Critical fluctuations in models with van der Waals interactions

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Critical Point and Onset of Deconfinement 2016

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Outline

[Introduction](#page-2-0)

² [Generalizations of Van der Waals equation](#page-7-0)

- [Grand Canonical Ensemble](#page-7-0)
- [Quantum statistics](#page-12-0)

³ [Applications](#page-14-0)

- [Critical fluctuations](#page-14-0)
- [Nuclear matter as VDW gas of nucleons](#page-14-0)
- [Interacting pion gas with van der Waals equation](#page-25-0)
- [Van der Waals interactions in Hadron Resonance Gas](#page-26-0)

[Summary](#page-27-0)

Van der Waals equation

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

Formulated in 1873.

Simplest model for 1st order phase transition and critical point.

Motivation: A toy model to study QCD critical point

E.-by-e. fluctuations can be used to study QCD phase transition¹

Nobel Prize in 1910.

Two ingredients:

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

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

2) Attractive interactions in mean-field approximation, *P* → *P* − *a n*²

¹Stephanov, Rajagopal, Shuryak, Phys. Rev. D (1999) Ejiri, Redlich, Karsch, Phys. Lett. B (2005)

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- VDW isotherms show irregular behavior below certain temperature T_C
- \bullet Below \mathcal{T}_C isotherms are corrected by Maxwell's rule of equal areas
- Results in appearance of mixed phase

Critical point

\n
$$
\frac{\partial p}{\partial v} = 0, \quad \frac{\partial^2 p}{\partial v^2} = 0, \quad v = V/N
$$
\n
$$
p_C = \frac{a}{27b^2}, n_C = \frac{1}{3b}, T_C = \frac{8a}{27b}
$$
\nReduced variables

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

VDW equation is quite successful in describing qualitative features of liquid-vapour phase transition in classical substances

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But can it provide insight on phase transitions in QCD?

Statistical ensembles

VDW equation originally formulated in canonical ensemble

Canonical ensemble (CE)

- System of *N* particles in fixed volume *V* exchanges energy with large reservoir (heat bath)
- State variables: *T*, *V*, *N*
- Thermodynamic potential free energy $F(T, V, N)$
- All other quantities determined from *F*(*T*, *V*, *N*)

Grand canonical ensemble (GCE)

- System of particles in fixed volume *V* exchanges both energy and particles with large reservoir (heat bath)
- State variables: T, V, μ
- *N* no longer conserved. Chemical potential μ regulates $\langle N \rangle$
- Pressure $P(T, \mu)$ as function of T and μ contains complete information

GCE is more natural for systems with variable number of particles GCE formulation opens possibilities for new applications in nuclear physics 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 $n(T, \mu)$

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

- 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 $\omega_{\text{id}}[N] = 1$.

ω [**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

Scaled variance

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

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

Skewness

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

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Kurtosis

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)

VDW equation with quantum statistics

Nucleon-nucleon potential:

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

Original VDW equation is for Boltzmann statistics Nucleons are fermions, obey Pauli exclusion principle Unlike for classical fluids, quantum statistics is important

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) $s > 0$ and $s \to 0$ as $T \to 0$

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VDW equation with quantum statistics in GCE

Ansatz: Take pressure in the following form

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

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

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

$$
s(T, \mu) = \left(\frac{\partial p}{\partial T}\right)_\mu = \frac{s^{id}(T, \mu^*)}{1 + b n^{id}(T, \mu^*)}
$$

$$
\varepsilon(T, \mu) = Ts + \mu n - p = [\varepsilon^{id}(T, \mu^*) - an]n
$$

This formulation explicitly satisfies requirements 1-3

Algorithm for GCE

1) Solve system of eqs. for p and n at given (T, μ) (there may be multiple solutions)

2) Choose the solution with largest pressure

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 $n = n_0 \cong 0.16$ fm⁻³ at $T = p = 0$ we obtain: *a* ≅ 329 MeV fm³ and *b* ≅ 3.42 fm³

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

VDW eq. now at very different scale!

VDW gas of nucleons: pressure isotherms

Behavior qualitatively same as for Boltzmann case Mixed phase results from Maxwell construction Critical point at $T_c \approx 19.7$ MeV and $n_c \approx 0.07$ fm⁻³ $\text{Experimental estimate}^2$: $\mathcal{T}_c = 17.9 \pm 0.4 \text{ MeV}, \, n_c = 0.06 \pm 0.01 \text{ fm}^{-3}$ ² J.B. Elliot, P.T. Lake, L.G. Moretto, L. Phair, Phys. Rev. C 87, 054622 (2013) Volodymyr Vovchenko (FIAS, Frankfurt & Kiev University) May 30, 2016 15 / 25

VDW gas of nucleons: (T, μ) plane

Density in (T, μ) plane³

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VDW gas of nucleons: (T, μ) plane

Density in (T, μ) plane³

Boltzmann: $T_c = 28.5$ MeV. Fermi statistics important even at CP

 $3V.$ Vovchenko et al., Phys. Rev. C 91, 064314 (2015)

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VDW gas of nucleons: scaled variance

Scaled variance in quantum VDW:

$$
\omega[\mathbf{M}] = \omega_{\mathrm{id}}(\mathbf{T}, \mu^*) \left[\frac{1}{(1 - b n)^2} - \frac{2 a n}{\mathbf{T}} \omega_{\mathrm{id}}(\mathbf{T}, \mu^*) \right]^{-1}
$$

VDW gas of nucleons: skewness and kurtosis

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 gas of nucleons: skewness and kurtosis

VDW Kurtosis -1 ⁰ ¹ 35 September 2014 - 1995 - 1995 - 1995 - 1995 - 1995 - 1996 - 1997 - 1998 - 1999 - 1999 - 1999 - 1999 - 1999 --10 300 St 200 S -100 T (MeV)
₁₅
T ₁₅ --100 No. 1 ----20 September 2010 and 2010 and 2010 1.00 15 Million St. 15 Million St. 15 Million ¹ 100 and 100 percent states and the states of the states of the states of gas liquid gas established and the second control of the second second control of the second the contract of the contract of the contract of 880 890 900 910 930 (MeV)

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

Fluctuation patterns in VDW very similar to effective QCD models

Beam energy dependence of skewness and kurtosis

There are measurements of higher-order cumulants with BES @ RHIC

Important to know dependence on centrality and kinematic acceptance

Strongly intensive measures near CP

Strongly intensive measures (Gorenstein, Gazdzicki, PRC 84, 014904 (2015))

- 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 program⁴

In classical VDW:

$$
\Delta[E^*, N] = 1 - \frac{an(2\bar{\epsilon}_{id} - 3an)}{\bar{\epsilon}_{id}^2 - \bar{\epsilon}_{id}^2} \omega[N], \quad \Sigma[E^*, N] = 1 + \frac{a^2n^2}{\bar{\epsilon}_{id}^2 - \bar{\epsilon}_{id}^2} \omega[N].
$$
\n• Critical behavior in VDW, same as for $\omega[N] \Rightarrow \Delta, \Sigma \sim |\tau|^{-\gamma}$ \n• Finite-size scaling: $\Delta[E^*, N], \Sigma[E^*, N] \sim \xi^{\gamma/\nu} \sim L^{\gamma/\nu}$

⁴Gazdzicki, Seyboth, Acta Phys. Polon. (2015); E. Andronov's talk at CPOD2016 Volodymyr Vovchenko (FIAS, Frankfurt & Kiev University) May 30, 2016 21 / 25

Strongly intensive measures in \mathcal{T} - μ plane

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Strongly intensive measures in $T-\mu$ plane

- Non-monotonous energy/system-size dependence of $Δ[E^*, N]$ and $Σ[E^*, N]$ in scenario with CP
- ∆[*E* ∗ , *N*] is more sensitive than Σ[*E* ∗ , *N*] to proximity of CP

Pion gas with van der Waals equation

Interacting pion gas as a VDW gas with Bose statistics

VDW parameters: $r = 0.3$ fm and $a/b = 500$ MeV

- Van der Waals attraction leads to emergence of limiting temperature
- Consequence of GCE and Bose statistics
- Suggestive similarity to Hagedorn mass spectrum
- Hint of phase transition to new state of matter?

R. Poberezhnyuk et al., arXiv:1508.04585

VDW interactions in hadron resonance gas

Hadron resonance gas – successful model for low density part of QCD

Gas of hadrons and resonances with eigenvolume VDW interactions

$$
P(T,\mu) = \sum_{i} P_i^{\rm id}(T,\mu_i - v_i P), \qquad n_i(T,\mu) = n_i^{\rm id}(T,\mu_i^*)/(1 + \sum_{i} v_i n_i^{\rm id}(T,\mu_i^*))
$$

- \bullet If eigenvolumes are same ratios are $= 0.3 \text{ fm}$: unaffected
	- If different ratios have non-monotonic dependence
	- A ratio "measurement" has two solutions
- $\frac{1}{100}$ $\frac{1}{150}$ $\frac{200}{150}$ $\frac{250}{150}$ $\frac{300}{150}$ \bullet Qualitatively similar behavior in full HRG
	- 0 100 200 300 400 500 0 $2 - r = 0.5$ fm 4 6 | City 8 | No. 1991 $10 \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow$ \mathbf{x}^2 r = 0.5 fm \cdots $r_1 - m_1^{1/3}$, $r_p = 0.5$ fm $p = 0.0$... $r_{\rm M}$ = 0.0 fm, $r_{\rm B}$ = 0.3 fm May 30, 2016 $24 / 25$ ALICE, Pb+Pb, $s_{NN}^{1/2} = 2.76$ TeV, 0-5% centrality

i

- Widening of χ^2 profile with two local minima
- Huge sensitivity of fits to VDW interactions, needs further studies
- V. Vovchenko, H. Stoecker, arXiv:1512.08046

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- ¹ Classical VDW equation is transformed to GCE and generalized to include effects of quantum statistics. New physical applications emerge.
- ² VDW equation with Fermi statistics for nucleons is able to describe properties of symmetric nuclear matter. VDW equation with Bose statistics for pions shows limiting temperature. Strong effect of VDW interactions in HRG.
- ³ Fluctuations are very sensitive to the proximity of the critical point. Gaseous phase is characterized by positive skewness while liquid phase corresponds to negative skewness. The crossover region is clearly characterized by negative kurtosis in VDW model. Role of repulsive and attractive interactions is clarified.
- ⁴ Strongly intensive measures of energy and particle number fluctuations show critical behavior in vicinity of CP and are suitable for the experimental study. Critical behavior is same as for the scaled variance, $Δ$ measure is shown to be more sensitive than $Σ$.
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Thanks for your attention!

Backup slides

Scaled variance in mixed phase region

Inside the mixed phase:

$$
V_g = \xi V, \quad V_l = (1 - \xi) V, \quad F(V, T, N) = F(V_g, T, N_g) + F(V_l, T, N_l)
$$

$$
\langle N \rangle = \langle N_g \rangle + \langle N_l \rangle = V[\xi n_g + (1 - \xi)n_l]
$$

$$
\omega[N] = \frac{\xi_0 n_g}{n} \left[\frac{1}{(1 - b n_g)^2} - \frac{2 a n_g}{T} \right]^{-1} + \frac{(1 - \xi_0) n_l}{n} \left[\frac{1}{(1 - b n_l)^2} - \frac{2 a n_l}{T} \right]^{-1} + \frac{(n_g - n_l)^2 V}{n} \left[\langle \xi^2 \rangle - \langle \xi \rangle^2 \right], \qquad \xi_0 = \frac{n_l - n_g}{n_l - n_g}
$$

In addition to GCE fluctuations in gaseous and liquid phases there are also fluctuations of volume fractions

$$
W(\xi) = C \exp\left[-\frac{1}{2T}\left(\frac{\partial^2 F}{\partial \xi^2}\right)_{\xi=\xi_0}(\xi-\xi_0)^2\right]
$$

$$
\langle \xi^2 \rangle - \langle \xi \rangle^2 = \frac{T}{V}\left[\frac{n_g T}{\xi_0 (1-bn_g)^2} - \frac{2an_g^2}{\xi_0} + \frac{n_I T}{(1-\xi_0)(1-bn_I)^2} - \frac{2an_f^2}{1-\xi_0}\right]^{-1}
$$

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 χ^2 still has a rather complicated non-parabolic structure Standard statistical methods of extracting the uncertainties become inapplicable