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Rarefaction waves in Van Der Waals Fluids

Albert Yuen
UC Berkeley – Department of Nuclear Engineering

John Barnard
Lawrence Livermore National Lab

Richard More
Lawrence Berkeley National Lab

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Introduction – Warm Dense Matter

Warm Dense Matter:

$$[0.01\rho_{solid} < \rho < 10\rho_{solid}]$$
$$[0.01\, eV < T < 10\, eV]$$

Where to find Warm Dense Matter?

A few examples:

Ablation of a metal by a laser or an ion beam

In the core of gaseous planets

During the early stages of an inertial confined fusion implosion

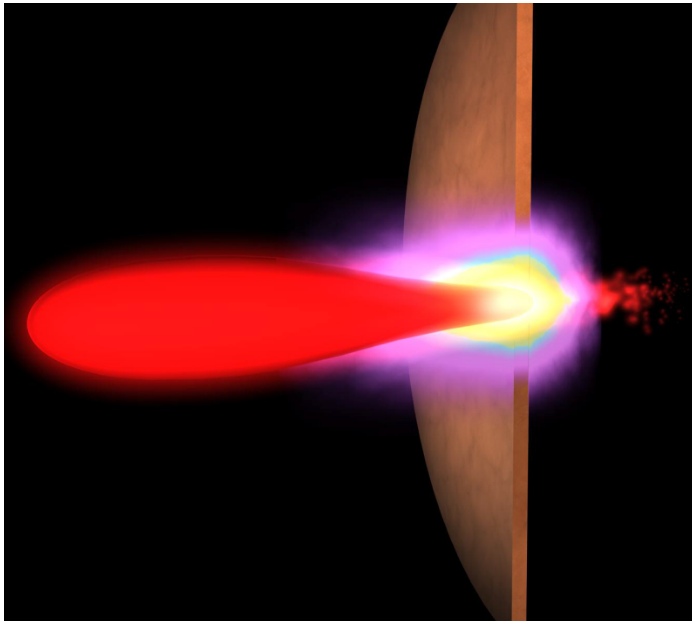
<u>One area of interest:</u>
Transition from a high temperature solid or liquid into the vapor state.

Motivation

- **For many material, the critical point above with there is no distinction between liquid and vapor is poorly known for many materials.**
- **Need to develop methods to experimentally measure these quantities.**
- **In this presentation, the 1D isentropic expansion into vacuum of a uniform semi-infinite layer of a heated metal in the WDM regime is studied semi-analytically.**

Geometry of our problem

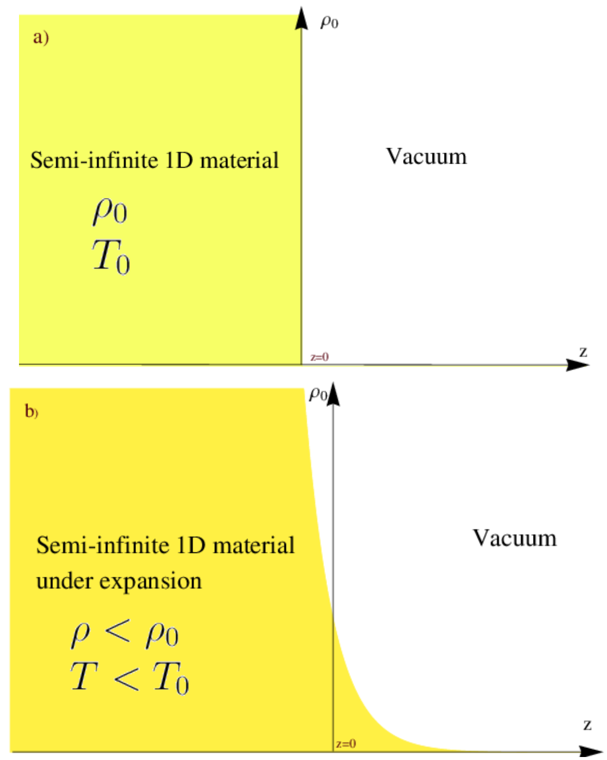
Real case:



Ion beam shining through a metallic foil.

Our case (Schematic):

$$t = 0$$



$$t > 0$$

Hydrodynamics of the VDW Fluid – Hydromotion (I)

- **1D cartesian Eulerian fluid equations**
- **No mass source/sink**
- **Non-viscous and neutral fluid**

Continuity equation: $$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial t} = 0$$

Momentum equation: $$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x}$$

$\rho : mass\ density$

$v : fluid\ velocity$

$t : time$

$z : longitudinal\ coordinate$

Hydrodynamics of the VDW Fluid – Hydromotion (II)

Let $\begin{aligned} P &= v + I \\ M &= v - I \end{aligned}$ **where** $I(\rho) = \int_{\rho_0}^{\rho} \frac{c_s(\rho')}{\rho'} \, \mathrm{d}\rho'$ **and** $c_s{}^2(\rho) = \left.\frac{\partial p}{\partial \rho}\right|_s$

The continuity and momentum equation can be transformed to:

$$\frac{\partial P}{\partial t} + (v + c_s)\frac{\partial P}{\partial z} = 0 \qquad \frac{\partial M}{\partial t} + (v - c_s)\frac{\partial M}{\partial z} = 0$$

As there is no natural time or space scale, let $\xi = \frac{z}{t}$ **. Then:**

$$(v + c_s - \xi)P'(\xi) = 0 \qquad (v - c_s - \xi)M'(\xi) = 0$$

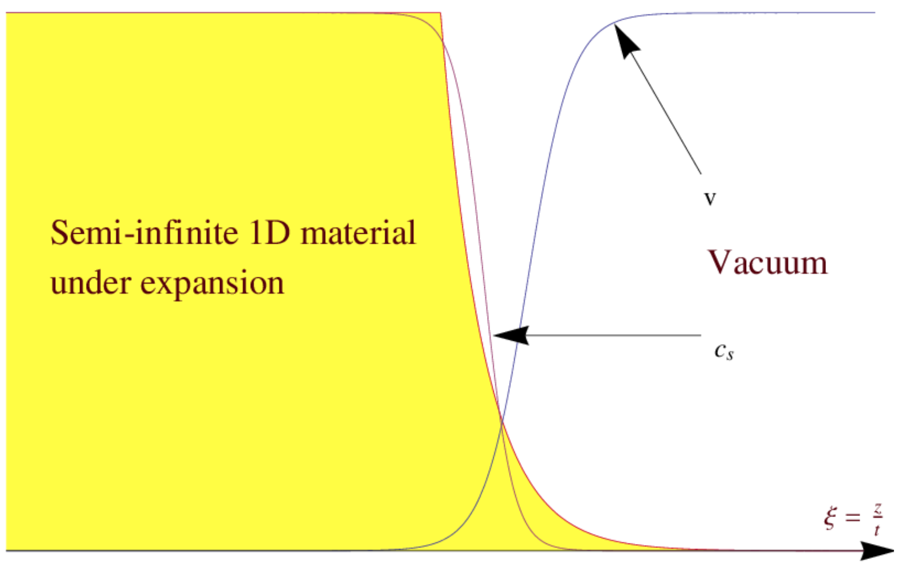
1. Zelodovich and Raizer, "Physics of High Temperature Hydodynamics Phenomena," (1962) 2. Anisimov, S.I. et al, Applied Physics A 69, 617 - 620 (1999) 3. R. More, T. Kato, H.Yoneda, NIFS Report (2005)

Hydrodynamics of the VDW Fluid – Hydromotion (III)

Solutions:

$$(v - c_s - \xi) = 0 \quad and \quad P'(\xi) = 0$$

$$\cancel{or \quad (v + c_s - \xi) = 0 \quad and \quad M'(\xi) = 0}$$



Boundary conditions:

$$For\ \xi < 0,\ c_s > 0\ and\ v \to 0$$

$$\cancel{For\ \xi > 0,\ c_s \to 0\ and\ v > 0}$$

$$\Downarrow$$

$$(v - c_s - \xi) = 0 \quad and \quad P'(\xi) = 0$$

$$\Downarrow$$

$$P(\xi) = constant \Rightarrow v(\rho) = -I(\rho) + constant$$

$$\Downarrow$$

$$@\ t=0, \rho=\rho_0 \Rightarrow v(\rho_0)=0 \Rightarrow constant=0$$

$$\boxed{\xi(\rho) = -I(\rho) - c_s(\rho)} \Leftarrow$$

But what are *I(ρ)* and *cs(ρ)* ? *Need Equation of State (EOS)*

Equation of State: the VDW model

Why VDW? Why not perfect gas? Or more advanced EOS such as QEOS?

- **Exhibits phase-transition behavior: first order gas-liquid transition**
- **Mathematically simple**

The VDW EOS is based on the perfect gas law but takes into account:

- **The non-zero size of the molecules**
- **The attraction between them**

Equation of State: the VDW model

VDW EOS: $$p = \frac{\rho k T}{A m_{amu}(1-b\rho)} - a\rho^2$$

$$S = \frac{k}{A m_{amu}} ln(A m_{amu} \frac{1-b\rho}{\rho\lambda^3}) \quad where \quad \lambda = \sqrt{\frac{h^2}{2\pi A m_{amu} k T}}$$

p : *pressure*
ρ : *mass density*
T : *temperature*
S : *entropy density*
ϵ : *energy density*

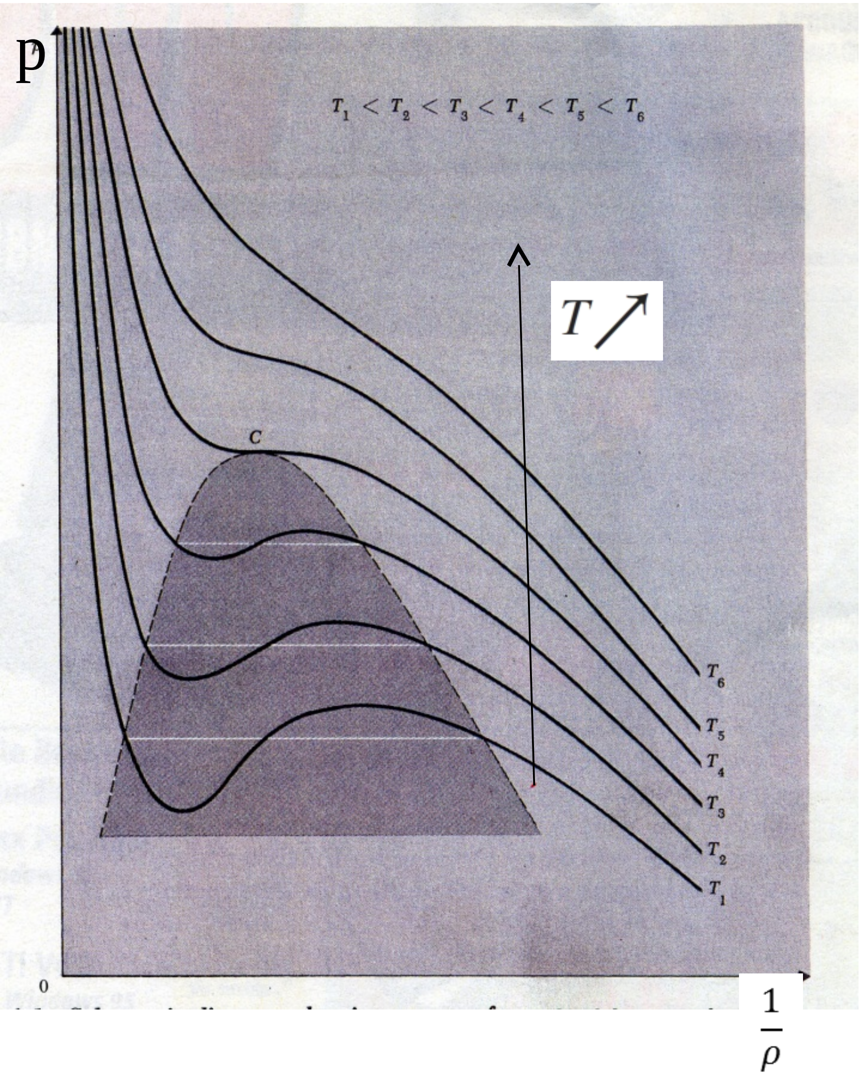
m_{amu} : *atomic mass unit*
A : *mass number*
a, b : *VDW parameters*

$$\epsilon = \frac{3}{2}\frac{kT}{A m_{amu}} - a\rho$$

For this EoS, the sound speed can be imaginary: $c_s^2(\rho) \equiv \left.\frac{\partial p}{\partial \rho}\right|_s$

$\frac{\partial P}{\partial V} > 0$ leads to instability

Maxwell construction replaces unstable region on isotherm curve with constant pressure 2-phase region where liquid and vapor coexist.



The liquid/gas border is determined by setting $pl = pg$ and $\int_{V_l}^{V_g} (p - p_g) dV = 0$

Dimensionless VDW EOS (I)

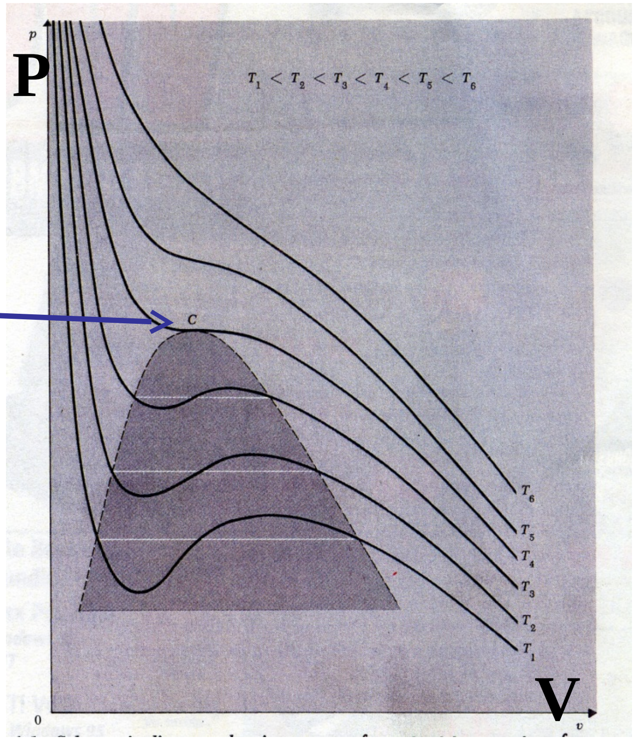
In order to treat the problem more generally,
we use dimensionless parameters.
We choose the critical parameters as the scaling parameters.

$$\frac{\partial p}{\partial \rho} = \frac{\partial^2 p}{\partial \rho^2} = 0$$

$$\rho_c = \frac{1}{3b}$$

$$p_c = \frac{1}{27}\frac{a}{b^2}$$

$$\frac{kT_c}{Am_{amu}} = \frac{8}{27}\frac{a}{b}$$



F. Reif, "Fundamentals of statistical and thermal physics"

define a characteristic sound speed ${c_{s,0}}^2 = \frac{p_c}{\rho_c}$ and a characteristic energy $\epsilon_0 = \frac{8}{27}\frac{a}{b}$

Dimensionless VDW EOS (2)

Define: $\tilde{\rho} = \frac{\rho}{\rho_c}$ $\tilde{p} = \frac{p}{p_c}$ $\tilde{T} = \frac{T}{T_c}$ $\tilde{c_s}(\tilde{\rho}) = \frac{c_s(\rho)}{c_{s,0}}$ $\tilde{\epsilon}(\tilde{\rho}, \tilde{T}) = \frac{\epsilon(\rho, T)}{\epsilon_0}$

A dimensionless form of the VDW EOS can be rewritten:

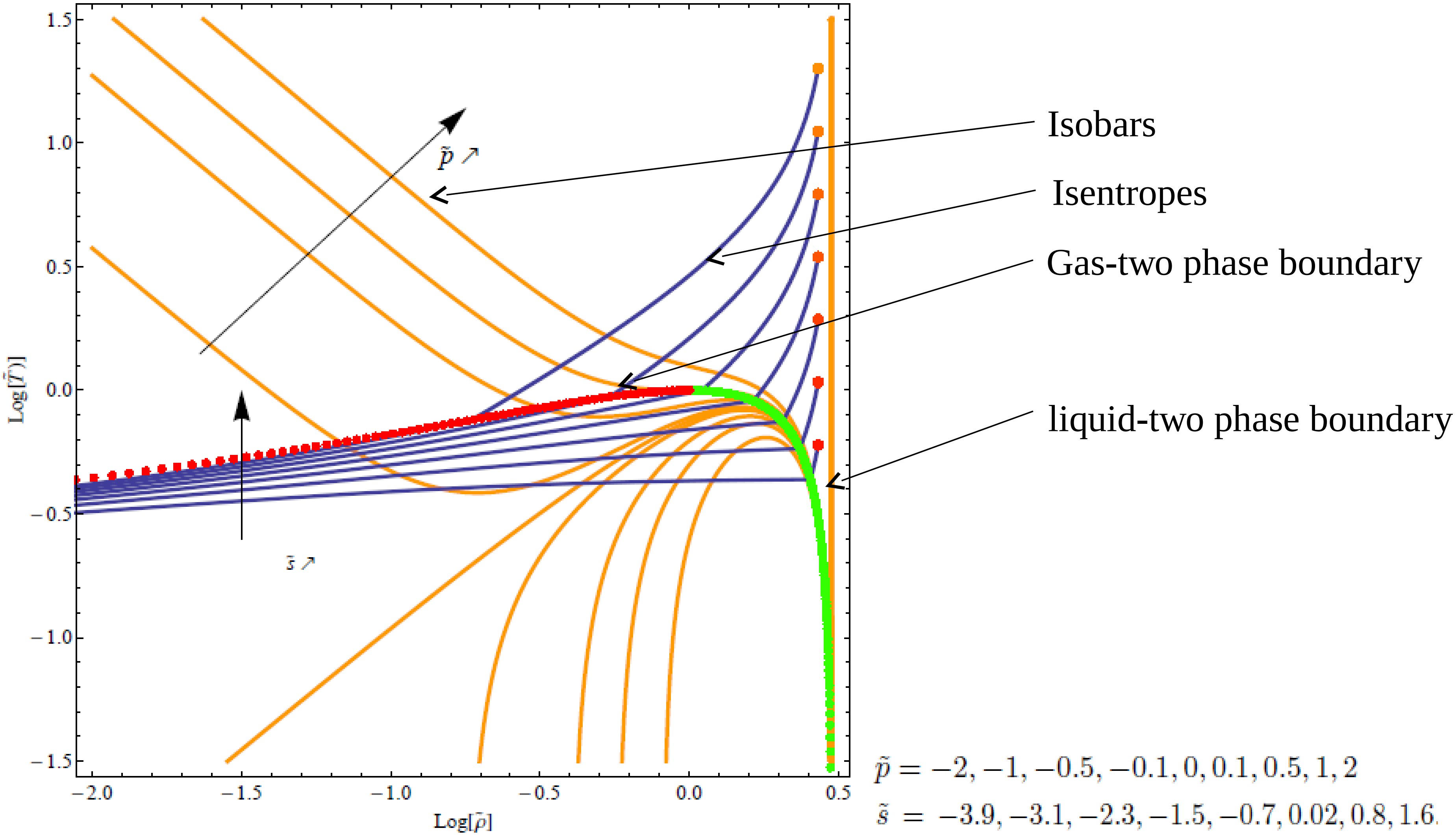
$$\tilde{p} = 8\frac{\tilde{\rho}\tilde{T}}{3-\tilde{\rho}} - 3\tilde{\rho}^2$$

$$\tilde{s} = \frac{s - s_c}{\frac{k}{Am_{amu}}} = ln(\frac{3-\tilde{\rho}}{2\tilde{\rho}}\tilde{T}^{\frac{3}{2}}) \quad where \quad s_c = S(\rho_c, T_c)$$

$$\tilde{\epsilon} = \frac{3}{2}(\tilde{T} - \frac{9}{12}\tilde{\rho})$$

+ Maxwell Construction

Dimensionless VDW EOS (II) + Maxwell Construction



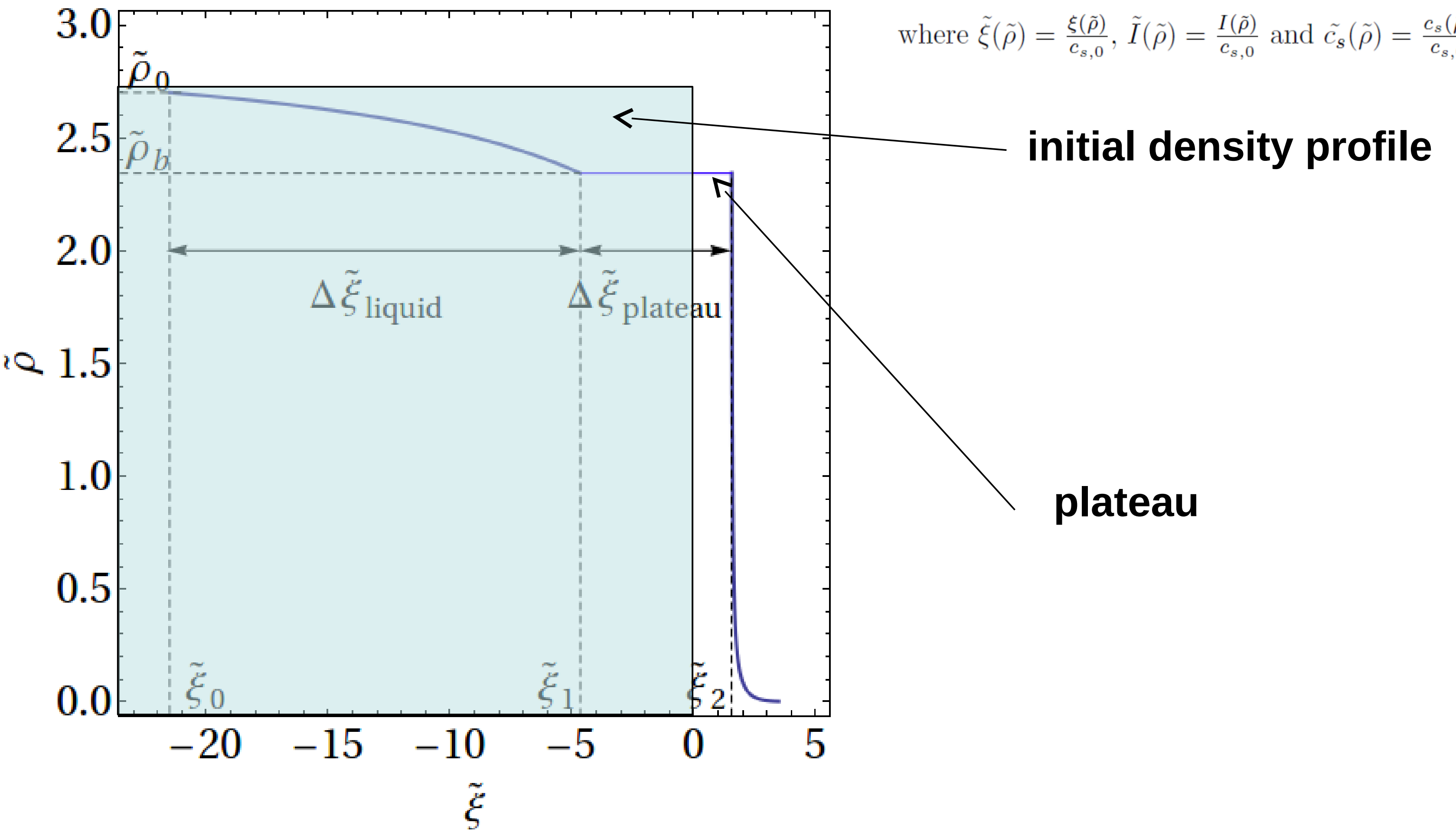
$\tilde{p} = -2, -1, -0.5, -0.1, 0, 0.1, 0.5, 1, 2$

$\tilde{s} = -3.9, -3.1, -2.3, -1.5, -0.7, 0.02, 0.8, 1.6.$

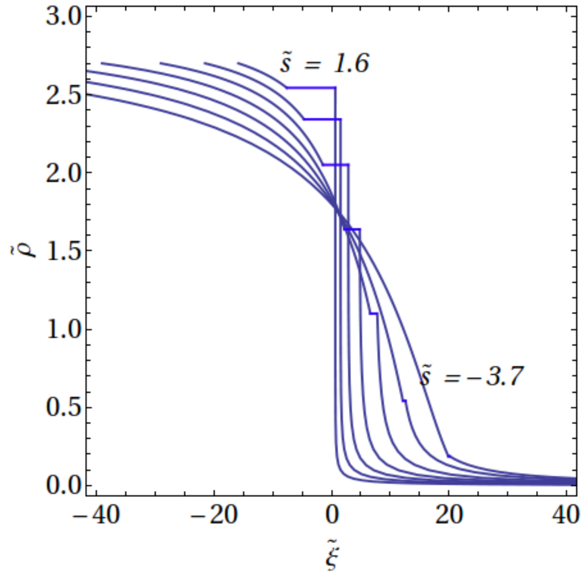
Results: a universal set of dimensionless curves (I)

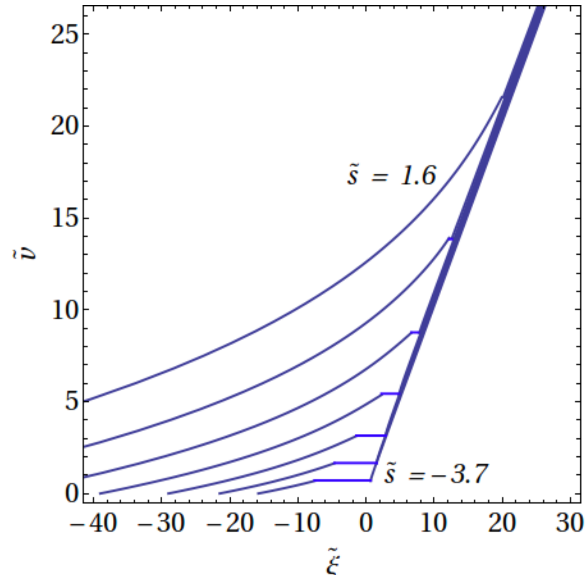
Dimensionless hydrodynamics equation: $\tilde{\xi}(\tilde{\rho}) = -\tilde{I}(\tilde{\rho}) - \tilde{c_s}(\tilde{\rho})$

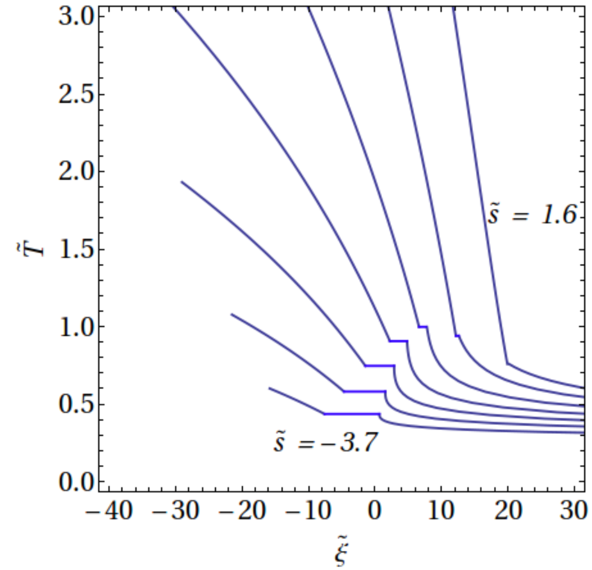
where $\tilde{\xi}(\tilde{\rho}) = \frac{\xi(\tilde{\rho})}{c_{s,0}}$, $\tilde{I}(\tilde{\rho}) = \frac{I(\tilde{\rho})}{c_{s,0}}$ and $\tilde{c_s}(\tilde{\rho}) = \frac{c_s(\tilde{\rho})}{c_{s,0}}$

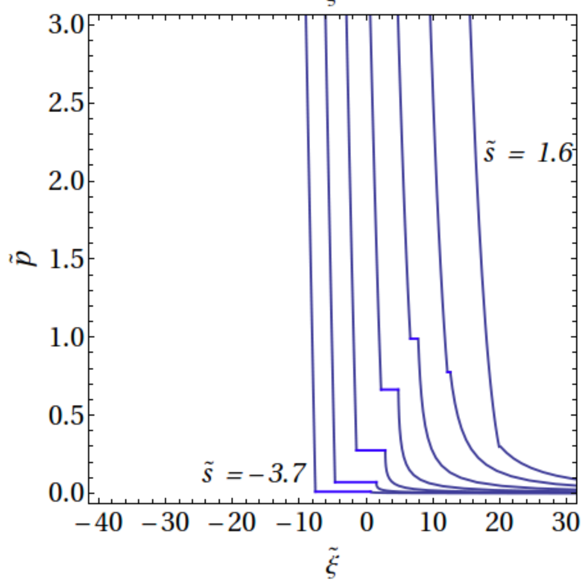


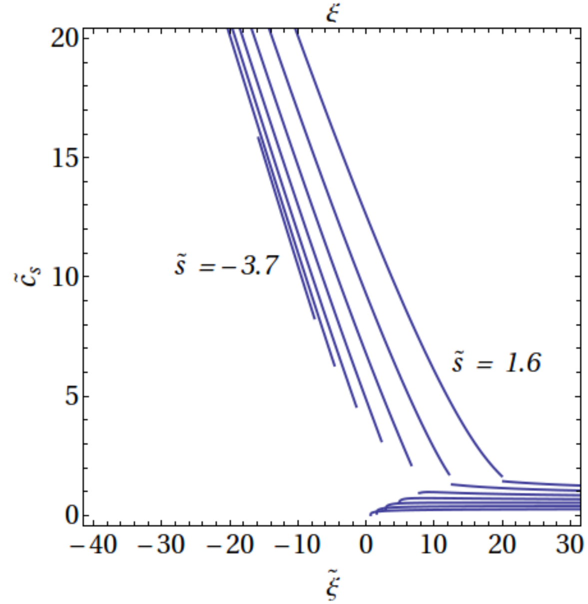
Results: a universal set of dimensionless curves (II)











$\tilde{\rho}_0 = 2.7$

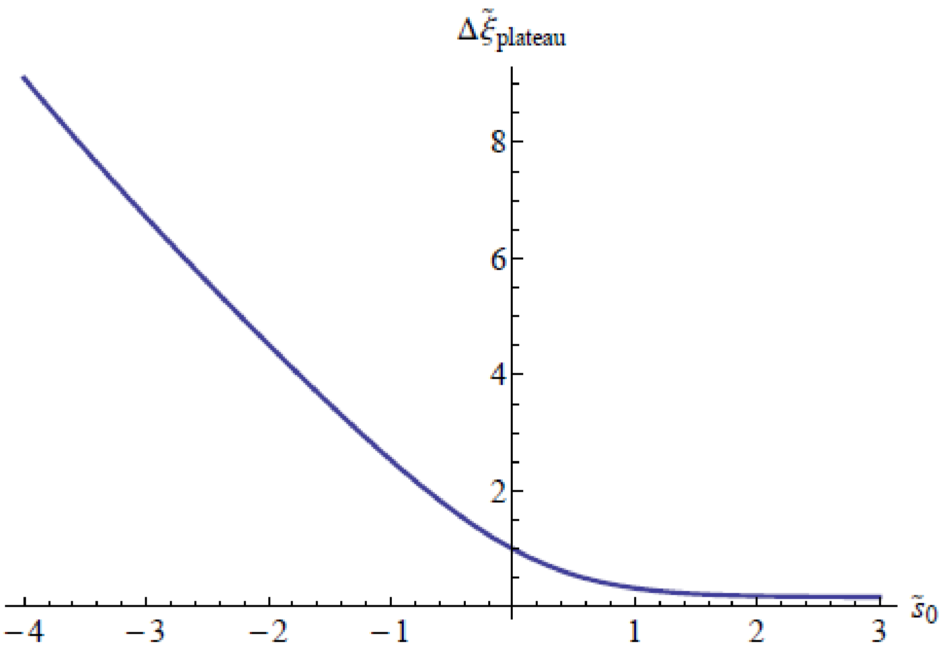
$\tilde{T}_0 = 0.5, 0.84, 1.43, 2.43, 4.11, 6.97, 11.9, 20$

$\tilde{s} = -3.9, -3.1, -2.3, -1.5, -0.7, 0.02, 0.8, 1.6$

Results: a universal set of dimensionless curves (III)

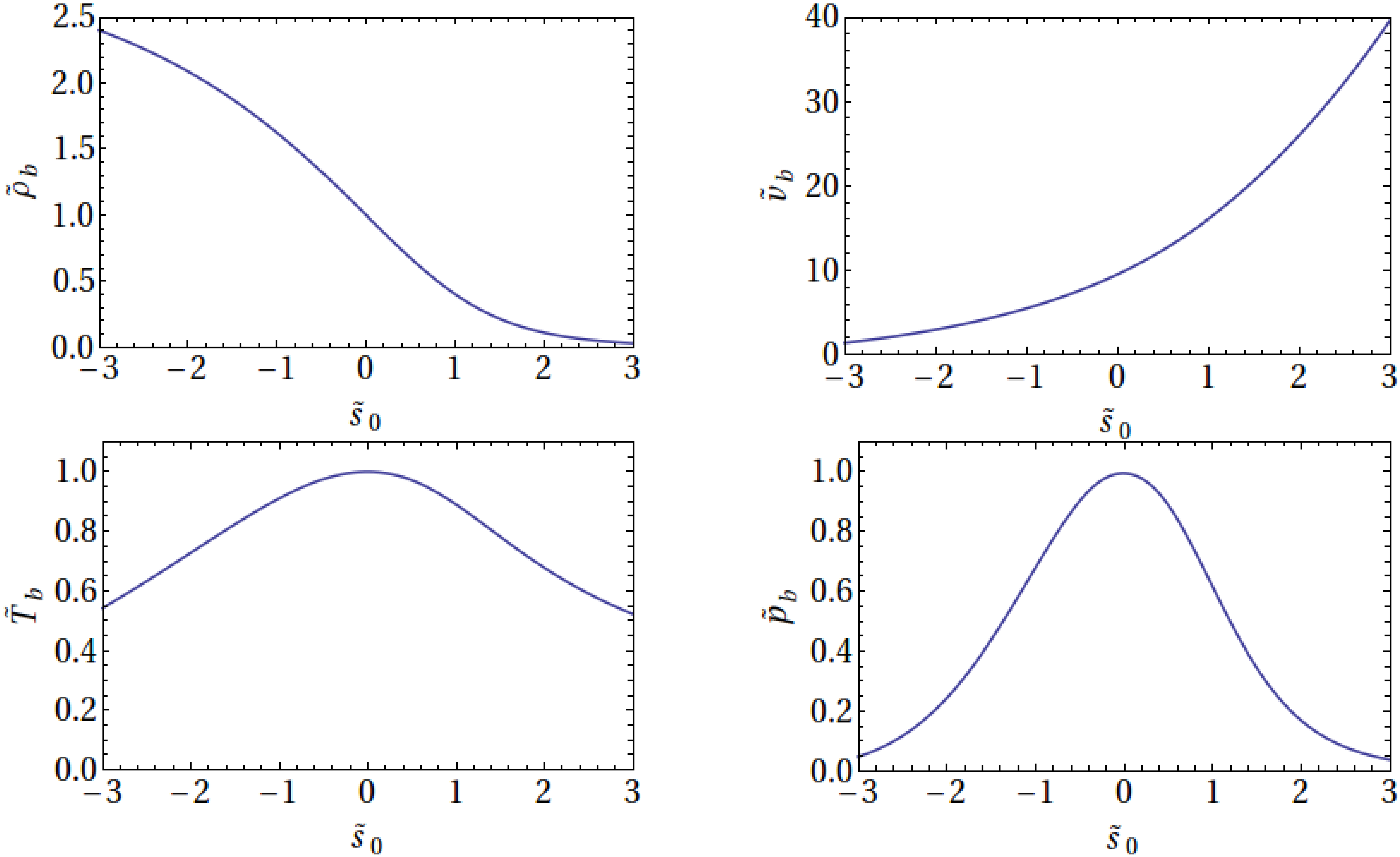
A surprising result:

The length of the plateaus depends ONLY on the initial entropy!



Results: a universal set of dimensionless curves (IV)

All the values at the the boundary of the liquid and the two-phase regions depend on the initial entropy.

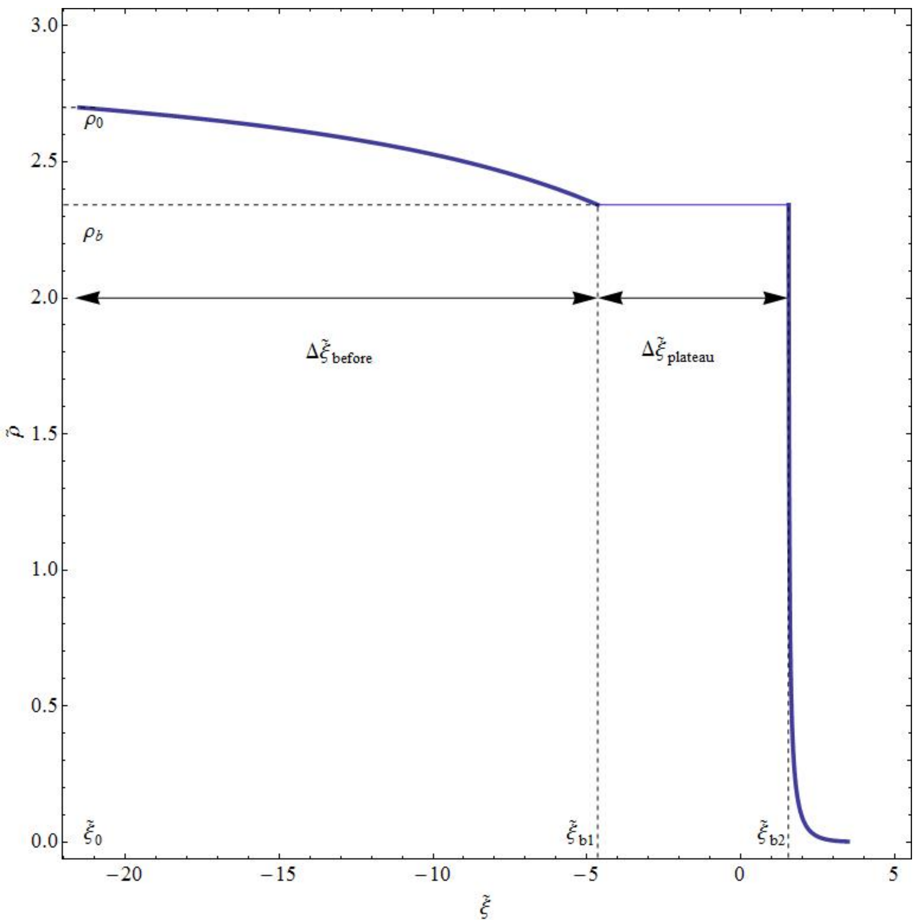


Method determining critical and initial parameters (I)

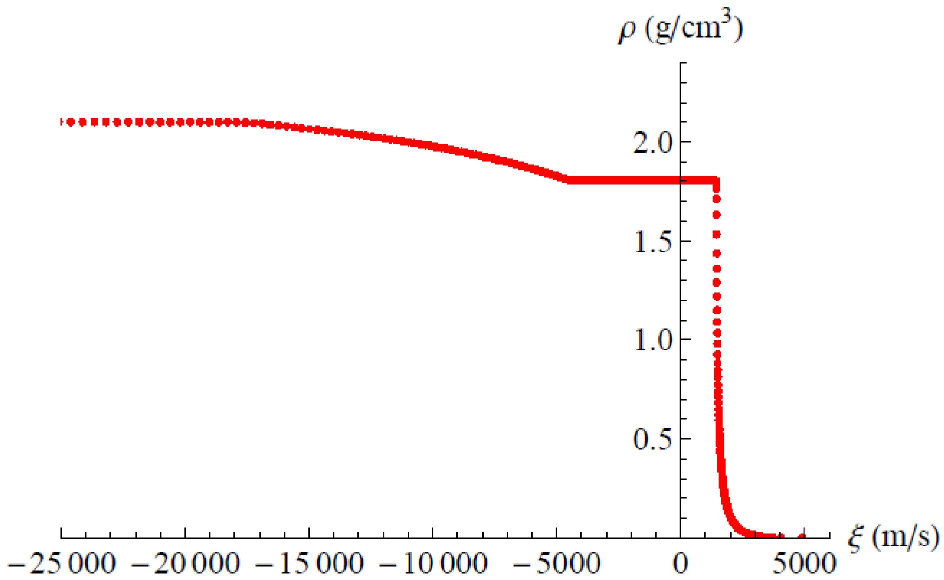
- **The dimensionless set of curves are theoretically applicable to any material**
- **The length of the plateaus in the previous section depends ONLY on the initial entropy.**

The critical and initial parameters from a single (dimensionful) density profile can be determined.

Method determining critical and initial parameters (II)



Dimensionless



Dimensionful

Method determining critical and initial parameters (III)

A dimensionful density profile matches only ONE dimensionless density profile by multiplying constant.

1. **From the dimensionful density profile, we get the two invariants** $R_\rho = \frac{\rho_0}{\rho_b} = \frac{\tilde{\rho}_0}{\tilde{\rho}_b}$ $\quad R_\xi = \frac{\Delta\xi_{plateau}}{\Delta\xi_{before}} = \frac{\Delta\tilde{\xi}_{plateau}}{\Delta\tilde{\xi}_{before}}$
2. **For any couple** (R_ρ, R_ξ) **, only one solution** $(\tilde{\rho}_0, \tilde{s}_0)$ **can be found.**
3. **This provides critical parameters:**

$$\rho_c = \frac{\rho_0}{\tilde{\rho}_0}$$

$$kT_c = \frac{8}{3}\left(\frac{\Delta\xi_{plateau}}{\Delta\tilde{\xi}_{plateau}}\right)^2 A m_{amu}$$

4. **…and initial parameters:**

$$kT_0 = kT_c\left(\frac{2\tilde{\rho}_0}{3-\tilde{\rho}_0} e^{\tilde{s}}\right)^{\frac{2}{3}}$$

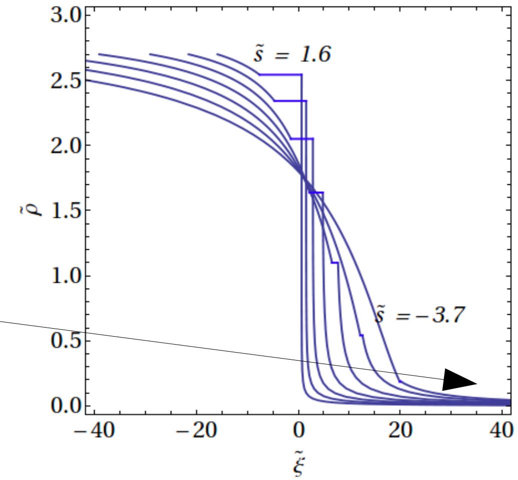
Robustness of the algorithm

If an offset of ξ_1 is introduced, the relevant calculated parameters change. The following table shows how robust this algorithm is.

T_0	0.5 eV	1 eV	2 eV
$\frac{\partial \rho_c}{\partial \xi_1}$	-0.320136	-0.242898	-0.645116
$\frac{\partial T_c}{\partial \xi_1}$	-3.85929	-3.08899	-6.60853
$\frac{\partial T_0}{\partial \xi_1}$	-3.78751	-4.9355	-4.19571

Note: the fluid velocity v (hence ξ) diverges and a cut-off must be used

Remember that $v(\rho) = -I(\rho) = -\int_{\rho_0}^{\rho} \frac{c_s(\rho')}{\rho'}\,\mathrm{d}\rho'$

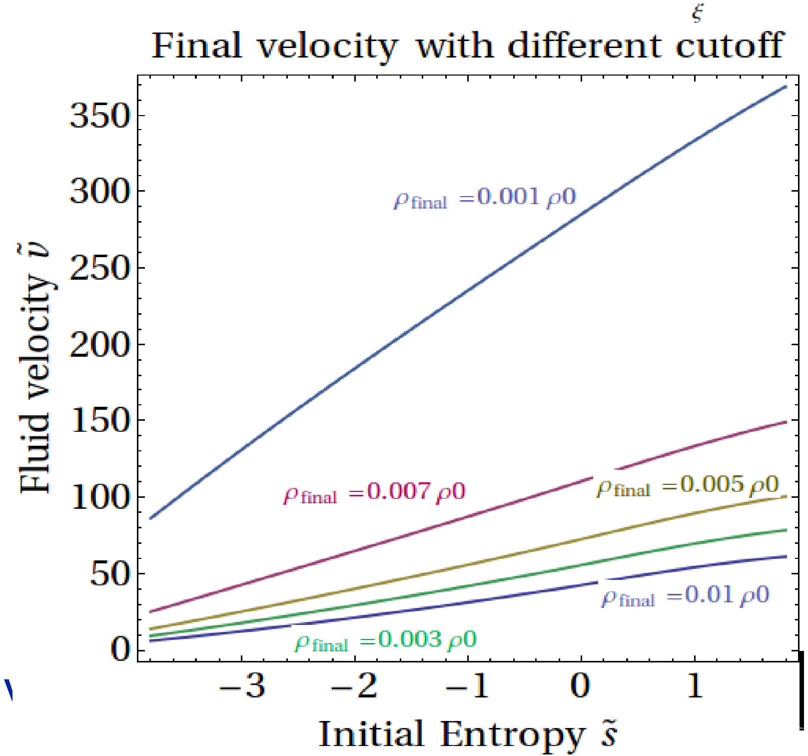


Logically, $\rho \to 0$.

However, $v(\rho) \to +\infty$ when $\rho \to 0$.

A cut-off must be introduced such as:

$$v(\rho) = -\int_{\rho_0}^{\rho_{final}} \frac{c_s(\rho')}{\rho'}\,\mathrm{d}\rho'$$



Conclusions

The universal set of dimensionless curves give us insight in experimental results.

We developed a method to find critical and initial parameters from a single density snapshot. This method is applicable for a snapshot of velocity profile, temperature profile or pressure profile.

The next step would be to study a 1D slab geometry (and not a 1D semi-infinite geometry). Two rarefaction waves from each side of the slab would meet and overlap, giving birth to complex waves.