^B_2$**
- **$\chi^{BQ}_{11}$**
- **$\chi^B_4 / \chi^B_2$**
- **$\chi^B_6 / \chi^B_2$**

- **Quantitative features of QCD captured by QvdW-HRG**
Critical point of nuclear matter shines brightly in fluctuation observables, across the whole region of phase diagram probed by heavy-ion collisions.

Subsequent work: outlook

LQCD crossover transition: Hagedorns + excluded volume?

Radius of convergence sees Roberge-Weiss transition?

With C. Greiner

A lot of Lattice QCD data requiring careful interpretation...
Summary I: Main results

- Thermal fits are very sensitive to excluded volume effects. Entropy per baryon is a robust observable.

- Quantum statistical van der Waals equation in the grand canonical ensemble opens new applications in high energy nuclear physics.

- Enhanced, non-monotonic behavior of high-order fluctuations is a promising signal of critical behavior.

- van der Waals like interactions between nucleons/baryons are surprisingly important for observables in high-temperature QCD.
Summary II: Selected Publications

Excluded volume effects

Equation of state

Thermal fits

Textbook extensions of van der Waals equation

Grand canonical ensemble

Quantum statistics

Mixtures (multi-component)
Summary II: Selected Publications

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Grand canonical ensemble

Quantum statistics
• V.V., Phys. Rev. C 96, 015206 (2017)

Mixtures (multi-component)
• V.V., Motornenko, Alba, Gorenstein, Satarov, Stoecker, Phys. Rev. C 96, 045202 (2017)

Thanks for your attention!
Backup slides
Excluded volume procedure

Let us start with the excluded volume only:

substitute volume by the available volume $V \rightarrow V - bN$

\[
\text{CE: } p(T, n) = \frac{Tn}{1 - bn}
\]

\[
\text{GCE: } p(T, \mu) = p^{\text{id}}[T, \mu - b p(T, \mu)], \quad n(T, \mu) = \frac{n^{\text{id}}(T, \mu^*)}{1 + b n^{\text{id}}(T, \mu^*)},
\]

\[
\mu^* = \mu - b p, \quad b = \frac{16\pi}{3} r^3
\]

- CE: Excluded volume effects increase CE pressure $p(T, n)$
- GCE: Excluded volume effects decrease GCE pressure $p(T, \mu)$

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D. Anchishkin, JETP (1992): Identical formulation with mean-field approach
Origin of the two minima

Where does the 2nd minimum come from?

Consider $p/\pi$ ratio in the EV model

\[
\frac{n_p^{ev}}{n_\pi^{ev}} = \frac{n_p^{id}}{n_\pi^{id}} e^{(v_\pi - v_p)P/T}
\]

Non-monotonic behavior when $v_\pi < v_p$, yielding two solutions

L.M. Satarov, V.V., P. Alba, M.I. Gorenstein, H. Stoecker, 1610.08753
The QCD phase diagram has many unknowns at finite density.

Does the critical point exist? Use fluctuations as its signal!

**Theory:** $\chi^{(n)} = \frac{\partial^n (p/T^4)}{\partial (\mu/T)^n} \sim \xi^k, \quad \xi \to \infty$ at the CP

In heavy-ion collisions $\xi \lesssim 2 - 3$ fm [M. Stephanov, PRL '09]
Critical point of nuclear matter

The QCD phase diagram

The QCD phase diagram is known to contain the critical point of nuclear matter at $T_c \sim 15$ MeV and $(\mu_B/T)_c \sim 40 \Rightarrow$ way beyond current lattice methods.

It is the only QCD critical point we know is there...

How does it influence the fluctuation observables in heavy-ion collisions?
van der Waals isotherms

- 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**
\[
\tilde{p} = \frac{p}{p_C}, \quad \tilde{n} = \frac{n}{n_C}, \quad \tilde{T} = \frac{T}{T_C}
\]
Non-Gaussian fluctuations: Skewness

(Normalized) skewness measures the degree of asymmetry of distribution

\[ S_\sigma = \frac{\kappa_3}{\kappa_2} = \frac{\langle (\Delta N)^3 \rangle}{\sigma^2}. \]

Baselines:
- Gaussian: \( S_\sigma = 0 \)
- Poisson: \( S_\sigma = 1 \) \( \leftarrow \) ideal gas in grand canonical ensemble

At CP: \( S_\sigma \sim \xi^{4.5} \)
Non-Gaussian fluctuations: Kurtosis

(Normalized) kurtosis measures “peakedness” of distribution

\[ \kappa \sigma^2 = \kappa_4 \frac{\kappa_4}{\kappa_2} = \frac{\langle (\Delta N)^4 \rangle - 3 \langle (\Delta N)^2 \rangle^2}{\sigma^2} . \]

Baselines:

- Gaussian: \( \kappa \sigma^2 = 0 \)
- Poisson: \( \kappa \sigma^2 = 1 \) \( \leftarrow \) ideal gas in grand canonical ensemble

At CP: \( \kappa \sigma^2 \sim \xi^7 \)
Classical vdW equation: Skewness

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

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

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

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

QvdW fluid of nucleons: \((T, \mu)\) plane

\((T, \mu)\) plane: structure of critical fluctuations \\
\[ \chi_i = \partial^i (p / T^4) / \partial (\mu / T)^i \]

\[ \chi_2/\chi_1 \]

\[ \chi_3/\chi_2 \]

\[ \chi_4/\chi_2 \]

\[ \kappa \sigma^2 \]
Fluctuation patterns in vdW very similar to effective QCD models
Fluctuation signals from nuclear matter critical point and from QCD critical point may very well look alike
Calculating fluctuations along the “freeze-out” curve

Acceptance effects (protons instead of baryons, momentum cut) modeled schematically, by applying the binomial filter [M. Kitazawa, M. Asakawa, PRC ’12; A. Bzdak, V. Koch, PRC ’12]

![Graphs showing the ratio of certain quantities as functions of collision energy](image)

**Effects of nuclear liquid-gas criticality:**
- Non-monotonic collision energy dependence
- Net proton quite different from net baryon
Can the scenarios be distinguished? Need data at lower energies...

Opportunities for HADES, CBM, NA61/SHINE, STAR!
Strongly intensive measures [M.I. Gorenstein, M. Gazdzicki, PRC ’11]

- Independent of volume fluctuations, mitigate impact parameter fluctuations
- Can be constructed from moments of two extensive quantities
  \[
  \Delta[A, B] = C_\Delta^{-1} [\langle A \rangle \omega[B] - \langle B \rangle \omega[A]]
  \]
  \[
  \Sigma[A, B] = C_\Sigma^{-1} [\langle A \rangle \omega[B] + \langle B \rangle \omega[A] - 2(\langle AB \rangle - \langle A \rangle \langle B \rangle)]
  \]

- For most models without PT and CP equal/close to unity
- Supposedly show critical behavior, but no model calculation
- Used in search for CP, e.g. NA61/SHINE program\(^1\)

SI measures of excitation energy and particle number fluctuations in vdW

\[
\Delta[E^*, N] = 1 - \frac{an(2\overline{\epsilon}_{id} - 3an)}{\epsilon_{id}^2 - \overline{\epsilon}_{id}^2} \omega[N], \quad \Sigma[E^*, N] = 1 + \frac{a^2 n^2}{\epsilon_{id}^2 - \overline{\epsilon}_{id}^2} \omega[N].
\]

- Critical behavior is present due to criticality of \(\omega[N]\) term\(^2\)
- If \(a=0\) then no signal at all! Deviations really stem from criticality.

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\(^1\)Gazdzicki, Seyboth, APP ’15; E. Andronov, 1610.05569; A. Seryakov, 1704.00751