# Equation of state of the H-He mixture under solar conditions

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# Outline

1. **Introduction**

2. **Equations of state derived in the physical approach**

   a) Virial equation

   b) OPAL equation of state (EOS) and the **act**ivity **ex**pansion (*ACTEX*) method

3. **The screened cluster (SC) method**

   Relation to ACTEX/OPAL

   Results on the equation of state:

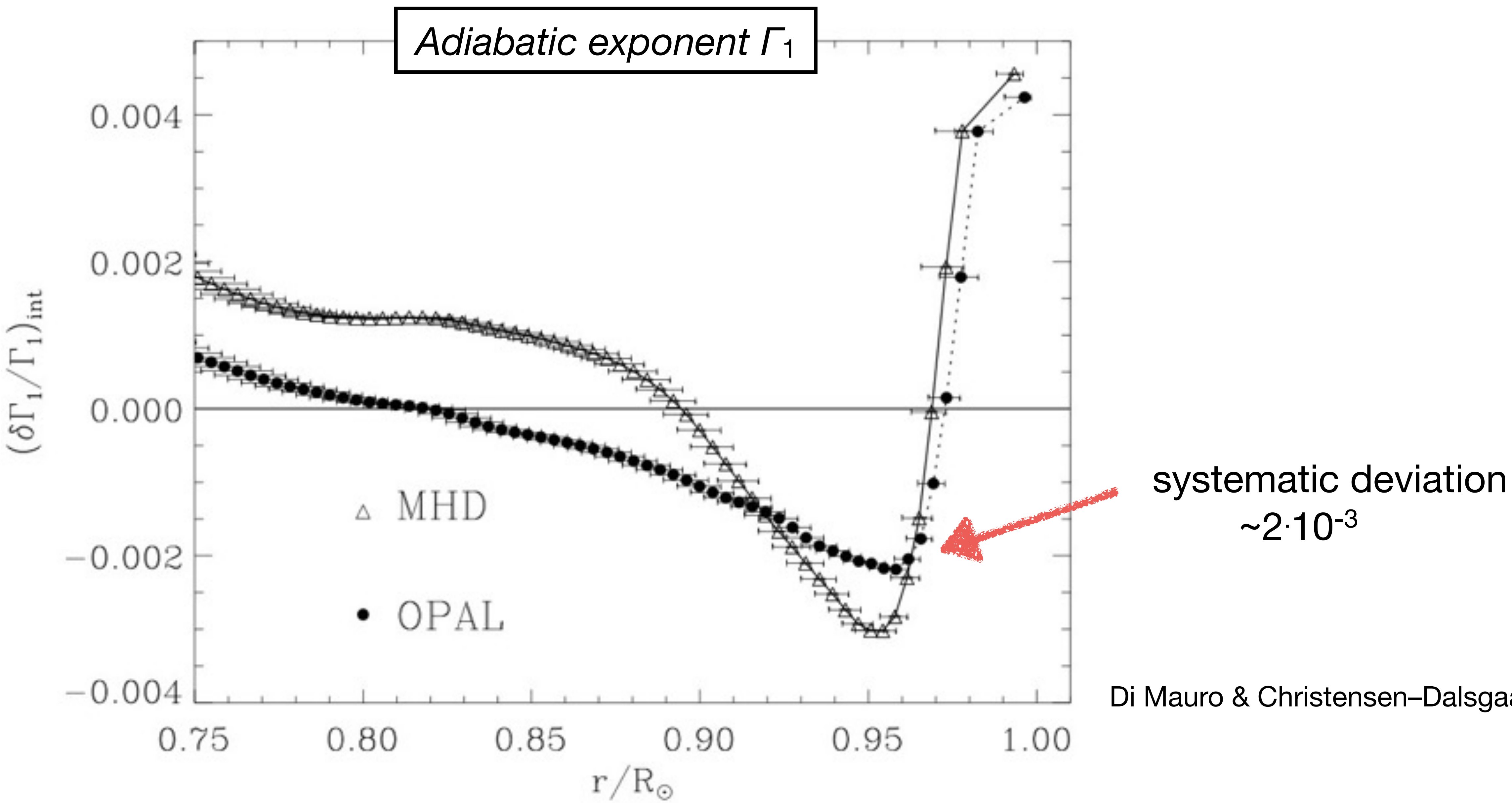
   - **SC3 EOS** (H-He mixtures)
   - **SLT expansion of the EOS** (pure H gas at *any ionization ratio*)

4. **Conclusions**

# 1. Introduction: Equation of state for the H-He gas

- Important ingredient in stellar modeling and helioseismology.

- Helioseismic inversions are sensitive to the EOS.




Di Mauro & Christensen–Dalsgaard (2000)

***Can inaccuracies in the OPAL EOS partly explain the systematic deviations ?***

# 2. Equations of state in the physical approach

**Hydrogen-helium gas (in the physical approach):**

Quantum gas of point particles, electrons (e), protons (p) and helium nuclei ($\alpha$), interacting only via the Coulomb interaction $e_i e_j / |\boldsymbol{r}_i - \boldsymbol{r}_j|$.

- Recombination/ionization phenomena for atoms and ions: H, He, $He^+$, $He^{2+}$, $H_2^+$, $H^-$…
- Screening effects:

  *Screened Coulomb interaction* $\phi(\vec{r}) = \dfrac{e^{-\kappa|\vec{r}|}}{|\vec{r}|}$

  *Modification of the atomic and molecular spectra*

## a) Virial equation of state

Exact expansion of the **pressure *P*** at low-densities:

$$\beta P = \sum_{\gamma=e,p,\alpha} \rho_\gamma - \frac{\kappa^{3/2}}{24\pi} + \sum_{\gamma_1}\sum_{\gamma_2} B_{\gamma_1,\gamma_2}(T)\,\rho_{\gamma_1}\rho_{\gamma_2} + \text{term order } \rho^{5/2} + O(\rho^3)$$

($\beta = 1/k_B T$)

ideal gas law (fully ionized)

exact treatment of 2-body effects (H and $He^+$)

3-body effects neglected (He, $H_2^+$, …)

Ebeling (1969)
Kraeft *et al*. (1986)
Alastuey & Perez (1992)

Valid if gas is weakly coupled and almost fully ionized (→ eq. applies in inner regions of the Sun).

# 2. **Equations of state** in the physical approach

## b) The OPAL EOS

Grand-canonical ensemble: variables $\{\mu_\gamma\}$, $V$, $T$

**Pressure:** $P = k_B T \lim_{V\to\infty} \frac{\ln(\Xi)}{V}$ where $\Xi(\{\mu_\gamma\}, V, T)$ = grand-canonical partition function

→ $P(\{z_\gamma\}, T)$ with $z_\gamma = e^{\beta\mu_\gamma}$ = **activity** of particles of species $\gamma$ ($\gamma$ = e, p or $\alpha$)

**Expand** $P\sim\ln(\Xi)$ in an **activity** series ( $\{z_\gamma\} \ll 1$ if gas not too dense)

→ Activity expansions:
- pressure: $P(\{z_\gamma\},T) = \ldots$
- densities: $\rho_\gamma(\{z_\gamma\},T) = \ldots$

⇒ Equation of state $\boldsymbol{P(\{\rho_\gamma\}, T)}$

The **ACTEX** method is an approximate, somewhat heuristic, activity expansion of $P$.
The precise formulas for the approx./models used in ACTEX are undisclosed.

> " The **ACTEX (OPAL) method** avoids the complexities of a fully quantum mechanical treatment by first carrying out a classical analysis and then replacing classical expressions with their quantum analogues.

F. Rogers [*High Pressure Research* **16** (2000), p.359]

# 3. The Screened Cluster (SC) method

- Feynman-Kac **path integral representation** of the quantum Coulomb system → equiv. classical system of ring polymers.
- Structure of the quantum activity series:

$$\beta P = \sum_{\gamma=e,p,\alpha} z_\gamma + \text{term order } z^{3/2} + \sum_{\gamma_1,\gamma_2} C_{\gamma_1,\gamma_2}(T;\kappa)\, z_{\gamma 1} z_{\gamma 2} + \text{term order } z^{5/2} + \sum_{\gamma_1,\gamma_2,\gamma_3} C_{\gamma_1,\gamma_2,\gamma_3}(T;\kappa)\, z_{\gamma 1} z_{\gamma 2} z_{\gamma 3} + \ldots$$

coeff. = screened **cluster functions**

The screening length $1/\kappa$ depends itself on $T$ and $\{z_\gamma\}$

Exact (path integral) formulas for these screened cluster functions

2-body effects ($C_{1,2}(T,\kappa)$) : charge-charge interactions, atom **H**, ion **$He^+$** *(with modified spectrum)*

3-body effects ($C_{1,2,3}(T,\kappa)$): 3-charge inter., atom-charge interactions, atom **He**, ions **$H_2^+$, $H^-$**

★ **Numerical calculation of the path integrals** for 2- and 3-body cluster functions

→ **SC3** EOS (accurate *tabulated* cluster functions at finite density)

★ Low-density low-temperature analysis of the activity series in the case of a **pure hydrogen** gas

→ **SLT expansion** of the EOS (*analytical* cluster functions in vacuum)

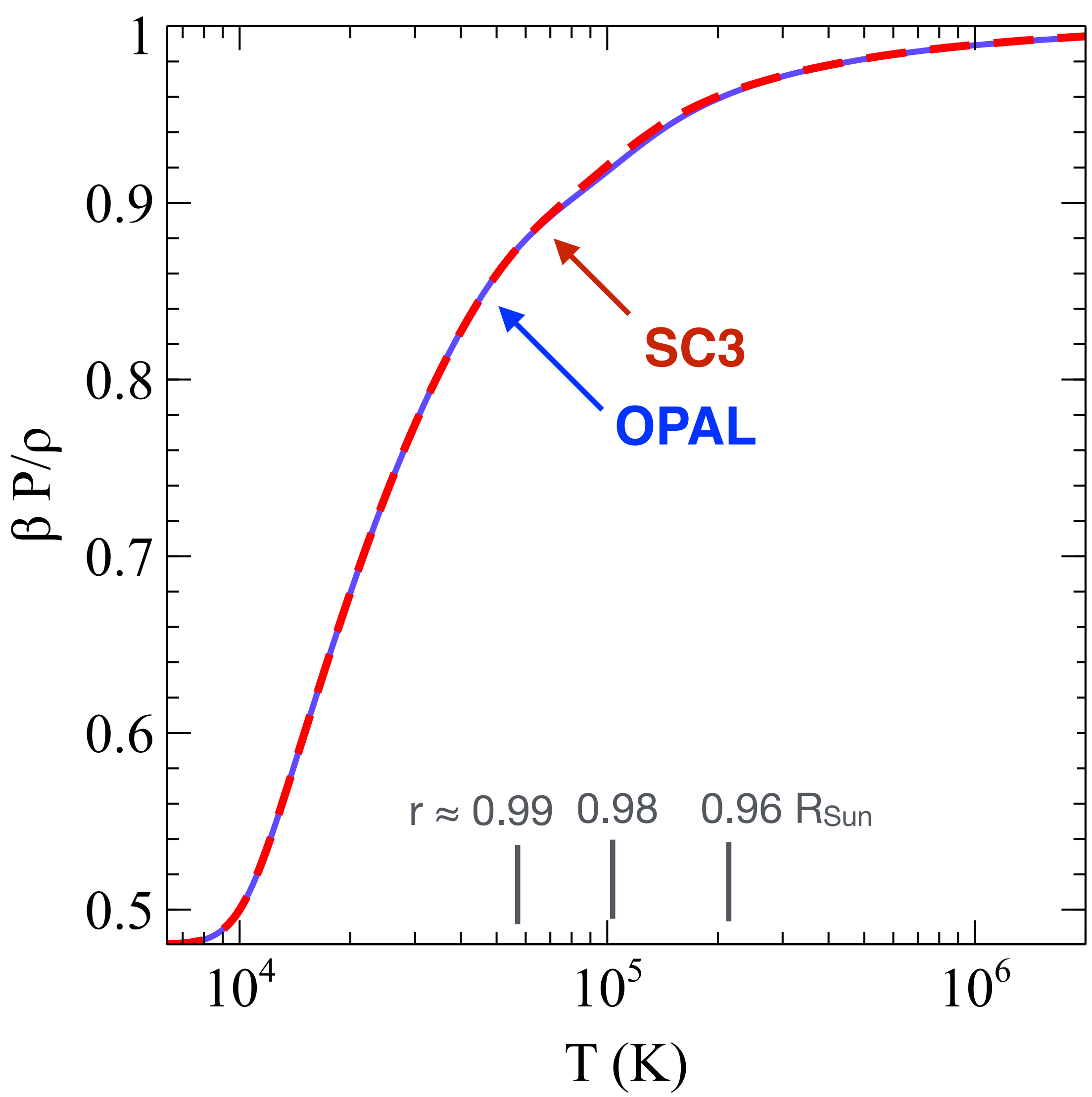
# 4. Result: SC3 equation of state

Effects up to 3-particle interactions are included: pressure: $P(\{z_\gamma\},T) = \ldots$(order 3)
densities: $\rho_\gamma(\{z_\gamma\},T) = \ldots$(order 3)

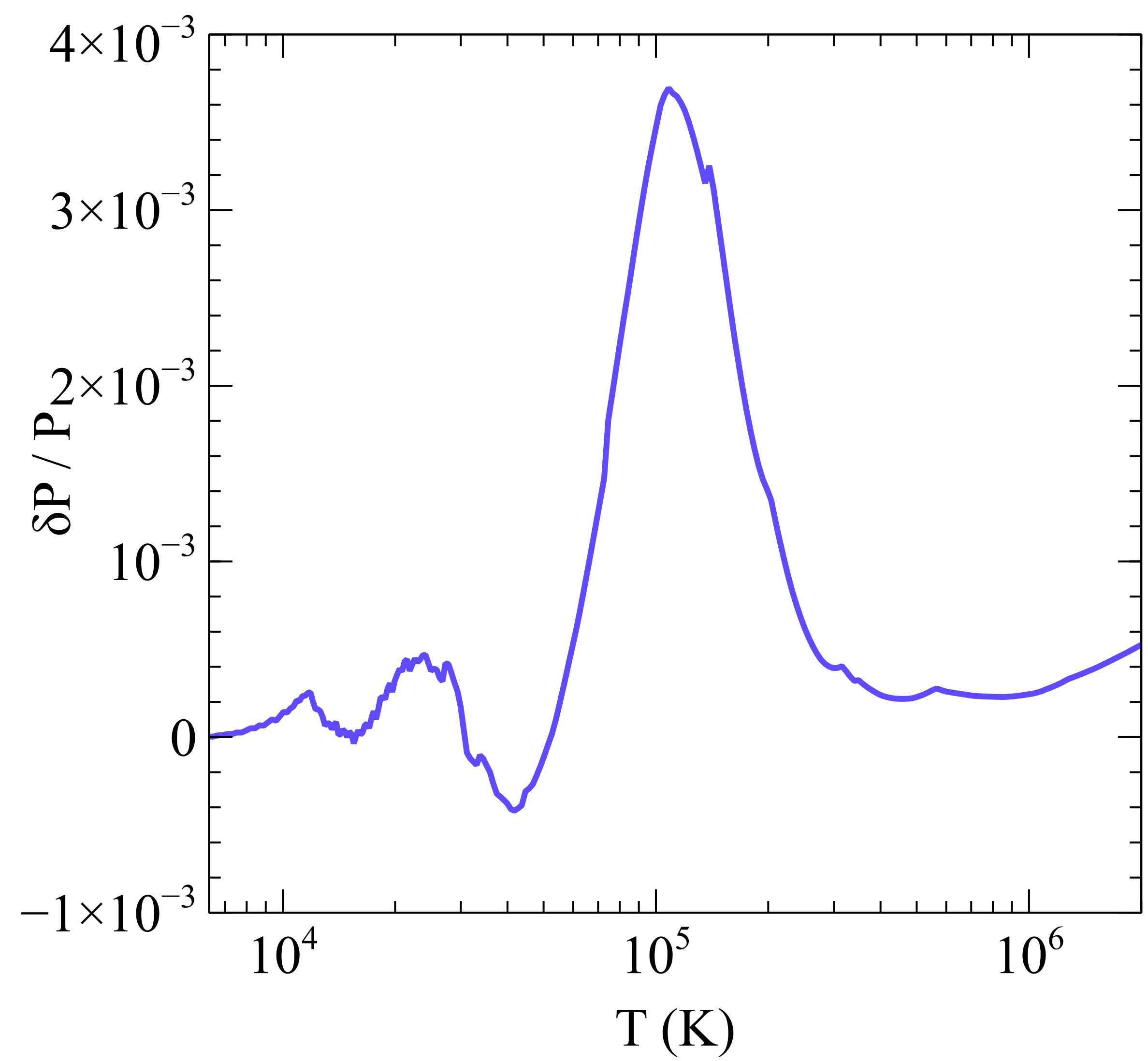
***Preliminary results***

## Pressure along the solar adiabat:

*Adiabat model: Christensen-Dalsgaard et al. (1996)*




Relative difference $\frac{P_{SC3} - P_{OPAL}}{P}$

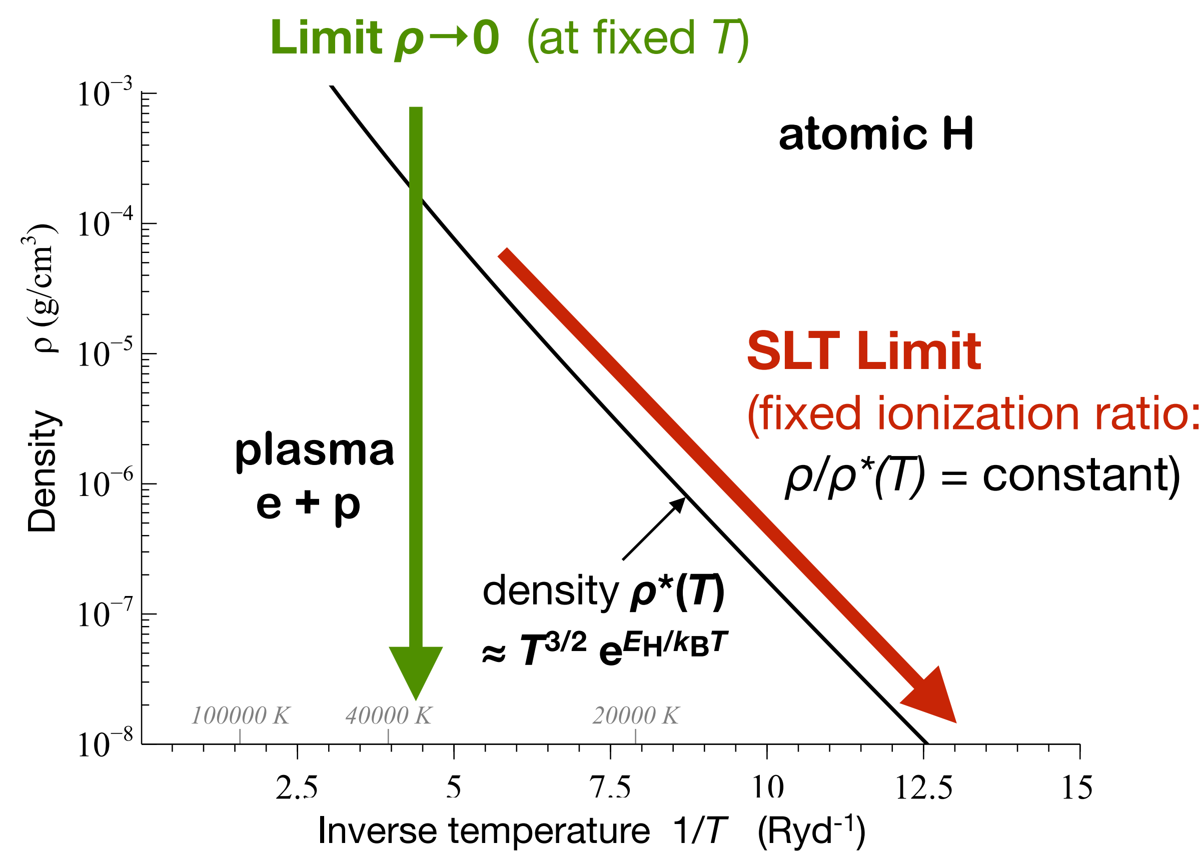



**SC3 versus OPAL :** difference $\delta P/P$ **< 4·10⁻³**.

Future work: Sound speed

D. Wendland, PhD thesis (2015), unpublished

# 4. Result: SLT expansion of the EOS




Case of (pure) **hydrogen gas**

in a dilute limit at fixed ionization ratio.

**Scaled Low Temperature (SLT) expansion**

Saha ionization theory for an ideal gas.

- Pressure: $P(\rho,T) = P_{Saha} + P_1 + P_2 + P_3 + P_4 + P_5 + \ldots$
- Internal energy $U(\rho,T) = U_{Saha} + U_1 + U_2 + U_3 + U_4 + U_5 + \ldots$
- Sound speed: $c^2 = \left.\frac{\partial P}{\partial \rho}\right|_S$

Alastuey, Ballenegger et al. (2008,2012)
Wendland, Ballenegger et al. (2014)

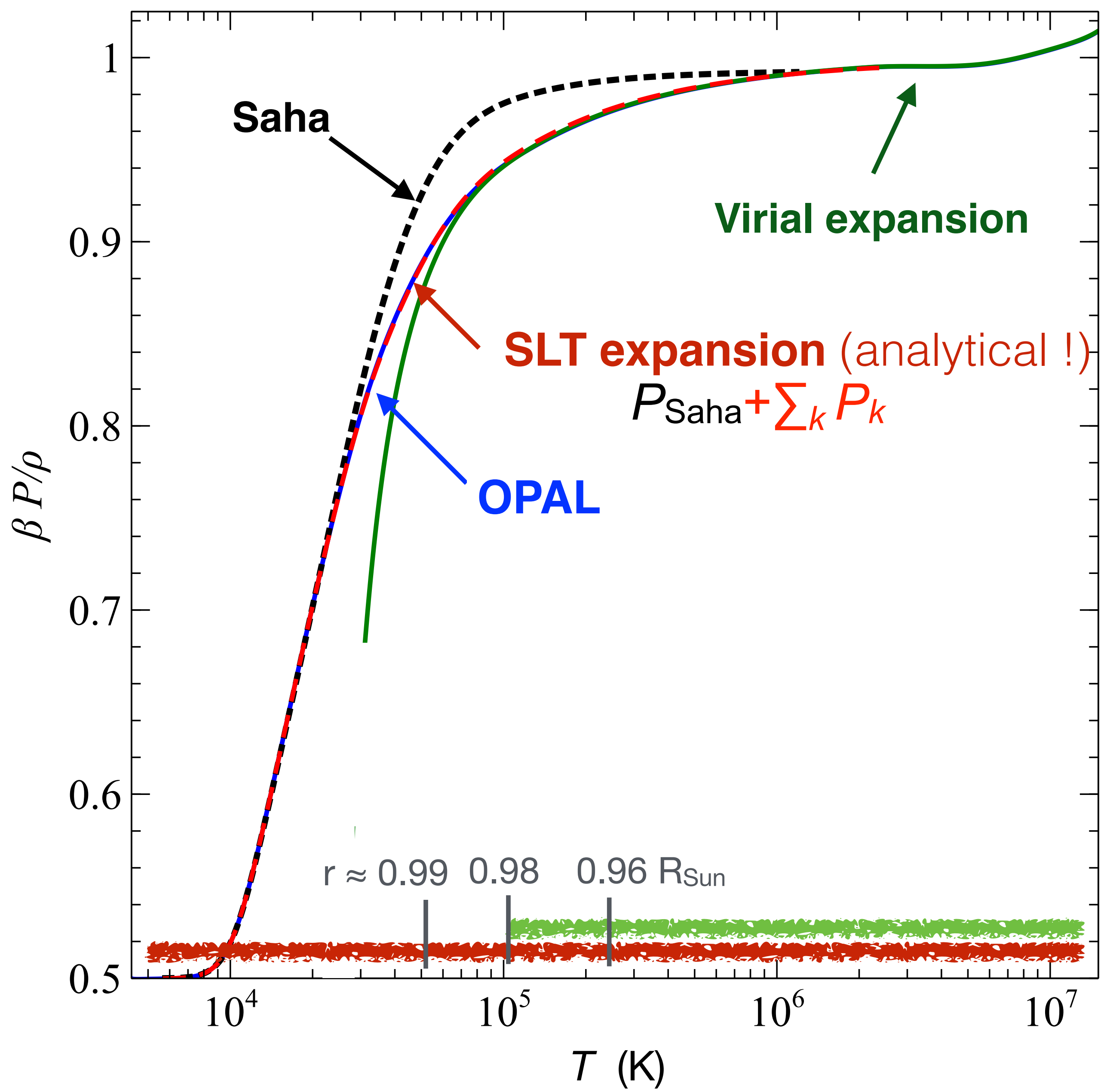
The explicit ***analytical*** formulas for the first 5 corrections ($P_k$ and $U_k$) to Saha theory involve 2-, 3- and 4-particle cluster functions *in vacuum.*

In the low-density limit $\rho \to 0$, the SLT expansion reduces to the virial expansion.

**Validity domain**: (atomic) hydrogen gas at ***any ionization ratio***.

# 4. Result: SLT expansion of the EOS

**Pressure along the adiabat** (fictious pure H Sun)




**Validity domains**
**virial** (pure H gas and H-He mixtures)
**SLT** (pure H gas)

Maximum rel. differences $P_{\mathrm{SLT}} - P_{\mathrm{OPAL}}$:

- pressure and internal energy: **< 0.4%**
- sound speed: $\delta\gamma_1/\gamma_1$ **< 0.3%**

The OPAL values (for pure H under solar conditions) can be fully predicted by the simple analytical SLT formulas.

# 5. Summary

**Two new equations of state:**

★ **SLT expansion of the EOS** for a partially ionized hydrogen gas (H ⇄ e + p)

**Exact first few corrections** to the **Saha theory** in a low-density limit.

**Analytic** formulas for the corrections to:
- pressure
- internal energy
- sound speed

★ **SC3 equation of state** (for H-He mixtures)


Based on quantum activity expansions truncated at 3rd order.

Uses highly-accurate screened cluster functions.

The validity domain includes stars with $M > 0.8\ M_\odot$.

- **The OPAL tables deviate at most ≈ 0.4% from our SC3 EOS.**

  *Is helioseismology sensitive to such small differences in the EOS ?*

## Perspective:

Add 4-particles effects: $H_2$ molecules, H-H interactions, charge-helium inter. → **SC4 EOS**