

Van der Waals equation on a nuclear scale

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Acknowledgements to

D. Anchishkin, M. Gorenstein, R. Poberezhnyuk, and H. Stoecker

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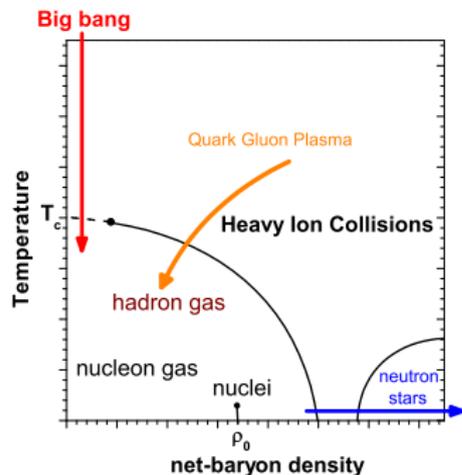
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 - Grand Canonical Ensemble
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Strongly interacting matter

- Protons and neutrons interact via **strong** force
- Not elementary, composed of **quarks**, interaction mediated by **gluons**
- Theory: Quantum Chromodynamics (QCD)



Scales

- Length: $1 \text{ fm} = 10^{-15} \text{ m} = 10^{-5} \text{ \AA}$
- Energy: $100 \text{ MeV} = 10^{10}$ times room T

Where is it relevant?

- Early universe
- Neutron stars
- Heavy-ion collisions (laboratory!)

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

Phenomenological tools are very useful

Thermodynamics

Put a lot of particles in a box and wait...

System will reach state of **thermodynamic equilibrium**, characterized by few macroscopic state variables

Equation of State – relation between different state variables

Ideal gas law

$$P(T, V, N) = \frac{N T}{V} = n T$$

- Good starting point for applying thermodynamic approach
- Simple mathematical properties
- With proper input (atoms, molecules, hadrons, ...) can describe well certain regions of corresponding phase diagram
- **Cannot** be used to describe **phase transitions** (no liquid-vapor)

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.
Nobel Prize in 1910.



Two ingredients:

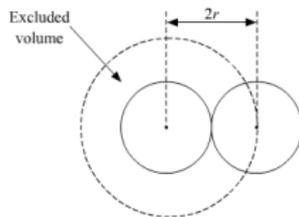
1) Short-range **repulsion**: particles are hard spheres,

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

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

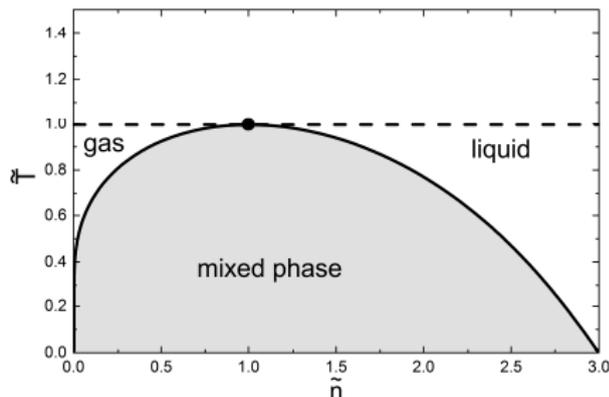
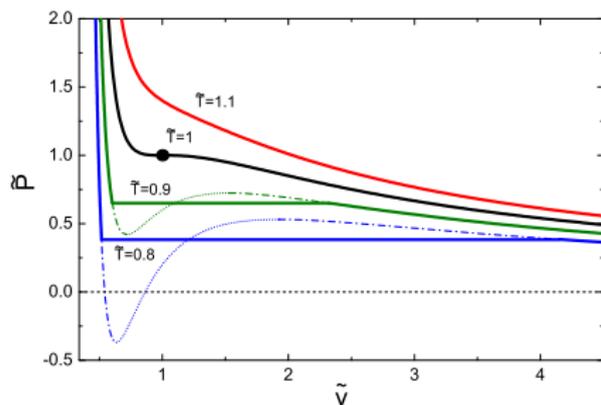
$$P \rightarrow P - an^2$$

Later derived from statistical physics



Van der Waals equation

- VDW isotherms show irregular behavior below certain temperature T_C
- Interpreted as the appearance of **phase transition**
- Below T_C isotherms are corrected by **Maxwell's rule of equal areas**



Critical point

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

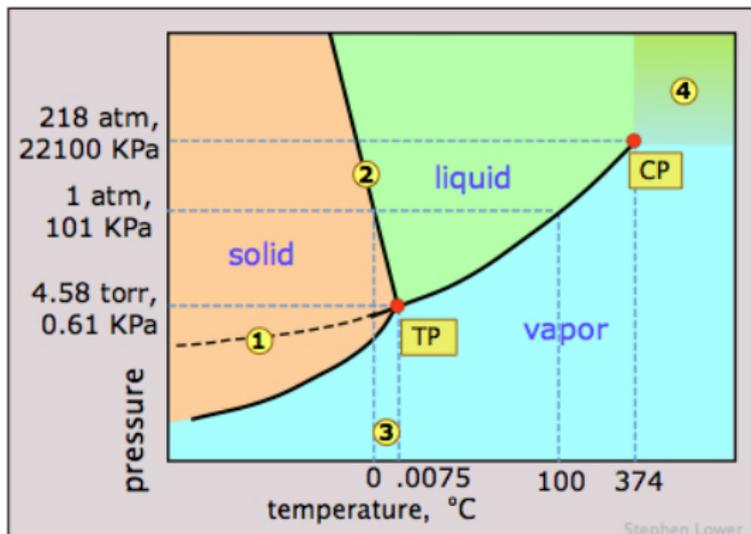
$$p_C = \frac{a}{27b^2}, \quad n_C = \frac{1}{3b}, \quad T_C = \frac{8a}{27b}$$

Reduced variables

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

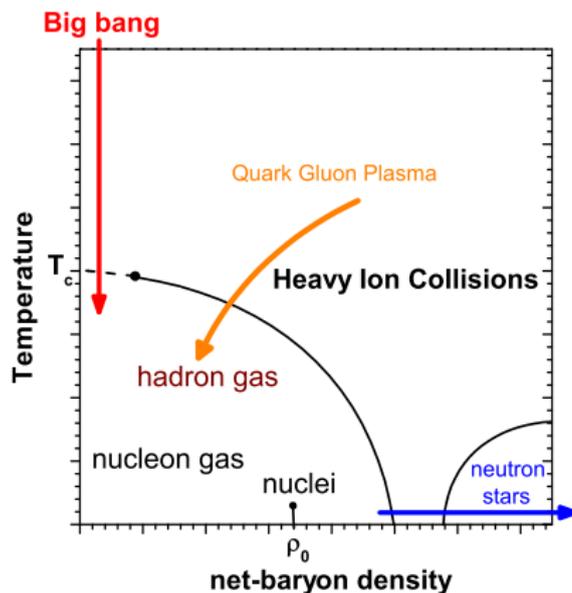
Van der Waals equation

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



Van der Waals equation

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



But can it provide insight on phase transitions in QCD?

VDW equation originally formulated in **canonical ensemble**

Canonical ensemble

- 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

- 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 $n(T, \mu)$

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

- Implicit equation in GCE, in CE it is 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

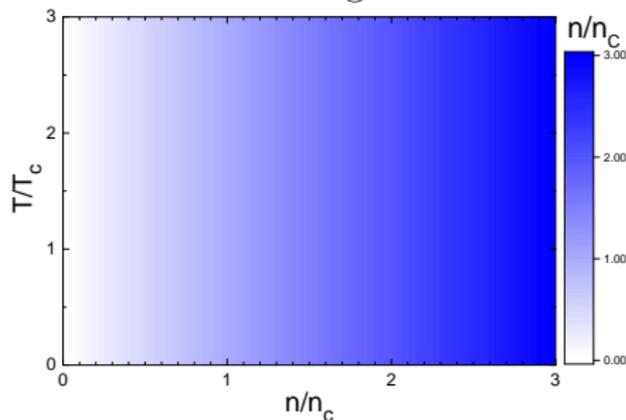
N-fluctuations are useful because they

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

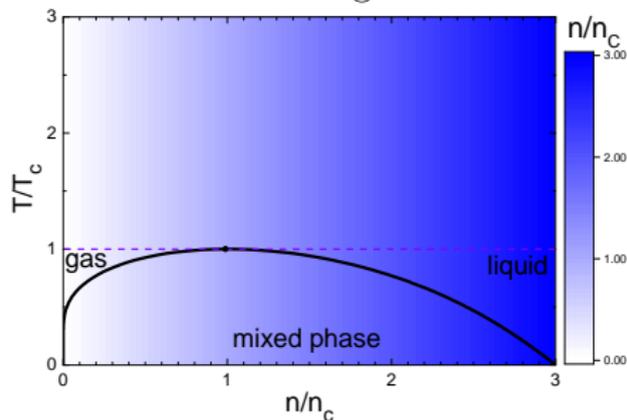
Phase transition signatures

Imagine we are measuring distribution of particle number

Ideal gas



VDW gas

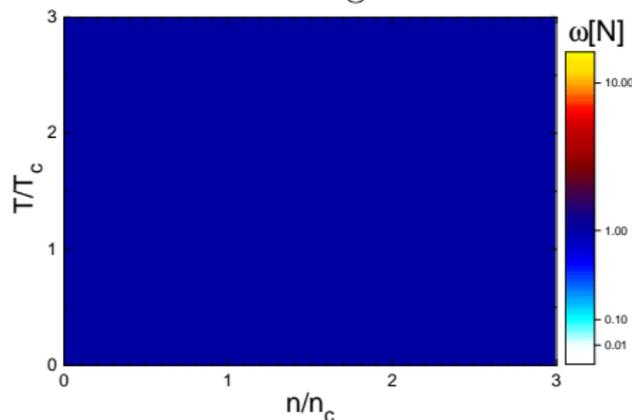


Measuring average $\langle N \rangle$ (or average energy) gives no information about phase transitions

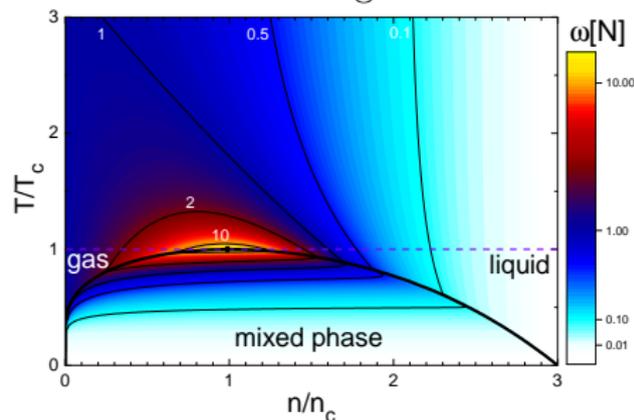
Phase transition signatures

What about fluctuations?

Ideal gas



VDW gas

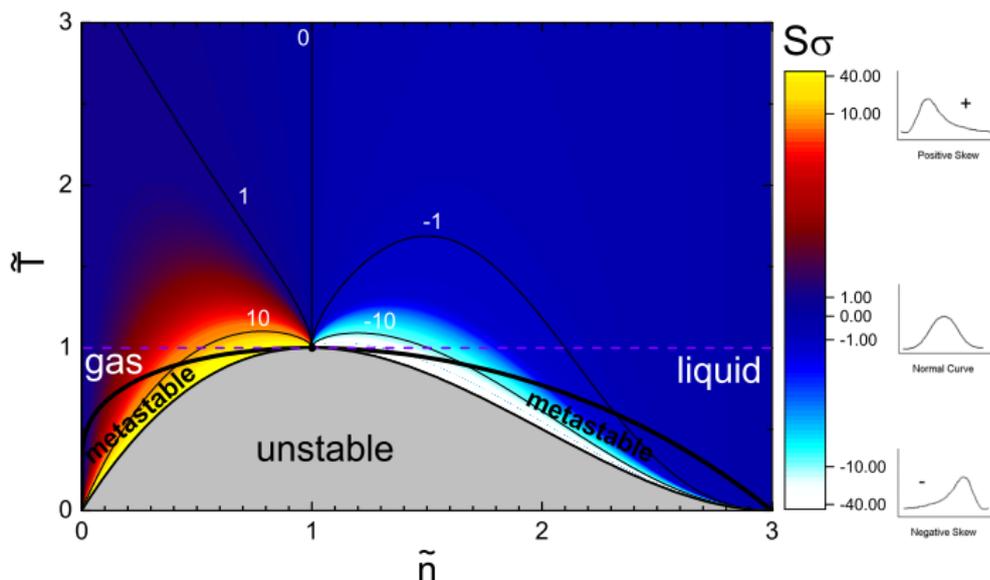


- Deviations from unity signal interaction effects
- Fluctuations grow rapidly near critical point

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

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

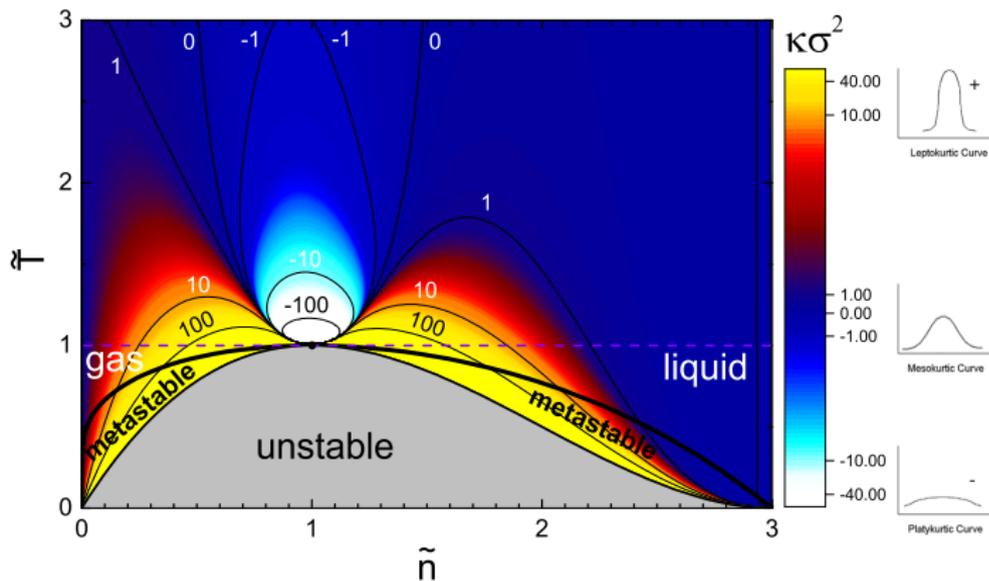


Skewness is

- **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

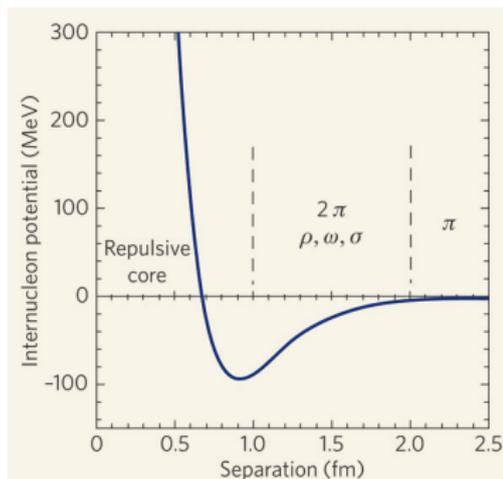


Kurtosis is **negative** (flat) above critical point (crossover), **positive** (peaked) elsewhere and very **sensitive** to the **proximity** of the critical point

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, uncertainty principle 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) $s \geq 0$ and $s \rightarrow 0$ as $T \rightarrow 0$

VDW equation with quantum statistics in GCE

Ansatz: Take pressure in the following form

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

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

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

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

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

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

Nuclear matter as a VDW gas of nucleons

Nuclear matter is known to have a liquid-gas phase transition at $T \leq 20$ MeV and exhibit VDW-like behavior

Usually studied analyzing nuclear fragment distribution

Has long history...

Theory:

Csernai, Kapusta, Phys. Rept. (1986)

Stoecker, Greiner, Phys. Rept. (1986)

Serot, Walecka, Adv. Nucl. Phys. (1986)

Bondorf, Botvina, Ilinov, Mishustin, Sneppen, Phys. Rept. (1995)

Experiment:

Pochodzalla et al., Phys. Rev. Lett. (1995)

Natowitz et al., Phys. Rev. Lett. (2002)

Karnaukhov et al., Phys. Rev. C (2003)

Our description: Nuclear matter as a **system of nucleons** ($d = 4$, $m = 938$ MeV) described by VDW equation with **Fermi** statistics. Pions, resonances and nuclear fragments are **neglected**

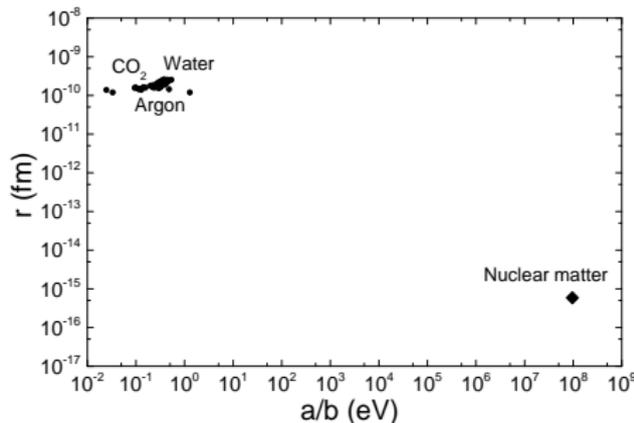
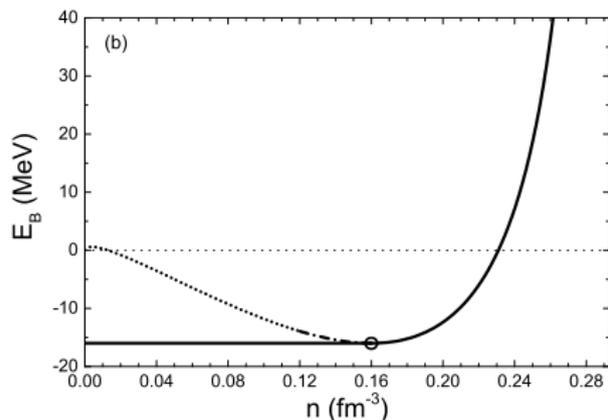
VDW gas of nucleons: zero temperature

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:

$$a \cong 329 \text{ MeV fm}^3 \text{ and } b \cong 3.42 \text{ fm}^3 \text{ (} r \cong 0.59 \text{ fm)}$$

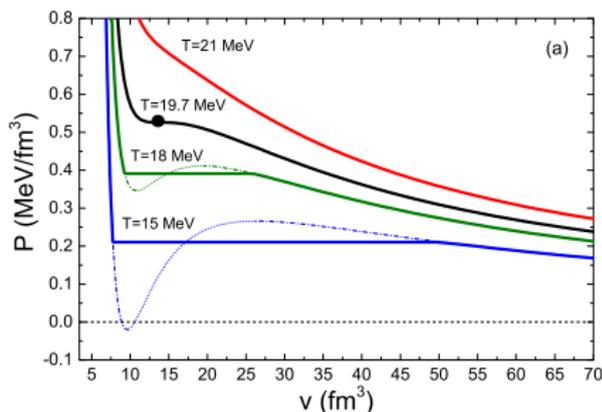
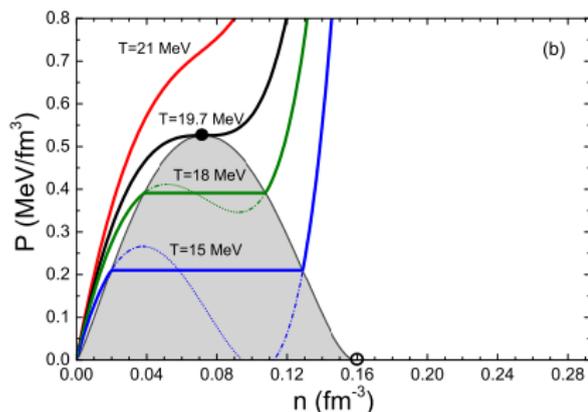


Mixed phase at $T = 0$ is **special**:
A mix of vacuum ($n = 0$) and liquid
at $n = n_0$

VDW eq. now at very different scale!

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**

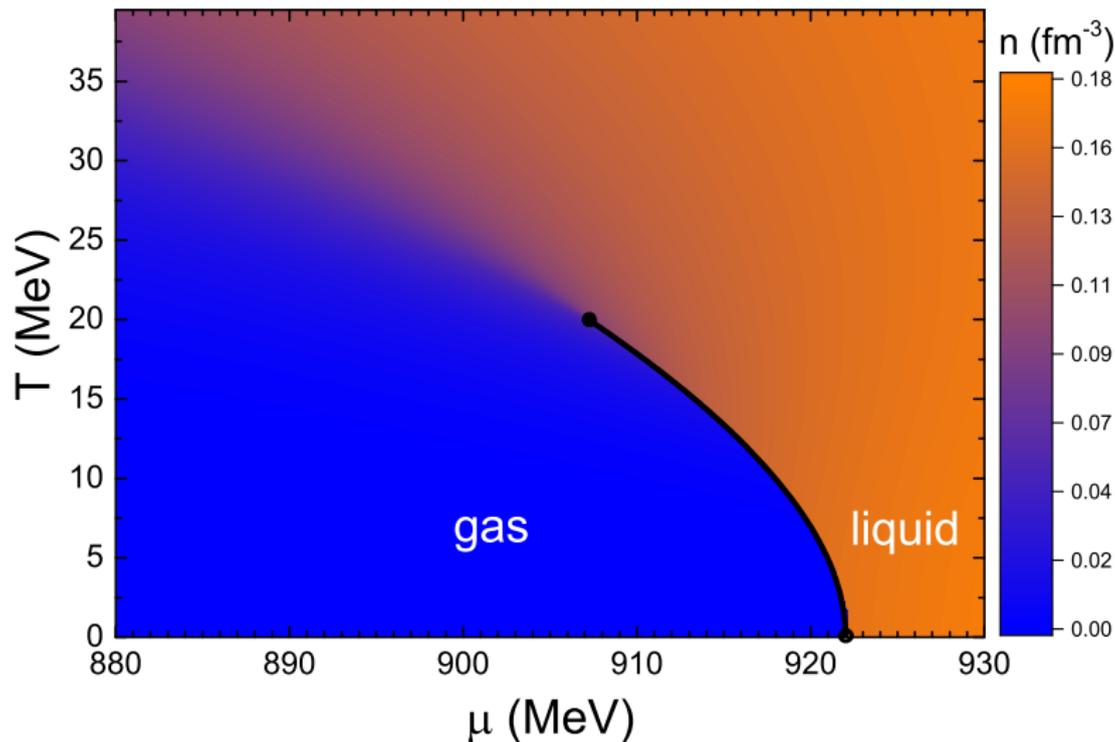
Critical point at $T_c \cong 19.7$ MeV and $n_c \cong 0.07$ fm⁻³

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

Density in (T, μ) plane²

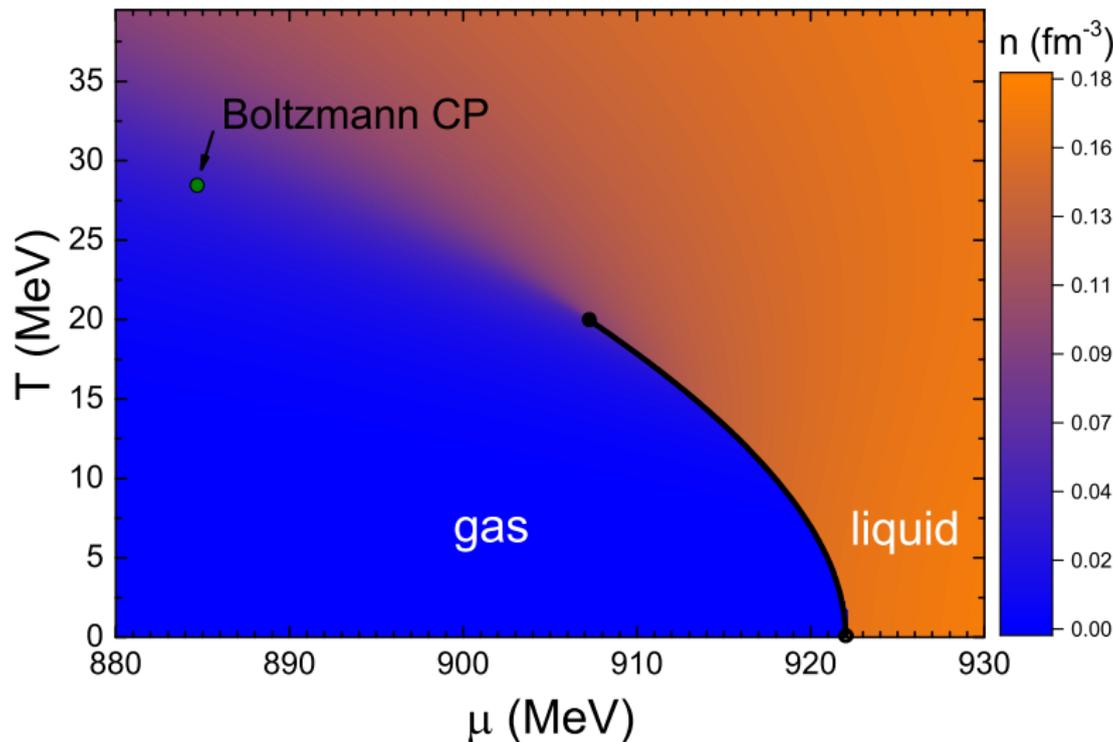


Crossover region at $\mu < \mu_C \cong 908$ MeV is clearly seen

¹V. Vovchenko et al., Phys. Rev. C 91, 064314 (2015)

VDW gas of nucleons: (T, μ) plane

Density in (T, μ) plane²



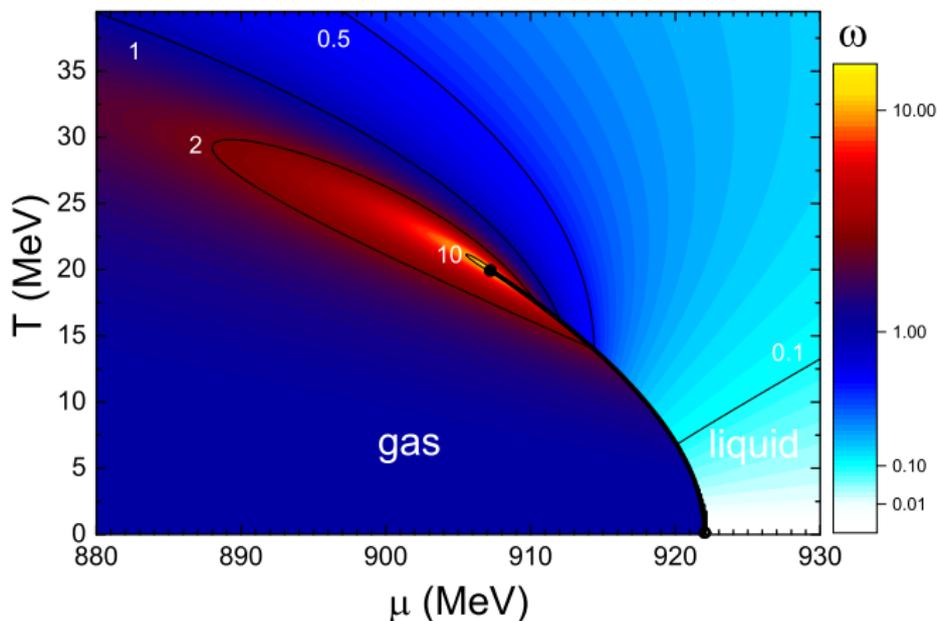
Boltzmann: $T_C = 28.5$ MeV. Fermi statistics **important** at CP

¹V. Vovchenko et al., Phys. Rev. C 91, 064314 (2015)

VDW gas of nucleons: scaled variance

Scaled variance in quantum VDW:

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



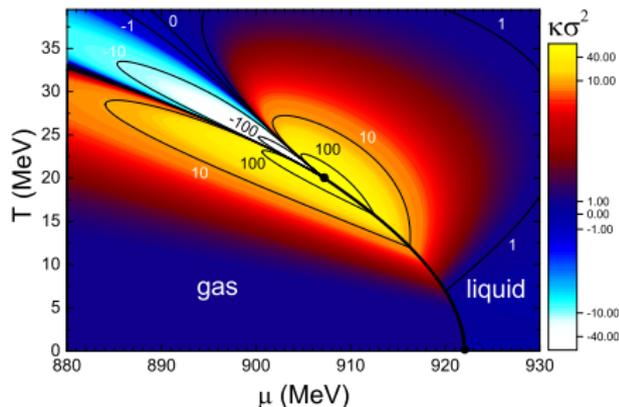
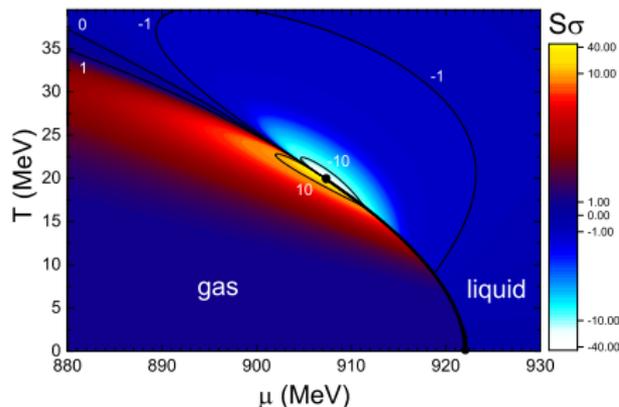
VDW gas of nucleons: skewness and kurtosis

Skewness

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

Kurtosis

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



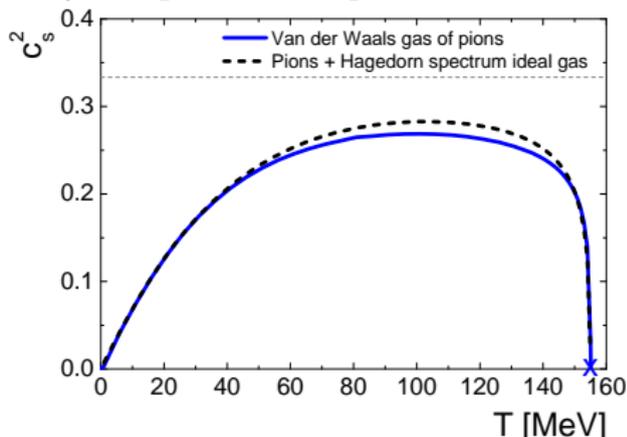
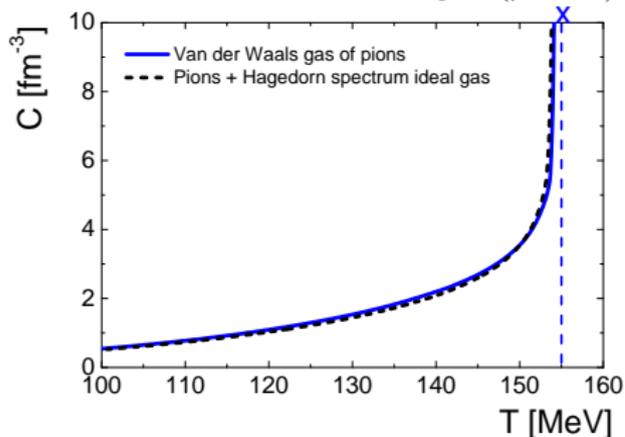
V. Vovchenko et al., Phys. Rev. C 92, 054901 (2015)

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

No conserved charges ($\mu = 0$), only temperature dependence



At some $T > T_0$ there are no solutions!

- 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?

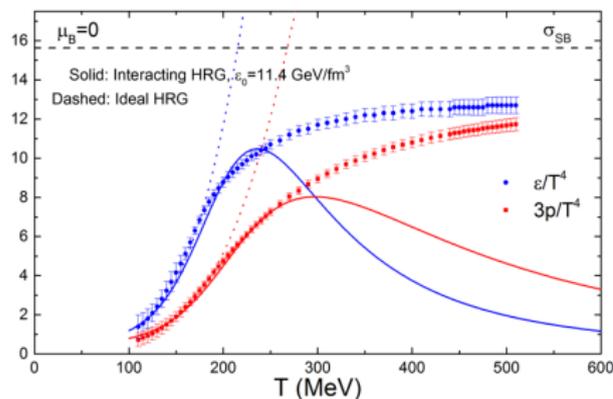
R. Poberezhnyuk et al., arXiv:1508.04585

VDW interactions in hadron resonance gas

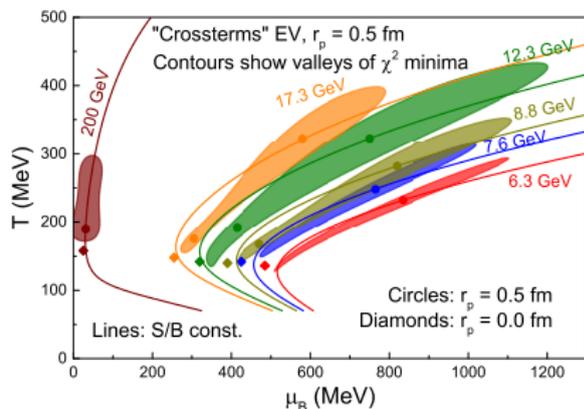
Hadron resonance gas – successful model for low density part of QCD

Usually modeled as non-interacting gas of hadrons and resonances

Add repulsive VDW interactions



Better agreement with lattice



Big change in fits to exp. data

Eigenvolume interactions had largely been overlooked in past!

V. Vovchenko, H. Stoecker, arXiv:1512.08046

- 1 Classical VDW equation is transformed to GCE and generalized to include effects of quantum statistics.
- 2 Scaled variance, skewness, and kurtosis of particle number fluctuations are calculated for VDW equation. Role of repulsive and attractive interactions is clarified.
- 3 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
- 4 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.

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Thanks for your attention!