EoS with IST

Equation of State (EoS) with Induced Surface and Curvature Tensions (ISCT)

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- Virial expansion for IST EoS
- IST EoS for one component system
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- Virial expansion for ISCT EoS
- ISCT EoS for one component system
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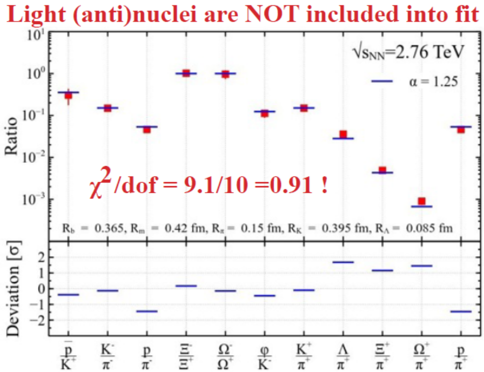
Motivation:Hadron Resonance Gas Model (HRGM)

- Succesfully describes hadron multiplicities measured in A+A collisions from $\sqrt{s_{NN}} \in [1\text{GeV}; 2.76\text{TeV}]$
- HRGM is EoS with hard core repulsion written for all known hadrons and hadronic resonances
- For given temperature T, baryonic chem. potential, strange charge chem. potential, chem. potential of isospin 3-rd projection $\Rightarrow$ thermodynamic quantities $\Rightarrow$ all charge densities, to fit data.
- HRGM allows one to find **Chemical Freeze-out** - moment after which hadronic composition is fixed and only strong decays are possible. I.e. there are no inelastic reactions.

Example of multicomponent hard-core repulsion



V. Sagun, K. Bugaev, L. Bravina, E. Zabrodin et al., Eur. Phys. J. A (2018) 54

- Radii are taken from the fit of AGS, SPS and RHIC data $\Rightarrow$ single parameter $T_{cfo} = 150 \pm 7$ MeV
- Combined fit of AGS, SPS, RHIC and LHC data gives $\chi^2_{tot}/dof \simeq 64.8/60 \simeq 1.08$. Best description achieved up to date.

Induced Surface Tension EoS

$$p = T \sum_{k=1}^{N} \phi_k \exp\left[\frac{\mu_k}{T} - v_k \frac{p}{T} - s_k \frac{\Sigma}{T}\right] \quad \rightarrow \text{Pressure}$$

$$\Sigma = T \sum_{k=1}^{N} L_k \phi_k \exp\left[\frac{\mu_k}{T} - v_k \frac{p}{T} - s_k \alpha \frac{\Sigma}{T}\right] \quad \rightarrow \text{Induced Surface Tension}$$

v_k and s_k are eigenvolume and eigensurface of hadron of sort k

$$\phi_k = g_k \int_{R^n} \frac{dp^n}{(2\pi\hbar)^n} e^{-\frac{\sqrt{p^2+m_k^2}}{T}} \rightarrow \text{thermal density}$$

Advantages:

- It allows us to go beyond the Van der Waals approximation since it reproduces 2-nd, 3-rd and 4-th virial coefficients of the gas of hard spheres.
- Number of equations does not depend on the number of different components.

Main problems to be resolved in this talk

So far, everything looks fine, but one has to:

- Derive the IST EoS in a more rigorous way
- Study whether the IST EoS can be improved further
- Find out whether IST EoS can be applyed to other objects (for example hard discs, spherocylinders and so on)

Derivation

Mean hard core radii: $\overline{R} = \frac{\sum\limits_{l} N_l R_l}{\sum\limits_{l} N_l}$

$\overline{R} \rightarrow \frac{\sum\limits_{l} \langle N_l \rangle R_l}{\sum\limits_{l} \langle N_l \rangle}$ - assumption for infinite system.

Introducing isobaric partition:

$$Z_{ISO}(T, \{\mu_k\}, V) \equiv \int_0^\infty dN e^{-\lambda V} Z_{GCE}(T, \{\mu_k\}, V)$$

One can get equation for pressure: $p = T \sum\limits_{k=1}^{n} \phi_k e^{\frac{\mu_k}{T} - \frac{pV_k}{T} - \frac{p\overline{R}S_k}{T}}$

Introducing induced surface tension with extrs α_k parameter:

$$p\overline{R} \rightarrow \Sigma S_k \rightarrow \Sigma S_k \alpha_k \text{ where } \alpha_k > 1$$

One component IST EoS

$$\begin{cases} p = T\phi_1 \exp\left[\frac{\mu_1}{T} - v_1\frac{p}{T} - s_1\frac{\Sigma}{T}\right] \\ \Sigma = TL_1\phi_1 \exp\left[\frac{\mu_1}{T} - v_1\frac{p}{T} - s_1\alpha_1\frac{\Sigma}{T}\right] \end{cases}$$

Introducing extra parameter k:

$$R_1 s_1 = 3v_1 \rightarrow L_1 s_1 = kv_1 \quad (1)$$

$$\text{Here } L_1 = \frac{k}{3}R_1 \quad (2)$$

Virial expansion

$$
\begin{aligned}
p &= T\left(A_1\rho + A_2\rho^2 + A_3\rho^3 + A_4\rho^4 + A_5\rho^5\right)\ ,\\
\Sigma &= RT\left(B_1\rho + B_2\rho^2 + B_3\rho^3 + B_4\rho^4 + B_5\rho^5\right)\ ,\\
A_1 &= 1\,.\\
A_2 &= \left(L_1 s_1 + v_1\right).\\
A_3 &= \left(L_1 s_1 + v_1\right)^2 - 2(\alpha-1)\left(L_1^2 s_1^2\right)\ ,\\
A_4 &= \left(L_1 s_1 + v_1\right)^3 + 6(\alpha-1)\left(L_1^2 s_1^2\left(L_1 s_1 + v_1\right)\right)\\
&\quad + \frac{9}{2}(\alpha-1)^2 L_1^3 s_1^3\,,\\
A_5 &= \left(L_1 s_1 + v_1\right)^4 - 12(\alpha-1)\left(L_1^2 s_1^2\left(L_1 s_1 + v_1\right)^2\right)\\
&\quad + 2(\alpha-1)^2 L_1^3 s_1^3\left(13L_1 s_1 + 9v_1\right) - \frac{32}{3}(\alpha-1)^3\left(L_1^4 s_1^4\right)\ .
\end{aligned}
$$

Hard Spheres

Compressibility

$$Z = \frac{p}{\rho T}, \qquad \rho = \left(\frac{\partial p}{\partial \mu}\right)_T$$

of gas of hard spheres very well described by Carnahan-Starling equation:

$$Z_{CS} = \frac{1 + \eta + \eta^2 - \eta^3}{(1-\eta)^3}, \qquad \eta = \rho v$$

Norman F. Carnahan and Kenneth E. Starling J. Chem. Phys. 51, 635 (1969); doi: 10.1063/1.1672048

Monte Carlo calculation for HS (van Rensburg, 1993):

$$Z = 1 + 4\eta + 10\eta^2 + 18.36\eta^3 + 28.23\eta^4 + 39.74\eta^5 + 53.5\eta^6 + 70.8\eta^7$$

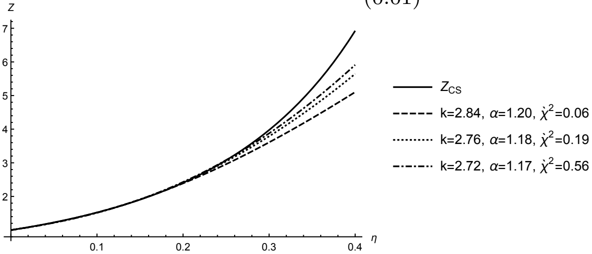
Carnahan-Starling eq. virial expansion:

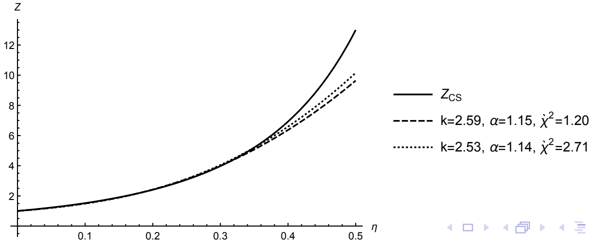
$$Z = 1 + 4\eta + 10\eta^2 + 18\eta^3 + 28\eta^4 + 40\eta^5 + 54\eta^6 + 70\eta^7$$

Hard Spheres

Z in virial expansion

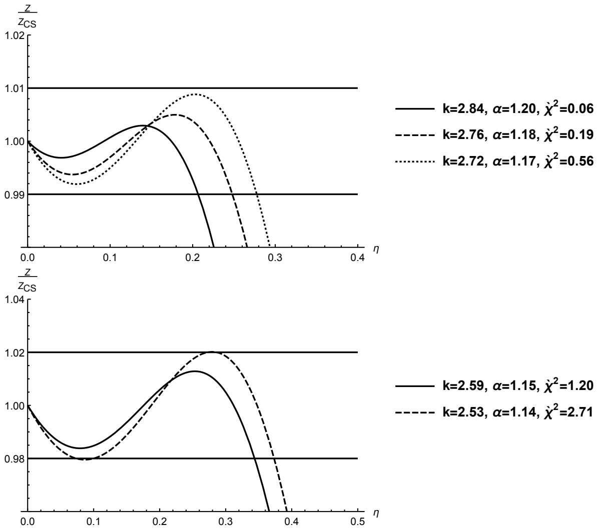
Here $\eta = \rho v_1$ - packing fraction, $\hat{\chi}^2 = \frac{\int (\frac{Z_{vir}}{Z_{CS}} - 1)^2 d\eta}{(0.01)^2}$





Hard spheres

Z to Z_{CS} ratio for virial expansion



Hard discs

Compressibility of gas of hard discs (2D case):

$$Z_S = \frac{1 + \frac{\eta^2}{8} - \frac{\eta^4}{10}}{(1-\eta)^2}$$

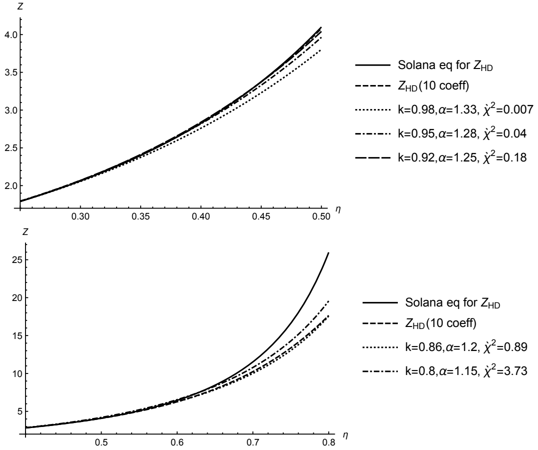
Numeric simulations for hard discs

$$Z_{VE} = 1 + 2\eta + 3.128\eta^2 + 4.25786\eta^3 + 5.3369\eta^4 + 6.36303\eta^5 + 7.35208\eta^6 + 8.31867\eta^7 + 9.27236\eta^8 + 10.2161\eta^9$$

C. Barrio and J.R. Solana, Phys. Rev. E 63, 011201 (2001)

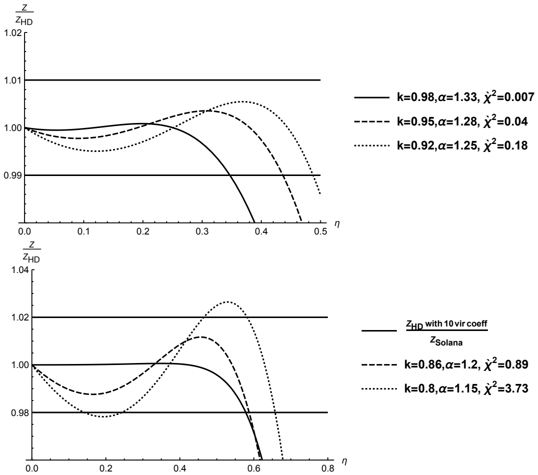
Hard discs

Z in virial expansion



Hard discs

Z to Z_S ration in virial expansion



Two component systems

Hard Spheres

Carnahan-Starling equation for multicomponent system:

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

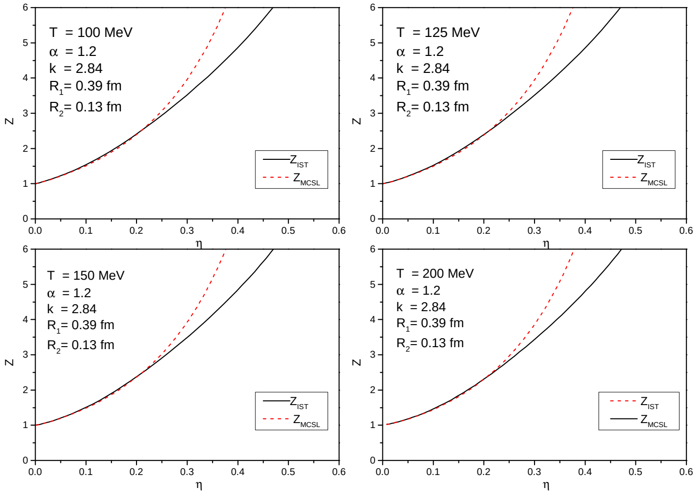
where $\xi_n = \frac{\pi}{6}\sum_{k=1}^{N}\rho_k(2L_k)^n$

IST EoS:

$$\begin{cases} p = T\sum_{k=1}^{N}\phi_k \exp\left[\frac{\mu_k}{T} - v_k\frac{p}{T} - s_k\frac{\Sigma}{T}\right] \\ \Sigma = T\sum_{k=1}^{N}L_k\phi_k \exp\left[\frac{\mu_k}{T} - v_k\frac{p}{T} - s_k\alpha\frac{\Sigma}{T}\right] \end{cases}$$

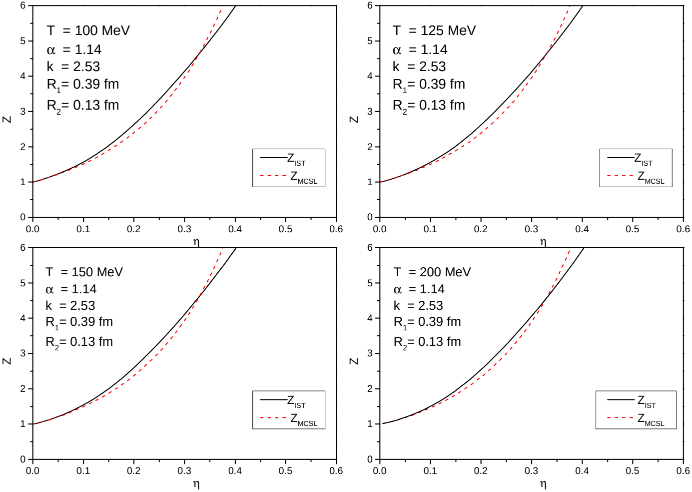
Hard Spheres

Z for different fit parameters and T



Hard Spheres

Z for different fit parameters and *T*



Hard Discs

Multicomponent Santos equation for hard discs mixture:

$$Z_{SHDM} = (1-\xi)\frac{1}{1-\eta} + \xi Z_S(\eta),$$

where

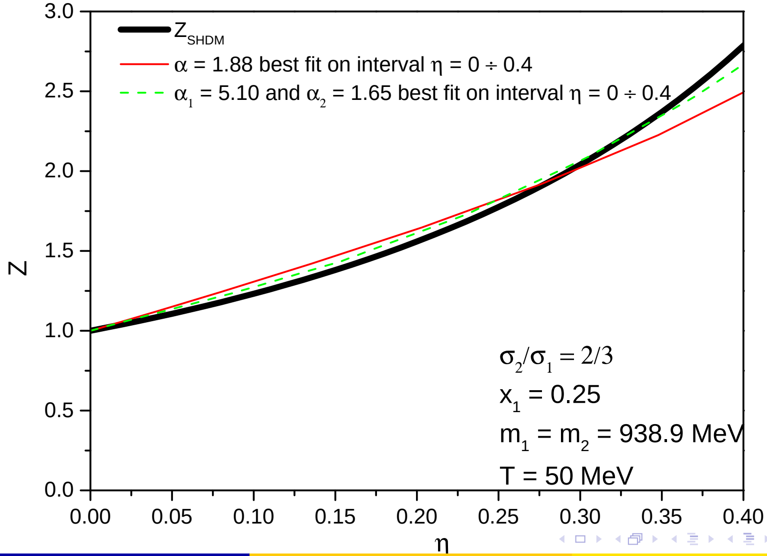
$$Z_S(\eta) = \frac{1+3\eta/\eta_0}{1-\eta/\eta_0} + \sum_{n=2}^{6}(b^n \eta_0^{n-1} - 4)\left(\frac{\eta}{\eta_0}\right)^{n-1}$$

- Woodcock's EoS, and $\xi = \overline{\sigma}^2/\overline{\sigma^2}$

Santos et al., PHYSICAL REVIEW E 66, 031202 (2002)

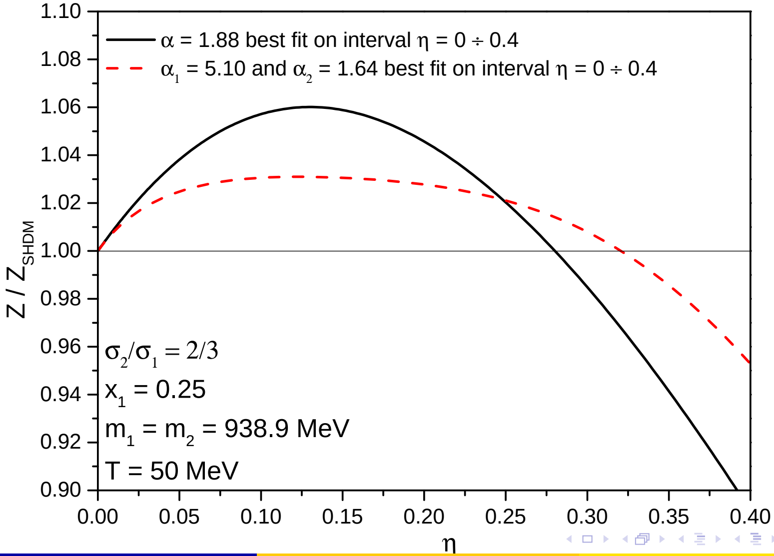
Hard Discs

Z with best fit parameters



Hard Discs

Z to Z_{SHDM} ratio with best fit parameters



IST EoS Conclusions

- Model consists of only 2 eq. for any number of components
- Can be used for different dimensions
- Relatively small number of fitting parameters
- Can be improved by intoducing extra equation for induced curvature tension

Induced Surface and Curvature Tension EoS

$$p = T\sum_{k=1}^{N}\phi_k \exp\left[\frac{\mu_k}{T} - v_k\frac{p}{T} - s_k\frac{\Sigma}{T} - c_k\frac{K}{T}\right]$$

$$\Sigma = AT\sum_{k=1}^{N}L_k\phi_k \exp\left[\frac{\mu_k}{T} - v_k\frac{p}{T} - s_k\alpha\frac{\Sigma}{T} - c_k\frac{K}{T}\right]$$

$$K = (1-A)T\sum_{k=1}^{N}L_k^2\phi_k \exp\left[\frac{\mu_k}{T} - v_k\frac{p}{T} - s_k\alpha\frac{\Sigma}{T} - c_k\beta_k\frac{K}{T}\right]$$

Here $c_k = \frac{s_k}{L_k}$

Hard Spheres

Virial expansion

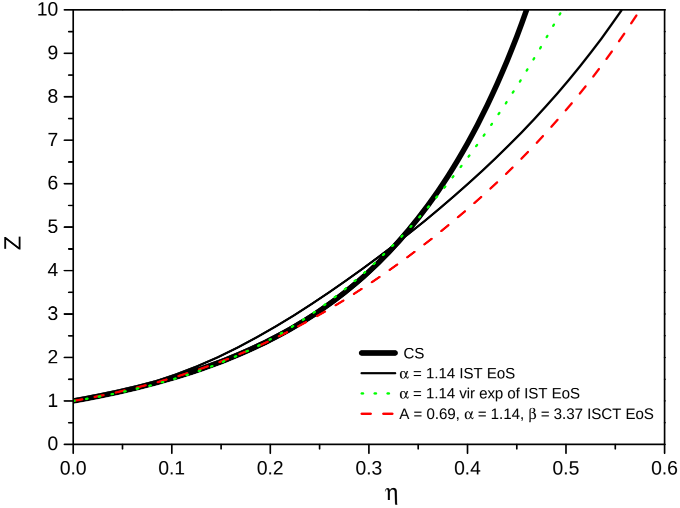
With virial expansion of ISCT EoS

$$p = T\left(A_1\rho + A_2\rho^2 + A_3\rho^3 + A_4\rho^4 + A_5\rho^5\right)$$
$$\Sigma = ART\left(B_1\rho + B_2\rho^2 + B_3\rho^3 + B_4\rho^4 + B_5\rho^5\right)$$
$$K = (1-A)RT\left(C_1\rho + C_2\rho^2 + C_3\rho^3 + C_4\rho^4 + C_5\rho^5\right)$$

we can exactly reproduce 5 virial expansion coefficients of Carnahan-Starling equation with $A = 0.68, \alpha = 1.14, \beta = 3.37$

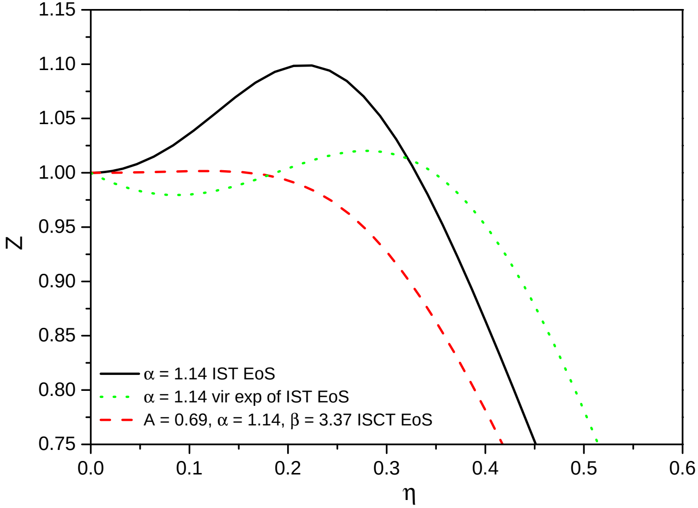
Hard Spheres

Z with different parameters



Hard Spheres

Z to Z_{CS} ratio



Conclusions

- 3 equations for any number of components
- Greatly describes CS and Solana equations just with few parameters
- Can be used for different dimensions