Van der Waals equation: event-by-event fluctuations, quantum statistics and nuclear matter

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In collaboration with Dmitry Anchishkin, Mark Gorenstein, and Roman Poberezhnyuk

based on:

Vovchenko, Anchishkin, Gorenstein,
arXiv:1501.03785 [nucl-th], J. Phys. A in print and
arXiv:1504.01363 [nucl-th], Phys. Rev. C in print

Transport Meeting

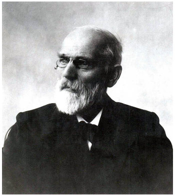
FIAS, Frankfurt
10 June 2015

Outline

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.

Is the simplest analytical model of interacting system with 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 transition

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

Van der Waals equation

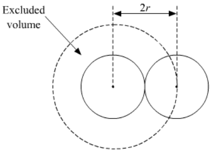
$$p(T,V,N) = \frac{NT}{V-bN} - a\frac{N^2}{V^2}$$

Two ingredients:

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

$b = 4\frac{4\pi r^3}{3}$

2) Attractive interaction in mean-field approximation



Critical point

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

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

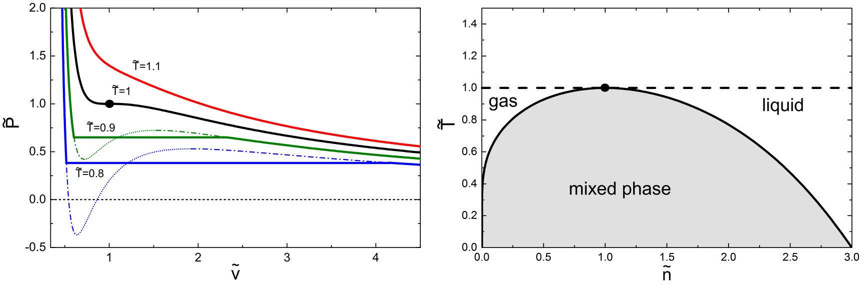
Reduced variables

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

Van der Waals equation

Van der Waals equation in reduced variables

$$p(\tilde{T}, \tilde{n}) = \frac{8\tilde{T}\tilde{n}}{3 - \tilde{n}} - 3\tilde{n}^2$$



Below T_C isotherms are corrected by Maxwell's rule of equal areas
This results in appearance of mixed phase

VDW equation in GCE

VDW equation has a simple and familiar form in canonical ensemble

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

In GCE one needs to define $p = p(T,\mu)$

What are the advantages of the GCE formulation?

1) Hadronic physics applications: number of hadrons usually not conserved, and GCE formulation is a good starting point to insert VDW interactions in multi-component hadron gas.

2) CE cannot describe particle number fluctuations. E.g., N-fluctuations in a small ($V \ll V_0$) subsystem follow GCE results.

3) GCE formulation is a good starting point to include effects of quantum statistics.

From CE to GCE

Variables T, V, N are not the natural variables for the pressure function.

Therefore $p(T, V, N)$ does not contain full information about system.

One needs instead free energy $F(T, V, N)$.

$$-\left(\frac{\partial F}{\partial V}\right)_{T,N} = p(T, V, N) \Rightarrow F(T, V, N) = F(T, V_0, N) - \int_{V_0}^{V} dV' \, p(T, V', N)$$

How to fix integration constant $F(T, V_0, N)$? Ideal gas at $V_0 \to \infty$!

VDW free energy

$$F(T, V, N) = F_{\rm id}(T, V - bN, N) - a\frac{N^2}{V}$$

$$F_{\rm id}(T, V, N) = -\, NT \left[1 \, + \, \ln \frac{V\,\phi(T; d, m)}{N}\right]$$

$$\phi(T; d, m) \;=\; \frac{d}{2\pi^2}\int_0^\infty k^2 dk \, \exp(-\sqrt{k^2 + m^2}/T) \;=\; \frac{d\, m^2\, T}{2\pi^2} K_2\left(\frac{m}{T}\right)$$

From CE to GCE

Chemical potential:

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} = -T \ln \frac{(V - bN)\,\phi(T; d, m)}{N} + b\,\frac{NT}{V - bN} - 2a\,\frac{N}{V}$$

Transcendental equation for $n(T, \mu)$

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

With $n(T, \mu)$ one then recovers $p(T, \mu)$:

$$p(T, \mu) = \frac{Tn}{1 - bn} - an^2 = p_{\rm id}(T, \mu^*) - an^2, \quad \text{where } n \equiv n(T, \mu)$$

Energy density:

$$\varepsilon(T, \mu) = [\epsilon_{id}(T) - an]\, n$$

Average energy per particle reduced by attractive mean field $-an$, excluded volume has no effect

Let $a = 0$: only repulsive interactions. Then

particle density: $$n(T,\mu) = \frac{n_{\rm id}(T,\mu^*)}{1 + b\,n_{\rm id}(T,\mu^*)}\,, \qquad \mu^* = \mu - b\,\frac{n\,T}{1 - b\,n}$$

pressure: $$p(T,\mu) = \frac{Tn}{1-bn} = p_{\rm id}[T, \mu - bp(T,\mu)]$$

energy density: $$\varepsilon(T,\mu) = \epsilon_{id}(T)\,n(T,\mu)$$

This reproduces the excluded-volume model
Rischke, Gorenstein, Stoecker, Greiner, Z. Phys. C51, 485

Scaled variance in VDW equation

Scaled variance is an intensive measure of N-fluctuations

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

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

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

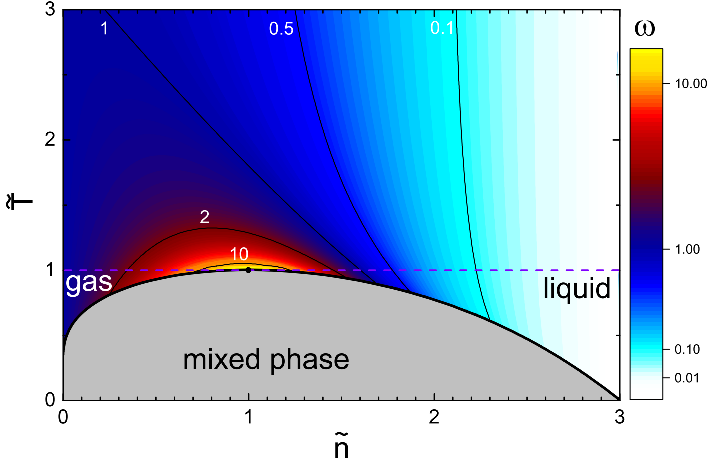
$$\omega[N] = \left[\frac{1}{(1 - bn)^2} - \frac{2an}{T} \right]^{-1}$$

Repulsive interactions suppress N-fluctuations while attractive interactions cause enhancement

Scaled variance outside mixed phase region

In reduced variables

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

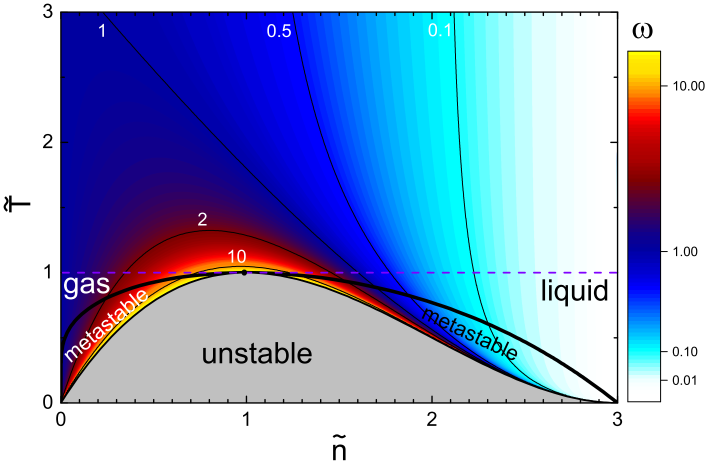


$\omega[N] \to \infty$ at the critical point

Scaled variance in metastable phases

VDW predicts existence of metastable liquid and gas phases

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



$\omega[N] \to \infty$ at the spinodal instability line, i.e. when $\partial p/\partial v = 0$

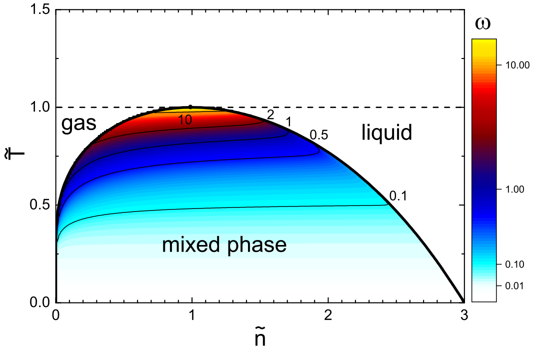
Scaled variance in mixed phase region

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

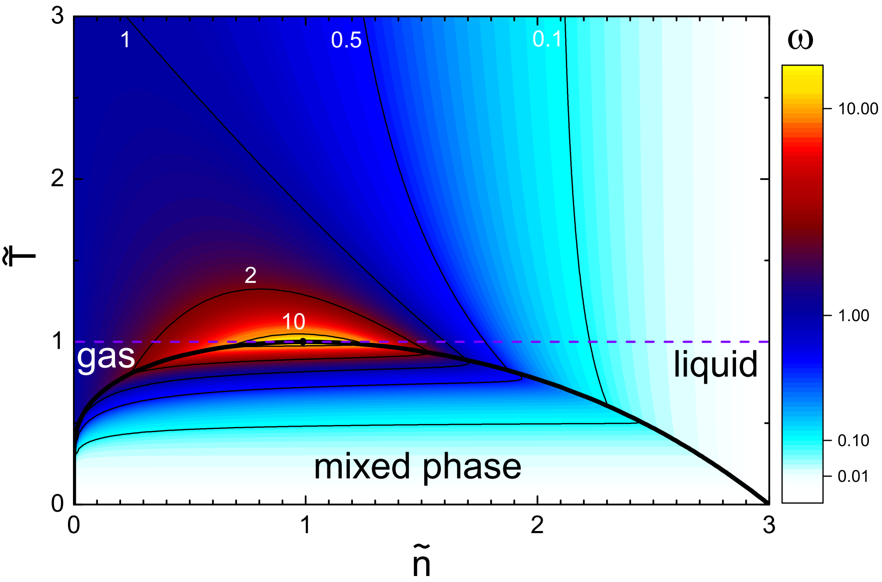
In addition to GCE fluctuations in gaseous and liquid phases there are also fluctuations of volume fractions

$$\omega[N] = \frac{\xi_0 \widetilde{n_g}}{9\widetilde{n}} \left[\frac{1}{(3-\widetilde{n_g})^2} - \frac{\widetilde{n_g}}{4\widetilde{T}}\right]^{-1} + \frac{(1-\xi_0)\widetilde{n}_l}{9\widetilde{n}} \left[\frac{1}{(3-\widetilde{n}_l)^2} - \frac{\widetilde{n}_l}{4\widetilde{T}}\right]^{-1}$$

$$+ \frac{(\widetilde{n_g}-\widetilde{n}_l)^2}{9\widetilde{n}} \left[\frac{\widetilde{n_g}}{\xi_0(3-\widetilde{n_g})^2} - \frac{\widetilde{n_g}^2}{\xi_0 4\widetilde{T}} + \frac{\widetilde{n}_l}{(1-\xi_0)(3-\widetilde{n}_l)^2} - \frac{\widetilde{n}_l^2}{(1-\xi_0)4\widetilde{T}}\right]^{-1}$$



Scaled variance in whole phase diagram



Non-gaussian fluctuations

Higher-order (non-gaussian) fluctuations are expected to be more sensitive to the proximity of the critical point

Stephanov, Phys. Rev. Lett. (2009); Karsch, Redlich, Phys. Lett. B (2010)

Skewness

$$s[N] = S\sigma = \frac{\kappa_3}{\kappa_2}$$

Kurtosis

$$\kappa[N] = \kappa\sigma^2 = \frac{\kappa_4}{\kappa_2}$$

Cumulants

$$\kappa_i = \frac{\partial^i (p/T^4)}{\partial(\mu/T)^i}$$

Skewness

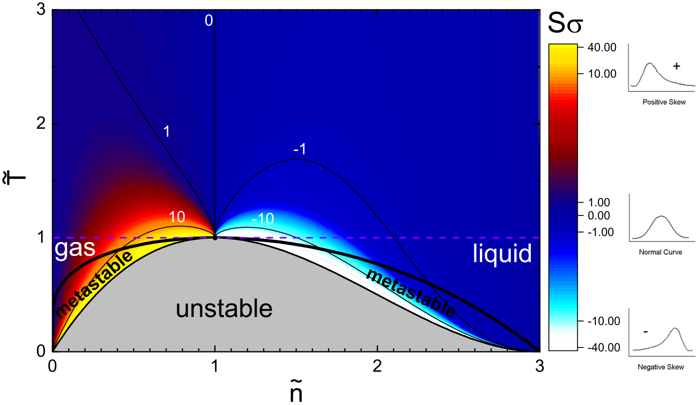
Skewness in VDW gas (pure phases)

$$s[N] = \omega^2[N]\left[\frac{1-3bn}{(1-bn)^3}\right] = \omega^2[N]\left[\frac{1-\widetilde{n}}{(1-\frac{1}{3}\widetilde{n})^3}\right]$$

Skewness

Skewness in VDW gas (pure phases)

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



Skewness is positive (right-tailed) in gaseous phase and negative (left-tailed) in liquid phase

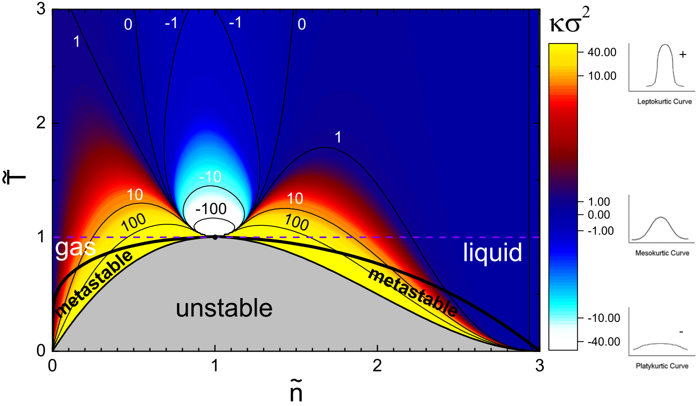
Kurtosis

Kurtosis in VDW gas (pure phases)

$$\kappa[N] = 3s^2[N] - 2\omega[N]s[N] - 6\omega^3[N]\frac{b^2 n^2}{(1-bn)^4}$$

Kurtosis in VDW gas (pure phases)

$$\kappa[N] = 3s^2[N] - 2\omega[N]s[N] - 6\omega^3[N]\frac{b^2 n^2}{(1-bn)^4}$$



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

Boltzmann statistics does not work well everywhere

Problems with Boltzmann statistics can already be seen on an ideal gas level

For non-relativistic gas

$$s^{\rm id}_{\rm Boltz} \cong \frac{n^{\rm id}}{T} \left[m + \frac{5}{2} T - \mu \right]$$

At $T \to 0$

$$s^{\rm id}_{\rm Boltz} \cong n_0 \left[\frac{5}{2} + \frac{3}{2} \ln(T/c_0) \right]$$

$s^{\rm id}_{\rm Boltz}$ can be negative at high n or at $T \to 0$

Quantum statistics needed in such case

Requirements for VDW equation with quantum statistics

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

VDW equation with quantum statistics in GCE

Ansatz: Take pressure in the following form

$$p(T,\mu) = p^{\rm id}(T,\mu^*) - an^2, \quad \mu^* = \mu - b\,p - a\,b\,n^2 + 2an$$

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

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

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

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

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

Quantum VDW: from GCE to CE

One can define pressure as a function of CE variables T and n

Recall that

$$n(T,\mu) = \frac{n^{\rm id}(T,\mu^*)}{1 + b\, n^{\rm id}(T,\mu^*)} \quad \Leftrightarrow \quad n^{\rm id}(T,\mu^*) = \frac{n(T,\mu)}{1 - b\, n(T,\mu)}$$

Therefore $\mu^*(n,T) = \mu^{\rm id}\left(\frac{n}{1-bn}, T\right)$ where $\mu^{\rm id}(n,T)$ is solution to

$$n \;=\; \frac{d}{2\pi^2} \int_0^\infty dk\, k^2 \left[\exp\left(\frac{\sqrt{m^2+k^2} - \mu^{\rm id}(n,T)}{T}\right) + \eta\right]^{-1}$$

VDW equation with quantum statistics in CE

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

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

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)

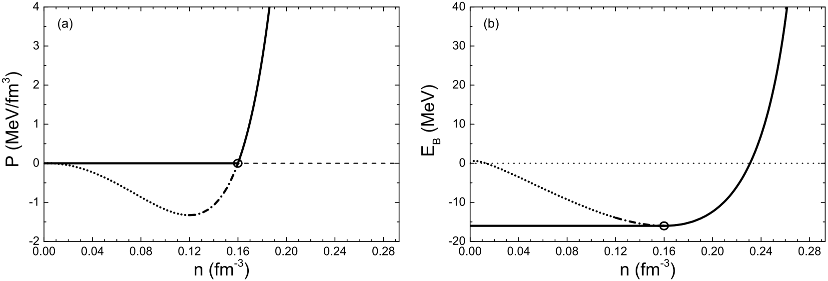
Our description: Nuclear matter as a system of nucleons ($d = 4$, $m = 938$ MeV) described by VDW equation with Fermi statistics. Pions, resonances and nuclear fragments are neglected

VDW gas of nucleons: zero temperature

How to fix a and b? Saturation density and binding energy at $T = 0$

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

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

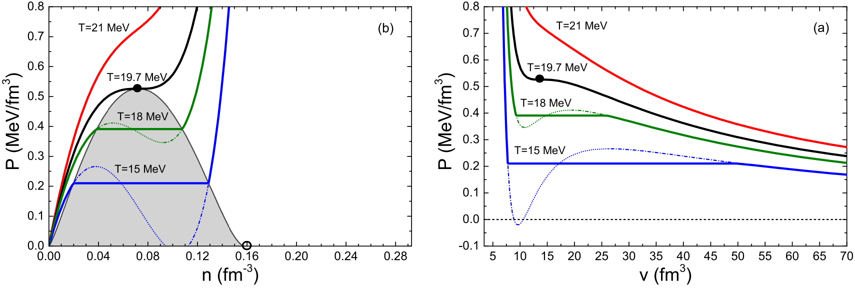


Mixed phase at $T = 0$ is rather special:
A mix of vacuum ($n = 0$) and liquid at $n = n_0$

VDW gas of nucleons: pressure isotherms

CE pressure

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

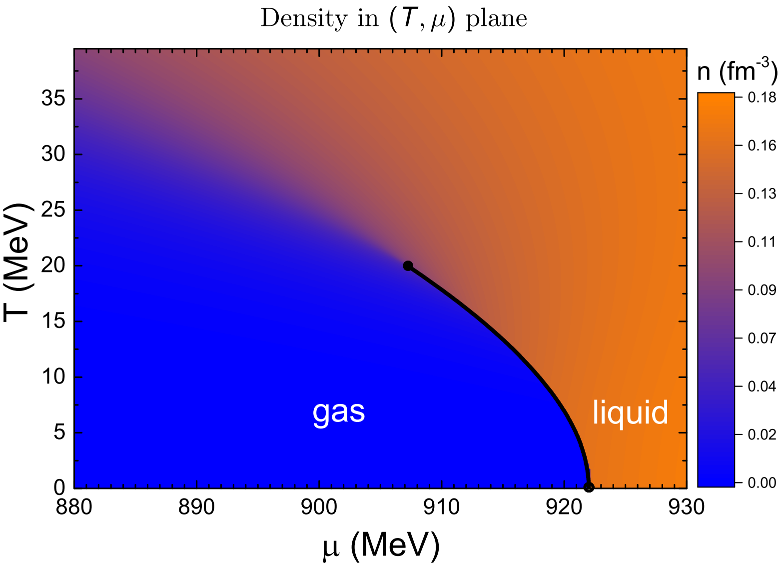


Behavior qualitatively same as for Boltzmann case

Mixed phase results from Maxwell construction

Critical point at $T_c \cong 19.7$ MeV and $n_c \cong 0.07$ fm^{-3}

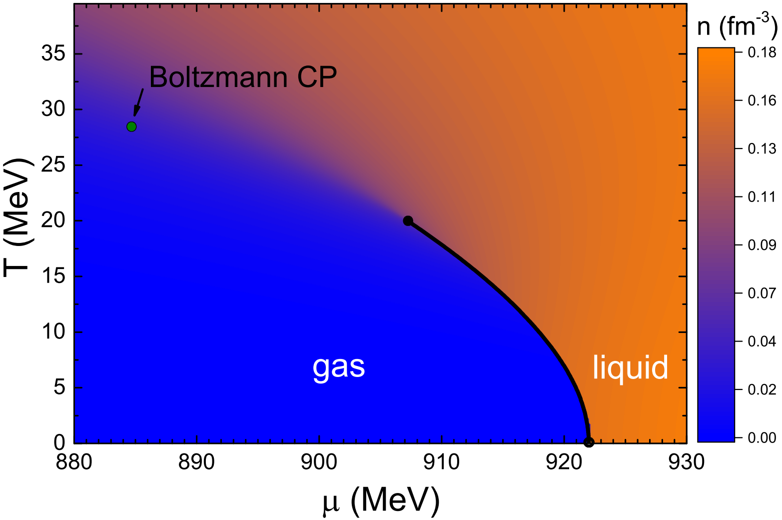
VDW gas of nucleons: (T, μ) plane



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

VDW gas of nucleons: (T, μ) plane

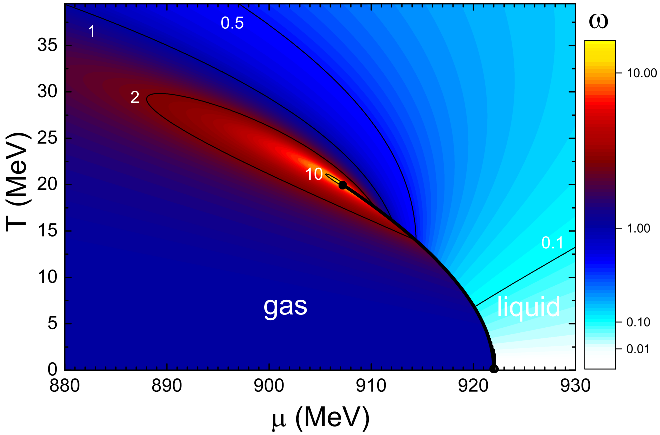
Density in (T, μ) plane



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

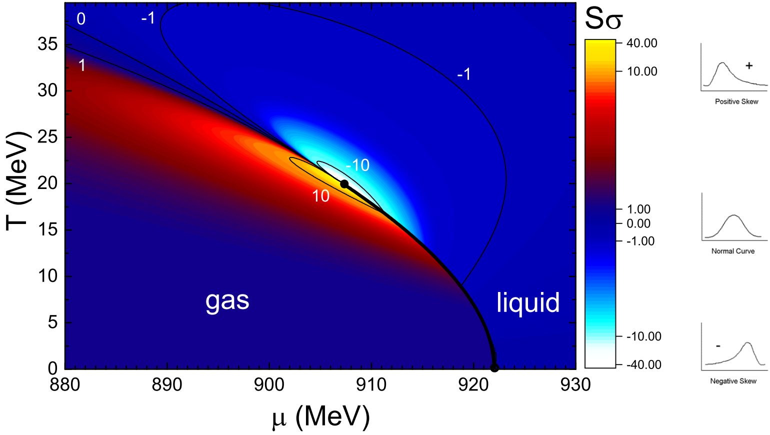
Scaled variance in quantum VDW:

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



Skewness in quantum VDW:

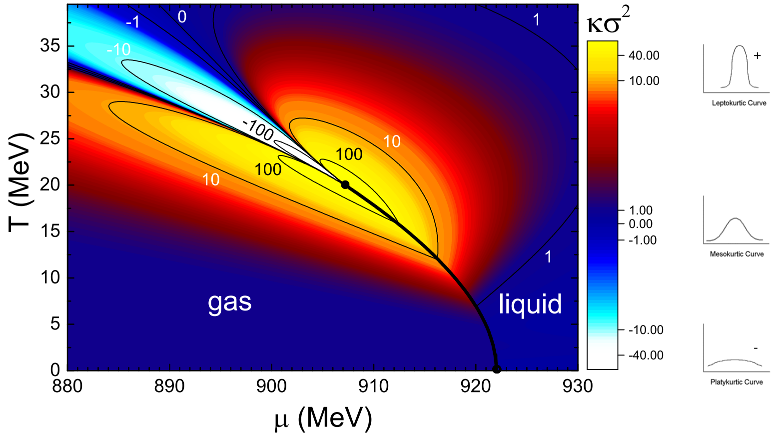
$$s[N] = \frac{\omega[N]}{[\omega_{\rm id}(T,\mu^*)]^2}\,\frac{T}{(1-bn)^2}\,\frac{\partial \omega_{\rm id}(T,\mu^*)}{\partial \mu} + \frac{\omega^2[N]}{\omega_{\rm id}(T,\mu^*)}\,\frac{1-3bn}{(1-bn)^3}$$



VDW gas of nucleons: kurtosis

Kurtosis in quantum VDW:

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



Crossover region is clearly characterized by large negative kurtosis
This also been suggested for QCD CP in Stephanov, PRL (2011)

Summary

1. Classical VDW equation is reformulated in GCE as a transcendental equation for particle density.
2. Scaled variance, skewness, and kurtosis of particle number fluctuations are calculated for VDW equation. Fluctuations remain finite both inside and outside the mixed phase region but diverge at the critical point.
3. VDW equation with Fermi statistics is presented and is able to qualitatively describe properties of symmetric nuclear matter. Fermi statistics effects remain quantitatively important near the critical point of nuclear liquid-gas transition.
4. Non-gaussian 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.

Possible tasks:

- Other fluctuation measures, e.g., strongly intensive quantities
- Inclusion of VDW interactions in multi-component systems, e.g., nuclear fragments, HRG etc.
- BEC in interacting VDW gas, e.g., gas of pions
- Transport coefficients

Thanks for your attention!

Backup slides

Scaled variance in mixed phase region

Inside the mixed phase:

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

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

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

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

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

$$\langle\xi^2\rangle - \langle\xi\rangle^2 = \frac{T}{V}\left[\frac{n_g T}{\xi_0\,(1-bn_g)^2} - \frac{2an_g^2}{\xi_0} + \frac{n_l T}{(1-\xi_0)(1-bn_l)^2} - \frac{2an_l^2}{1-\xi_0}\right]^{-1}$$