

Induced surface tension within novel equation of state of nuclear and hadron matter

O. Ivanytskyi

collaborators: K. Bugaev and V. Sagun

Refs: Nucl. Phys. A 924, 24 (2014)
arXiv:1611.07569 [nucl-th]

Budapest, 7 December 2016

Zimaniy School

Models of hadronic/nuclear matter EoS

- **Relativistic Mean Field models** - Walecka Model, Chiral Perturbation Theory, etc.
Advantage: QCD symmetries are preserved
Problems: 1. NO fluctuations \Rightarrow unrealistic critical point
2. Only few particle species
- **Statistical Cluster models** - Fisher Droplet Model, Gas of Bags Model, Statistical Multifragmentation Model, Hadron Resonance Gas Model
Advantage: fluctuations \Rightarrow physical critical point
Problems: Hard core repulsion violates causality
- **Hybrid approach** - Walecka model with nonrelativistic proper volume of nucleons

$$p(T, \mu) = p_{Walecka}(T, \mu - pV_{eigen})$$

D.H. Rischke, M.I. Gorenstein, H. Stoecker and W. Greiner, Z. Phys. C 51(1991) 485

Why hard core repulsion?

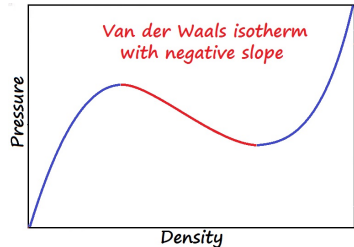
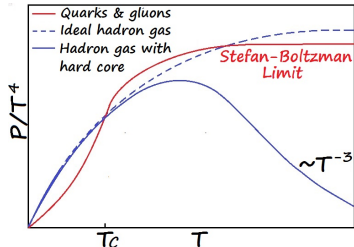
Hadronic hard core

- Prevents phenomenological EoS of QCD from quark confinement at high temperatures

ideal gas : $p \sim T^4$

hard core : $p \sim T$

- Accounts for short range repulsion between the constituents (hadrons, nuclear fragments, etc.)
- Is necessary for statistical (not Van der Waals) liquid-gas phase transition in cluster models
- Important element in description of particle yields (ideal hadron gas is proven to be inadequate at high A+A collision energies)



J. Cleymans and H. Satz, Z. Phys. C 57, 135 (1993)

J. Cleymans, M.I.Gorenstein, J. Stalnacke and E.Suhonen, Phys. Scripta 48, 277 (1993)

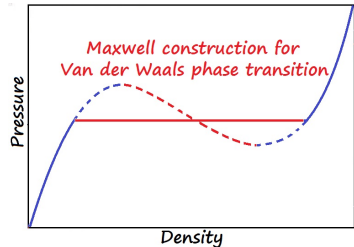
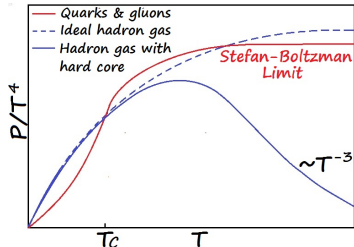
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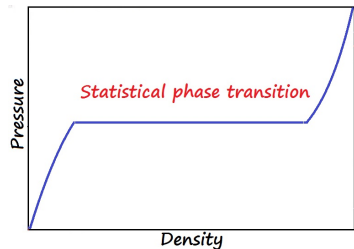
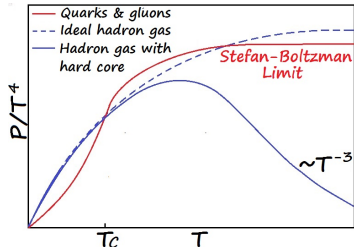
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J. Cleymans, M.I.Gorenstein, J. Stalnacke and E.Suhonen, Phys. Scripta 48, 277 (1993)

Constraints on hadronic/nuclear matter EoS

- **Multicomponent EoS** \Rightarrow Grand Canonical Ensemble (GCE) is natural choice
- **Thermodynamic consistency** (in GCE pressure is function of T and μ only)
 $p = p(T, \mu, n) \Rightarrow$ contradiction with thermodynamic relation $n = \frac{\partial p}{\partial \mu}$
 L. van Hove, *Physica* 15, 951 (1949) and *Physica* 16, 137 (1950)

- **Switching between excluded and eigen volumes (per particle)**



high order virial coefficients are needed

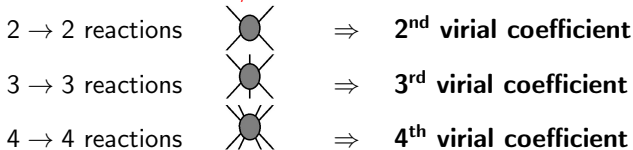
- **Causality:** $c_{\text{sound}} \leq c_{\text{light}} = 1$, where $c_{\text{sound}}^2 = \left. \frac{dp}{d\epsilon} \right|_{s/n=\text{const}}$
 Existing approaches to restore causality violated by hard core are rather complicated
 K. Bugaev, *Nucl. Phys. A* 807 (2008)

Something more convenient for practical applications is needed

Application to compact astrophysical objects

- Hadronic EoS used for modeling of the neutron star interiors **violates causality**
 H. Grigorian, COST Action @ CPOD 2016, Wroclaw

- Three, four, ... particle forces are needed - **high order virial coefficients**
 G. Baym, COST Action @ CPOD 2016, Wroclaw

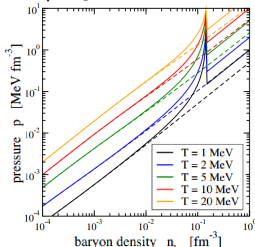


- Observational constrains require soft/stiff EoS at low/high densities

T. Kojo, COST Action @ CPOD 2016, Wroclaw
 hyperons ⇒ softening of the hadronic EoS
multicomponent EoS in GCE is needed

- Thermodynamically inconsistent suppression of deuterons in the neutron star interiors ⇒ **pressure discontinuity = zero order PT**

S. Typel, Eur. Phys. J. A (2016) 52, 16



Objectives

- Simple multicomponent EoS with hard core repulsion
- Thermodynamic consistency
- Correct asymptotics of excluded volume EoS at low and high densities
- Higher virial coefficients
- Causality up to densities where QGP is expected

Multicomponent mixture of Boltzmann hard spheres

- Virial expansion in powers of one particle thermal densities $\{\phi_i\}$

$$\begin{aligned}
 \frac{p}{T} &= \sum_i \phi_i e^{\frac{\mu_i}{T}} - \sum_{i,j} \overbrace{\frac{2\pi}{3} (R_i + R_j)^3}^{2^{nd} \text{ virial coefficient}} \phi_i \phi_j e^{\frac{\mu_i + \mu_j}{T}} + \mathcal{O}(\phi^3) \\
 &= \sum_i \phi_i e^{\frac{\mu_i}{T}} \left(1 - \underbrace{V_i \sum_j \phi_j e^{\frac{\mu_j}{T}}}_{\text{bulk term}} - \underbrace{S_i \sum_j R_j \phi_j e^{\frac{\mu_j}{T}}}_{\text{surface term}} \right) + \mathcal{O}(\phi^3)
 \end{aligned}$$

- VdW like extrapolation (gives exponentials)

$$\begin{cases} \sum_j \phi_j e^{\frac{\mu_j}{T}} \simeq \frac{p}{T} \\ \sum_j R_j \phi_j e^{\frac{\mu_j}{T}} \simeq \frac{\Sigma}{T} \end{cases} \Rightarrow \begin{cases} \frac{p}{T} = \sum_i \phi_i \exp\left(\frac{\mu_i - \rho V_i - \Sigma S_i}{T}\right) - \text{pressure} \\ \frac{\Sigma}{T} = \sum_i \phi_i \exp\left(\frac{\mu_i - \rho V_i - \Sigma S_i}{T}\right) R_i - \text{surface tension} \end{cases}$$

V.Sagun, A.Ivanytskyi, K. Bugaev, I. Mishustin, Nucl. Phys. A 924, 24 (2014)

- Hard core repulsion only in part is accounted by eigen volume.

The rest corresponds to **induced surface tension**

Extrapolation to high densities

- Extrapolation to high densities is not unique \Rightarrow equations for p and Σ can differ

$$\frac{p}{T} = \sum_i \phi_i \exp\left(\frac{\mu_i - pV_i - \Sigma S_i}{T}\right)$$

$$\frac{\Sigma}{T} = \sum_i R_i \phi_i \exp\left(\frac{\mu_i - pV_i - \Sigma S_i}{T}\right) \cdot \overbrace{\exp\left(\frac{(1-\alpha)S_i\Sigma}{T}\right)}^{\text{not uniqueness of extrapolation}}, \quad \alpha = \text{const}$$

- Meaning of $\alpha > 1$: one component case

$$\Sigma = pR \exp\left(\frac{(1-\alpha)S\Sigma}{T}\right)$$

$$p = T\phi \exp\left(\frac{\mu - pV_{\text{eff}}}{T}\right)$$

$$V_{\text{eff}} = V \left[1 + 3 \exp\left(\frac{(1-\alpha)S\Sigma}{T}\right) \right]$$

\Rightarrow low densities ($\Sigma \rightarrow 0$): $V_{\text{eff}} = 4V$
 high densities ($\Sigma \rightarrow \infty$): $V_{\text{eff}} = V$

α switches excluded and eigen volume regimes

high order virial coefficients?

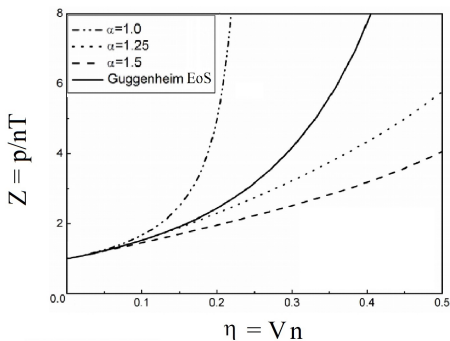
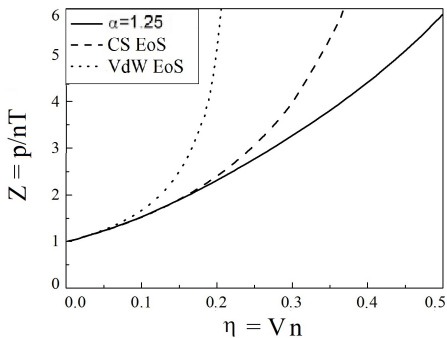


- Higher virial coefficients of hard spheres

- **Second virial coefficient** – reproduced for any α
- **Third virial coefficient** – reproduced for $\alpha = 1.245$ within 16%
- **Fourth virial coefficient** – reproduced for $\alpha = 1.245$

Comparison with other one component EoS

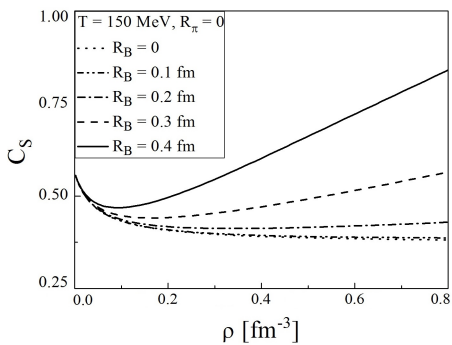
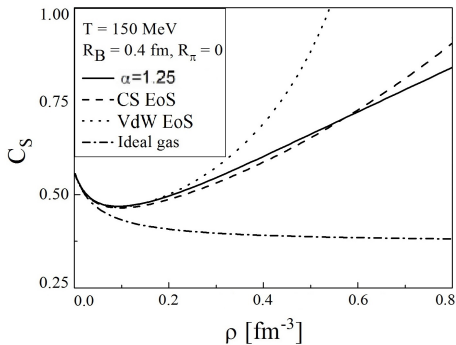
- One component Boltzmann gas of hard spheres



- VdW EoS: $Z = (1 - 4\eta)^{-1}$ - is rather stiff
- Guggenheim EoS: $Z = (1 - \eta)^{-4}$ - reproduced up to $\eta \simeq 0.2$
- Carnahan-Starling EoS (reproduces 7 virial coefficients): $Z = \frac{1+\eta+\eta^2-\eta^3}{(1-\eta)^3}$
- reproduced up to $\eta \simeq 0.22$

Causality of IST EoS at very extreme cases

- Boltzmann mixture of baryons (N and Δ) and pions



At $\alpha = 1.25$ multicomponent EoS is causal up to $\simeq 7$ normal nuclear densities where quark matter is expected

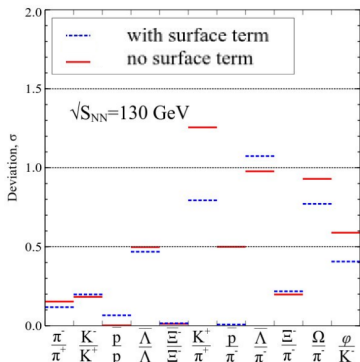
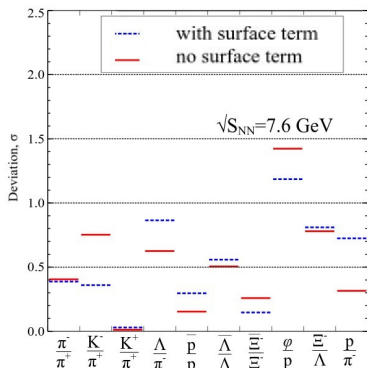
EoS with Induced Surface Tension

$$p = \sum_i p_0(T, \mu_i) \Rightarrow \begin{cases} p = \sum_i p_0(T, \mu_i - pV_i - \Sigma S_i) \\ \Sigma = \sum_i p_0(T, \mu_i - pV_i - \alpha \Sigma S_i) R_i \end{cases}$$

- Advantages compared to other EoS with hard core repulsion:
 - Multicomponent character and thermodynamic consistency
 - Correct asymptotic of excluded volume at high and low densities, higher virial coefficients
 - Wide range of causality
 - Straightforward generalization to quantum statistics and mean field models
- Questions
 - Value of α in case of quantum statistics? Medium dependent α ?
 - ...

Hadron Resonance Gas

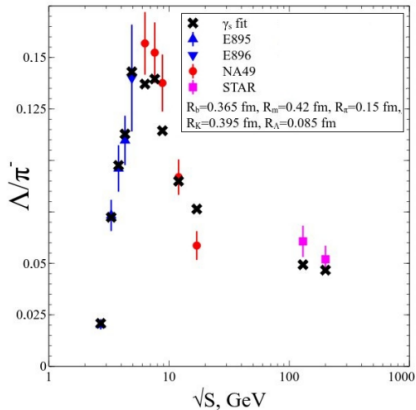
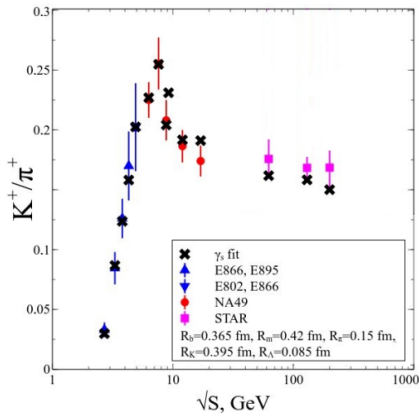
- Hadrons with masses ≤ 2.5 GeV (widths, strong decays, zero strangeness)
- 111 independent particle ratios measured at 14 energies
- 14×4 local parameters ($T, \mu_B, \mu_{13}, \gamma_s$) + 5 global parameters (hard core radii)



$R_b = 0.365$ fm, $R_m = 0.42$ fm, $R_\pi = 0.15$ fm, $R_K = 0.395$ fm, $R_\Lambda = 0.085$ fm

Overall $\chi^2/\text{dof} \simeq 1.038$

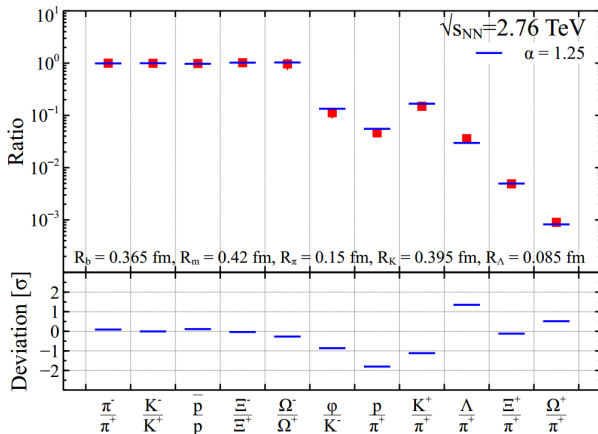
K^+/π^+ and Λ/π^- ratios



- Induced surface tension correction improves quality of the data description
- Advantage in multicomponent case - **EoS includes just two equations**
EoS of earlier HRG model versions - N equations for N components

Hadron Resonance Gas at ALICE energies

- 11 independent particle yields, 6 parameters (temperature + 5 hard core radii)
- Overall $\chi^2/dof \simeq 1.038$
- Freeze out temperature $T_{FO} = 154 \pm 7 \text{ MeV}$



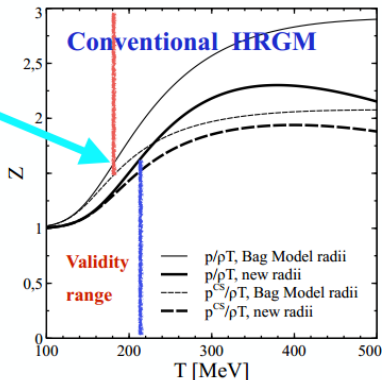
Applicability test with multicomponent Carnahan-Starling EOS

5 % deviation from MCSL EOS

compressibility $Z = p/(\rho T)$ total pressure of the system is p ,total particle density is $\rho = \sum_{k=1}^N \rho_k$

$$p^{CS} = \frac{6T}{\pi} \left[\frac{\xi_0}{1-\xi_3} + \frac{3\xi_1\xi_2}{(1-\xi_3)^2} + \frac{3\xi_2^3}{(1-\xi_3)^3} - \frac{\xi_3\xi_2^3}{(1-\xi_3)^3} \right],$$

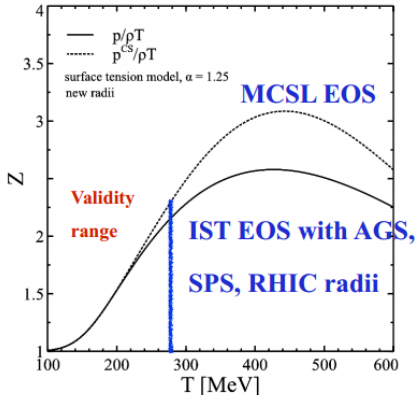
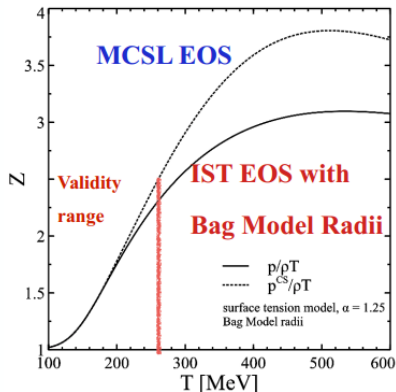
$$\xi_n = \frac{\pi}{6} \sum_{k=1}^N \rho_k [2R_k]^n.$$



Using densities, T and hard-core radii we calculated compressibility for each EOS and compared them with Z of MCSL EOS

MCSL EOS: G. A. Mansoori, N. F. Carnahan, K. E. Starling and T. W. Leland, Jr., J. Chem. Phys. 54, 1523 (1971)

Same Applicability Test for IST EOS



IST EOS with Bag Model radii is valid for $T < 260$ MeV

IST EOS with new radii is valid for $T < 280$ MeV

IMPORTANT: IST EOS is much softer than MCSL EOS at high densities!

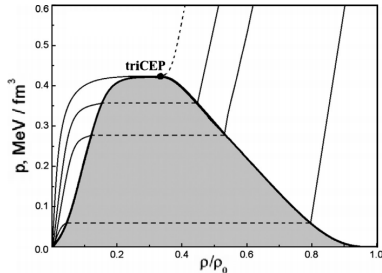
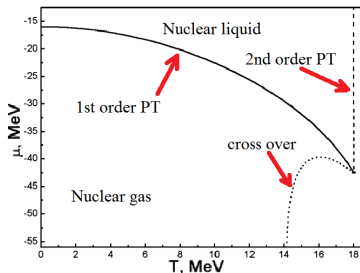
Summary

- Thermodynamically consistent approach to account for the excluded volume effects is proposed.
- Developed EoS reproduces 3rd and 4th virial coefficients and provides causality up to 7 normal nuclear densities.
- Approach to study induced surface tension. is developed.
Tolman length caused by curvature effects is evaluated. **Not in this talk :(**
- Novel EoS is applied to study properties of hadronic matter.
Phase diagram of nuclear matter is analyzed. **Not in this talk :(**
- Generalization of EoS with induced surface tension is discussed.

Thank you for attention

Nuclear matter in Statistical Multifragmentation Model

- Degrees of freedom: nucleons and composite nuclear fragments
- Interaction: hard-core repulsion, effective attraction due to large number of constituents like in the original Statistical Bootstrap Model
 J. P. Bondorf et al., *Phys. Rep.* 257, 131 (1995) and references therein
- Phase diagram with statistical liquid-gas phase transition and critical point



- Properties of normal nuclear matter
- Compressible nuclear liquid \Rightarrow critical density $\approx \frac{\rho_0}{3}$ which is typical for liquid-gas PT (standard SMM with incompressible nuclear liquid predicts $\rho_{cep} = \rho_0$)

V. V. Sagun, A. I. Ivanytskyi, K. A. Bugaev, I. N. Mishustin, *Nucl. Phys. A* 924, 24 (2014)

Thermodynamic consistency

- Grand Canonical Ensemble \Rightarrow pressure is function of T, μ and V only, $p = p(T, \mu, n) \Rightarrow$ contradiction with thermodynamic relation $n = \frac{\partial p}{\partial \mu}$
 L. van Hove, *Physica* 15, 951 (1949) and *Physica* 16, 137 (1950)
- van der Waals EoS is thermodynamically consistent

$$p = \underbrace{\frac{Tn}{1-nb}}_{CE} = \underbrace{T\phi \exp\left(\frac{\mu - pb}{T}\right)}_{GCE} \text{ if } n = \frac{\partial p}{\partial \mu}, \phi = \underbrace{g \int \frac{d\vec{k}}{(2\pi)^3} e^{-\frac{\omega(\vec{k})}{T}}}_{\text{one particle thermal density}}$$

- Available volume fraction commonly used to account for hard core repulsion

motivated by VdW EoS in CE : $p = \frac{Tn}{V\Phi_{VdW}(n)}, \Phi_{VdW}(n) = 1 - bn$

GCE generalizations : $p = \frac{p_{id}(T, \mu)}{\Phi(n)}$ – **not thermodynamically consistent**

S. Typel, *Eur. Phys. J. A* (2016)52:16

- GCE is much more suitable for multicomponent mixtures than CE

Thermodynamic consistency should be provided

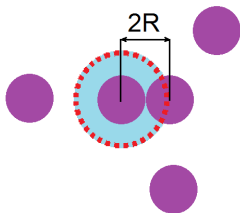
Excluded or eigen volume?

*hard core repulsion blocks
 the part of space for particle motion*

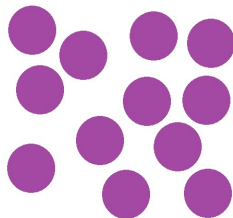


**excluded
 volume**

Low densities



High densities



translation of one particle around another

motion of particles is restricted

$$V_{excl} = \frac{1}{2} \cdot \frac{4\pi}{3} (2R)^3 = 4V_{eigen}$$

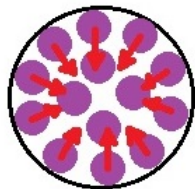
$$V_{excl} \simeq V_{eigen}$$

- replacement $\mu \rightarrow \mu - pV_{eigen}$ is based on the **high density approximation**
- VdW EoS is extrapolation of the **low density expansion**

Contradiction?

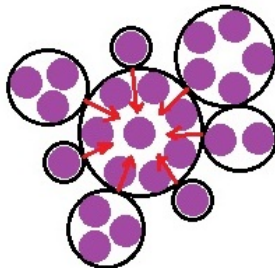
Physical origin of the induced surface tension

Vacuum



attraction of constituents
⇒ **eigen surface tension**

Medium



repulsion of clusters
⇒ **induced surface tension**



- Hard core repulsion only in part is accounted by eigen volume
- The rest corresponds to surface tension and curvature tension
Curvature tension can be accounted explicitly or implicitly
- Physical clusters tend to have spherical (in average) shape

Causality

- Causality condition: $c_{sound} \leq c_{light} = 1$, where $c_{sound}^2 = \left. \frac{dp}{d\epsilon} \right|_{\frac{\bar{s}}{n} = const}$
- VdW EoS violates causality:

$$p = T\phi(T) \exp\left(\frac{\mu - pb}{T}\right) \Rightarrow \begin{cases} p \rightarrow \mu/b \\ n \rightarrow 1/b \\ s \rightarrow T\phi'/b\phi \\ \epsilon = Ts + \mu n - p \rightarrow T^2\phi'/b\phi \end{cases} \Rightarrow c_{sound} \rightarrow \infty$$

dense packing ($\mu \rightarrow \infty$)

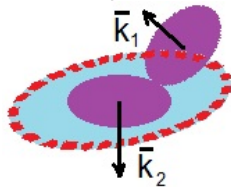
absolutely rigid objects are absent in nature due to Lorentz contraction

- Lorentz contraction of hard spheres is accounted for non-quantum VdW EoS
 K. Bugaev, Nucl. Phys. A 807 (2008)

relativistic hard core potential
 is momentum dependent



prescription is rather complicated



One should look for something
 more convenient for practical applications

High order virial coefficients

- Virial expansion of one component EoS with induced surface tension

$$p = nT \left[1 + \overbrace{4V}^{a_2} n + \overbrace{\left(16 - 18(\alpha - 1) \right)}^{a_3} V^2 n^2 \right. \\ \left. + \overbrace{\left(64 - 216(\alpha - 1) + \frac{243}{2}(\alpha - 1)^2 \right)}^{a_4} V^3 n^3 \right] + \mathcal{O}(n^5)$$

- Second virial coefficient of hard spheres $a_2 = 4V$ is reproduced always
- Third virial coefficient of hard spheres

$$a_3 = 10V^2 \Rightarrow \alpha = \frac{4}{3}, \quad a_4 = \frac{11V^3}{2} - \text{not reproduced}$$

- Fourth virial coefficient of hard spheres

$$a_4 \simeq 18.365V^3 \Rightarrow \alpha \simeq 2.537, \quad a_3 \simeq -11.666V^2 - \text{not reproduced} \\ \alpha \simeq 1.245, \quad a_3 \simeq 11.59V^2 - \text{reproduced with 16 \% accuracy}$$

**One parameter reproduces two (3rd and 4th) virial coefficients
and allows generalization for multicomponent case**

Tolman correction

- Extrapolation to high densities is not unique \Rightarrow surface and curvature terms can be treated separately

$$\frac{P}{T} = \sum_i \phi_i e^{\frac{\mu_i}{T}} \left(1 - V_i p - \overbrace{\frac{S_i}{2} \sum_j R_j \phi_j e^{\frac{\mu_j}{T}}}^{\text{surface term}} - \overbrace{2\pi R_i \sum_j R_j^2 \phi_j e^{\frac{\mu_j}{T}}}^{\text{curvature term}} \right) + O(\phi^3)$$

- Term proportional to circumference $L_i = 2\pi R_i^2$ is accounted explicitly

$$\frac{P}{T} = \sum_i \phi_i \exp\left(\frac{\mu_i - \rho V_i - \Sigma S_i - C L_i}{T}\right) - \text{pressure}$$

$$\frac{\Sigma}{T} = \sum_i \phi_i \exp\left(\frac{\mu_i - \rho V_i - \Sigma S_i - C L_i}{T}\right) \frac{R_i}{2} - \text{surface tension}$$

$$\frac{C}{T} = \sum_i \phi_i \exp\left(\frac{\mu_i - \rho V_i - \Sigma S_i - C L_i}{T}\right) \frac{R_i^2}{2} - \text{curvature tension}$$

- Tolman correction to surface tension

$$\Sigma_i^{\text{tot}} = \Sigma \left(1 - \frac{2\delta}{R_i} \right), \quad \delta = \frac{C}{\Sigma} - \text{Tolman length}$$

R.C. Tolman, J. Chem. Phys. 17, 333 (1949)

Negative values of surface tension

Surface Free Energy: $F = E - TS$

To find surface F one has to count for ALL surface deformations together with energy costs
 Can be exactly done within Hills and Dales Model for v-volume cluster:

K.A. Bugaev et al, PRE 72 (2005)

$$\underbrace{\exp\left[-\frac{\sigma_0 v^{2/3}}{T}\right]}_{\text{Energy part}} \underbrace{\exp(S)}_{\text{Entropy part}} = \underbrace{\exp\left[-\frac{\sigma_0 v^{2/3}}{T}\right]}_{\text{Sphere's Energy}} \times \left\{ 1 + \left(\frac{w_H N_H}{1 \text{ Hill}} + \frac{w_D N_D}{1 \text{ Dale}} \right) \exp\left[-\frac{\sigma_0 \Delta S_1}{T}\right] + 2, 3, \text{ etc deformations} \right\}$$

$$= \underbrace{\exp\left[-\frac{\sigma_0 v^{2/3}}{T}\right]}_{\text{Energy part}} \underbrace{\exp\left[\frac{\sigma_0 v^{2/3}}{T_c}\right]}_{\text{Entropy part}}$$

Simplest case (M. Fisher)

Also one can find supremum and infimum for surface F and surface partition

$$\sigma_0(1 - \lambda_L T) v^{\frac{2}{3}} \geq F \geq \sigma_0(1 - \lambda_U T) v^{\frac{2}{3}}, \quad \lambda_L \approx 0.28 T_c^{-1}, \quad \lambda_U \approx 1.06 T_c^{-1}$$

K.A. Bugaev & J. Elliott, UJP 52 (2007)

Thus, there is NOTHING wrong, if surface free energy $F < 0$ for high T!

This means only that entropy contribution dominates!