



Thermodynamics of non-ideal plasma in the SAHA model

V.K.Gryaznov, I.L.Iosilevskiy, A.N.Ivanova, **A.N.Starostin**

Institute of Problems of Chemical Physics RAS

Joint Institute for High Temperature RAS

SRC RF Troitsk Institute for Innovation and Fusion Research

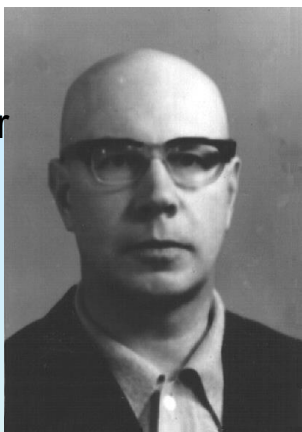


ТРИНИТИ
РОСАТОМ

Development of a gas-phase nuclear reactor

(1950-1980)

corr.-member
AS USSR



V.M. Ievlev

Heated Shock Tube



B.N. Lomakin



V.E. Fortov

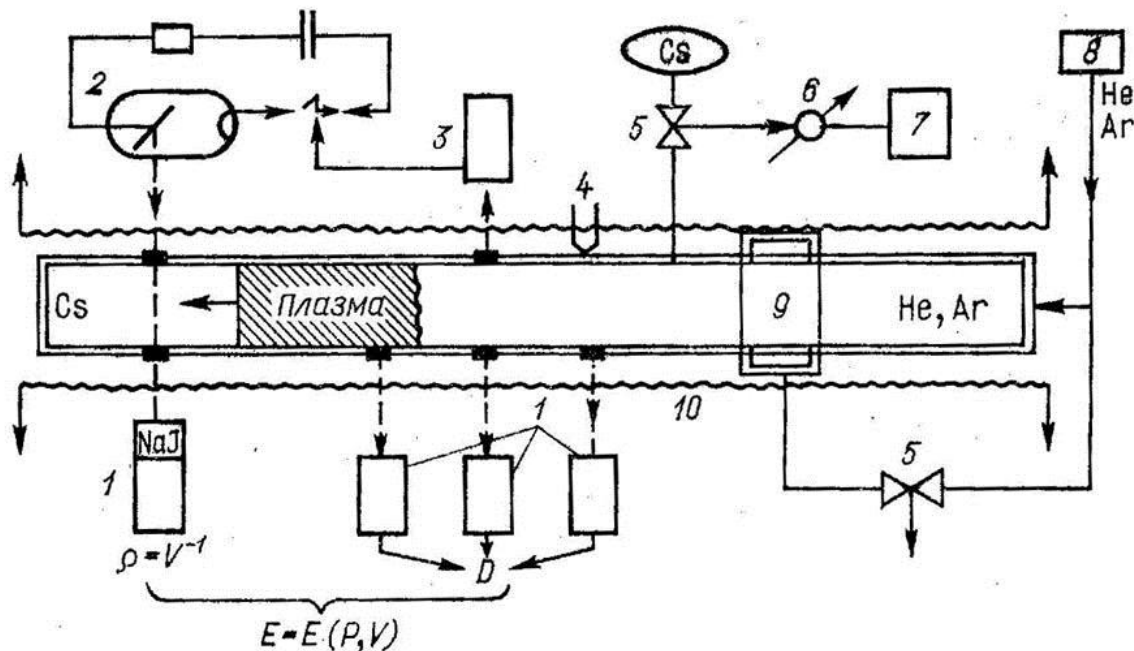
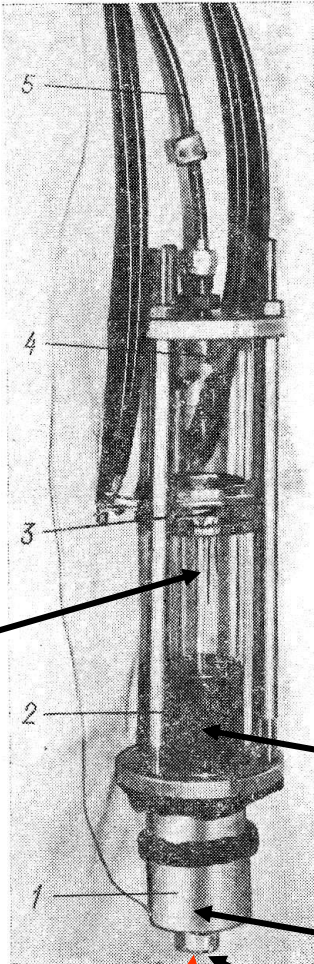


Схема подогреваемой ударной трубы:

1 — ФЭУ с катодным повторителем; 2 — рентгеновская трубка; 3 — схема импульсной рентгенографии; 4 — термопары; 5 — кран; 6 — вакуумметр; 7 — вакуумные насосы; 8 — компрессор; 9 — мембраны; 10 — обмотка обогревателя

ICP(Branch) AS USSR. Explosive Shock Tube



Ar, Xe,
Ne

Energy
~ 3MJ

Power
~ 100 GW

High
Explosive
Charge

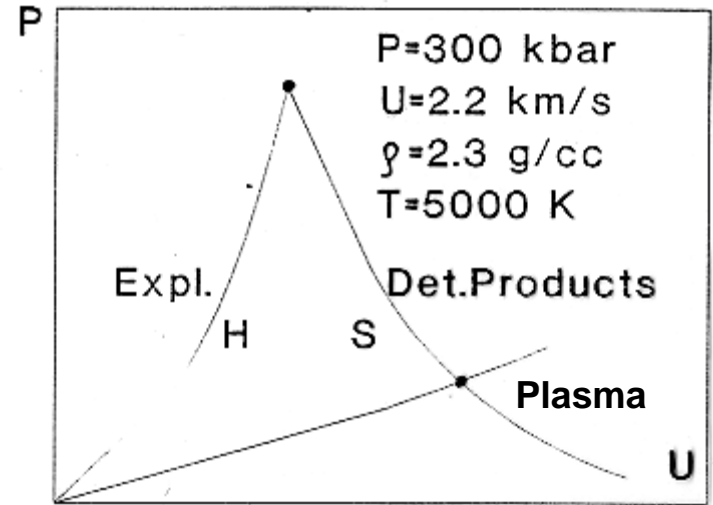
Lens

Detonator

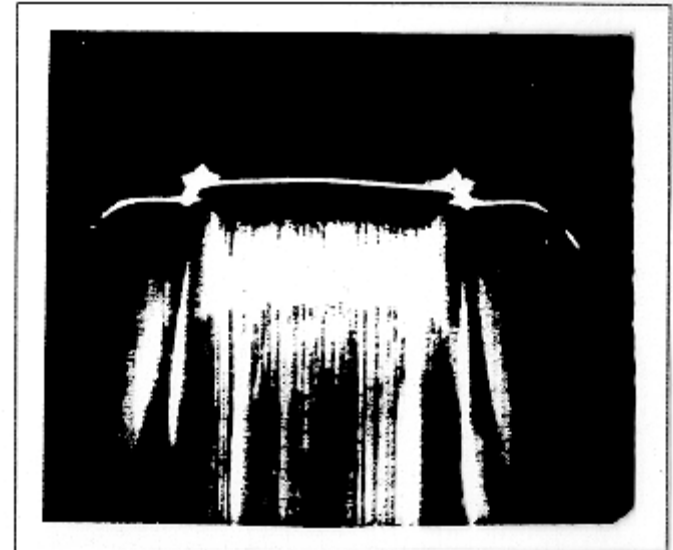
взрывной
грубы:

1 — детонационная линза;
2 — заряд ВВ; 3 — кольцо-
вставка с электроконтактны-
ми датчиками и окном для
рентгеновских измерений;
4 — зеркало для оптических
регистраций; 5 — трубка для
подачи газа

Фотография
ударной
грубы



Shock Front Curvature



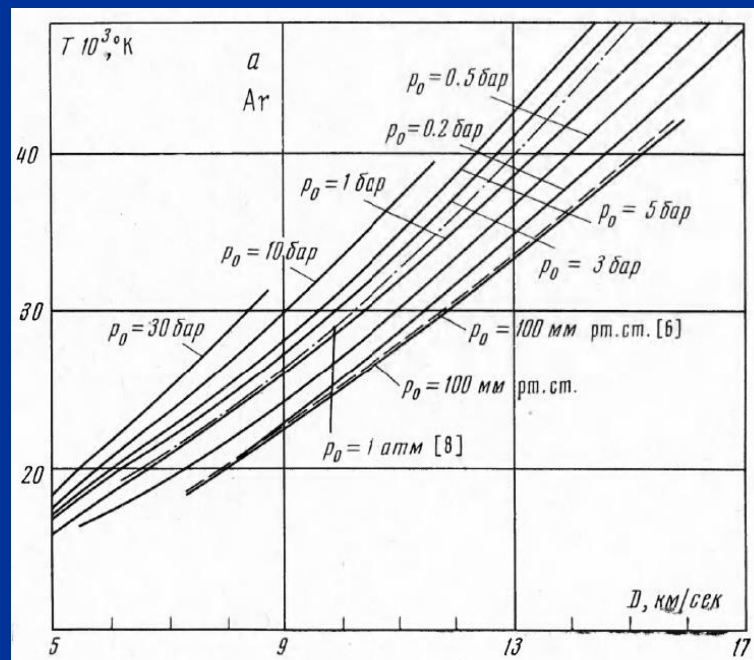
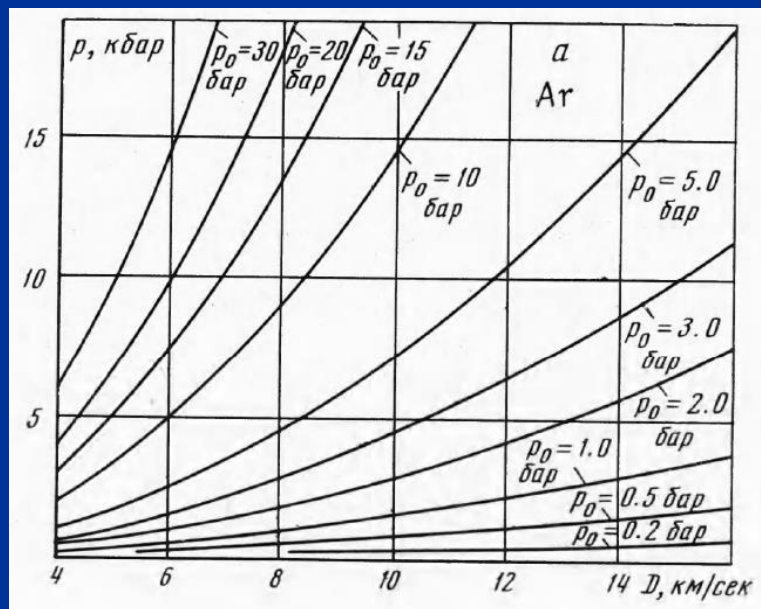
РАСЧЕТ УДАРНЫХ АДИАБАТ АРГОНА И КСЕНОНА

В. К. Грязнов, И. Л. Носилевский, В. Е. Фортвов
(Москва)

$$D = V_0 \left(\frac{P - P_0}{V_0 - V} \right)^{1/2}$$

$$u = [(P - P_0)(V_0 - V)]^{1/2}$$

$$H - H_0 = 1/2 (P - P_0)(V_0 + V)$$



Quasi-chemical representation for describing the thermodynamics of high-temperature highly compressed media

High temperature highly compressed media:
mixture of L components
electrons, atoms, molecules, ions
(atomic and molecular)

Given:
volume V , temperature T
and the number of nuclei K of chemical elements

$$F \equiv F_i^{(id)} + F_e^{(id)} + F_{ii,ie,ee,\dots}^{(int)}$$

Quasi-chemical representation

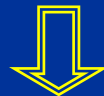
Thermodynamic equilibrium conditions

$$F(\{n_i\}, V, T) \xrightarrow{\{n_j\}} \min$$

$$\sum_{j=1}^L \nu_k^j N_j = N_k^0; \quad k = 1, 2, \dots, K + 1$$



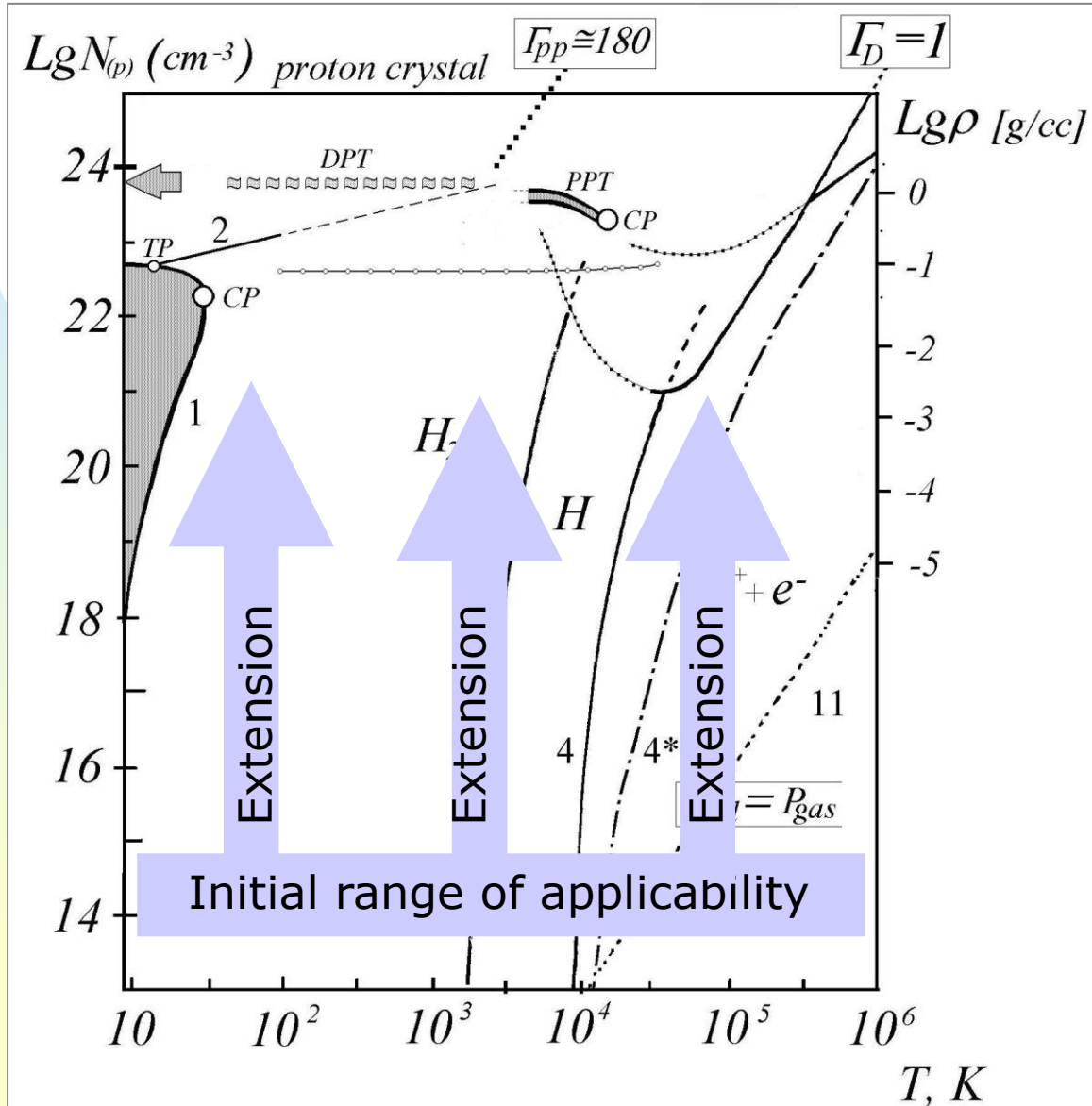
$$\sum_{j=1}^L \left(\frac{\partial F}{\partial N_j} \right)_{V, T} dN_j = 0; \quad \frac{\partial F}{\partial N_j} = \mu_j$$



Equilibrium equations

Chemical picture. Applicability problem

Hydrogen phase diagram



Coulomb non-ideality

Short-range repulsion

Short-range attraction

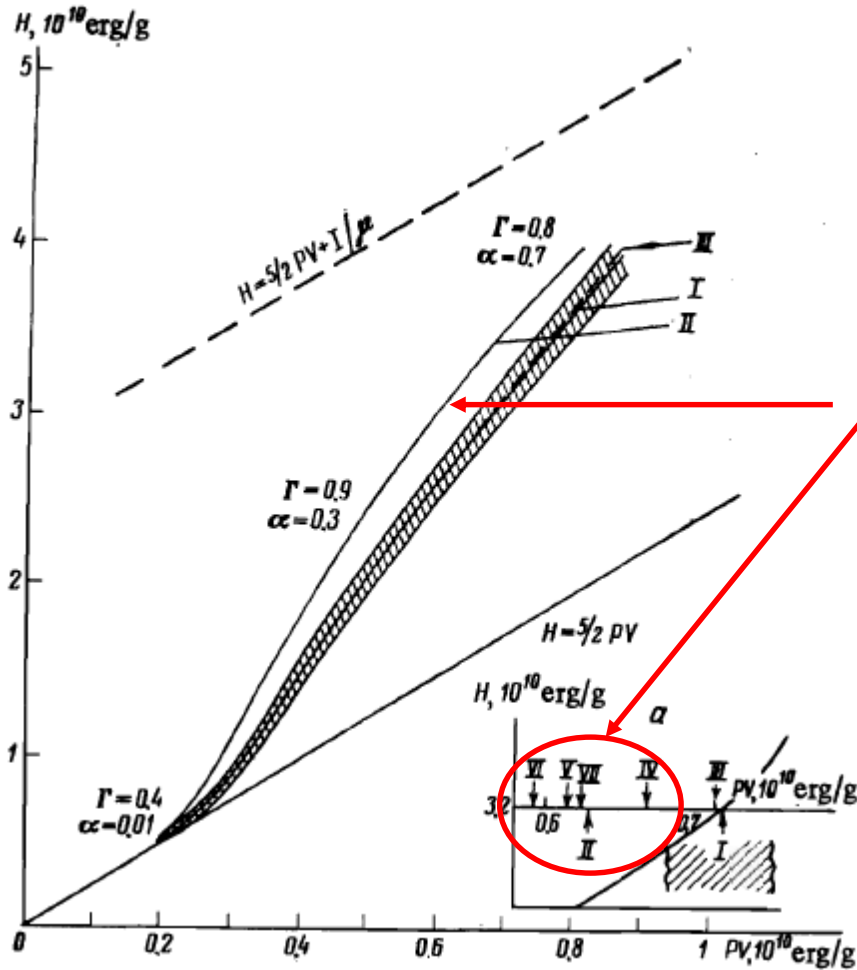
Electron degeneracy



Confined Atom Model

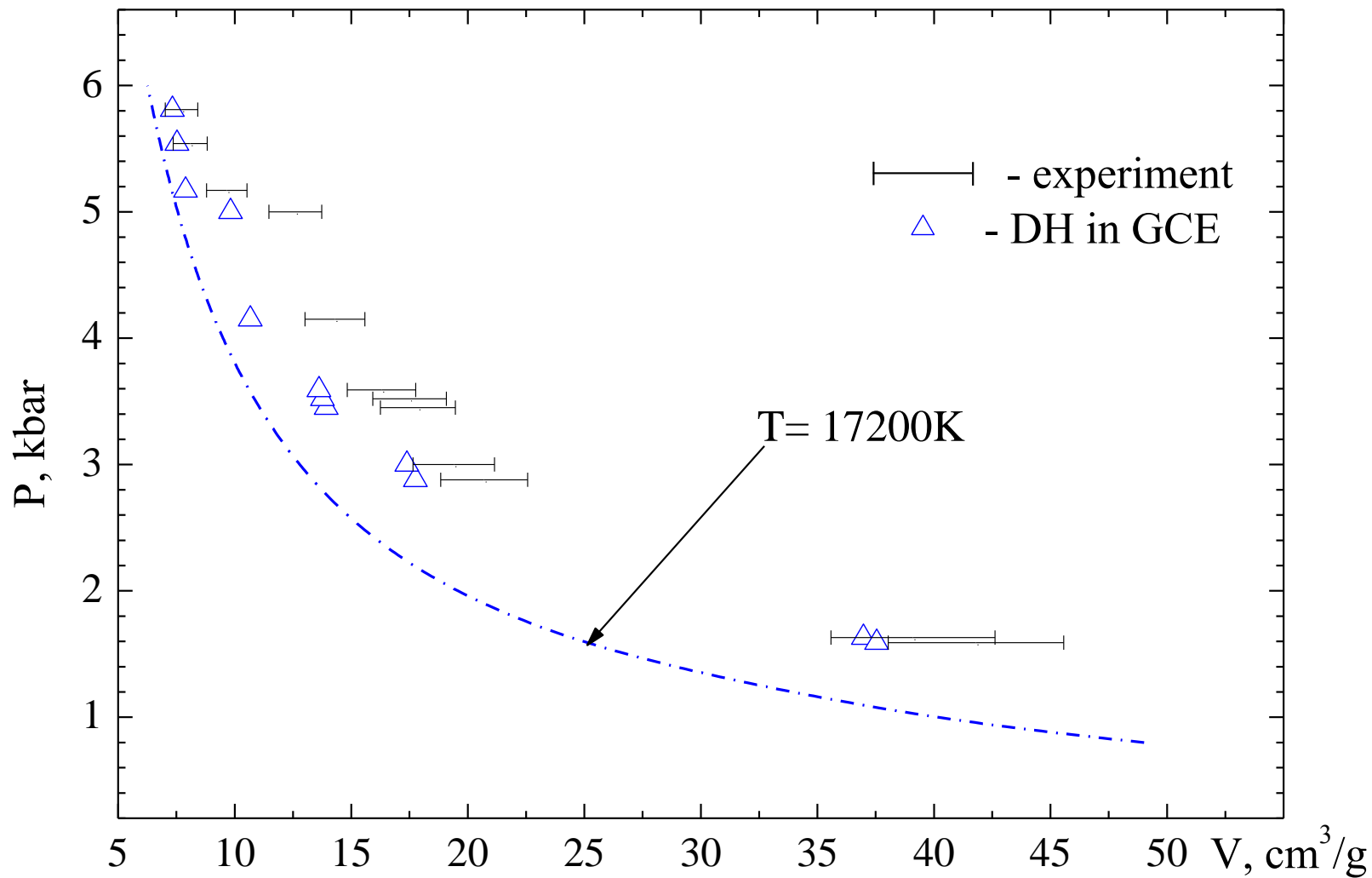
Thermodynamics of nonideal cesium plasma

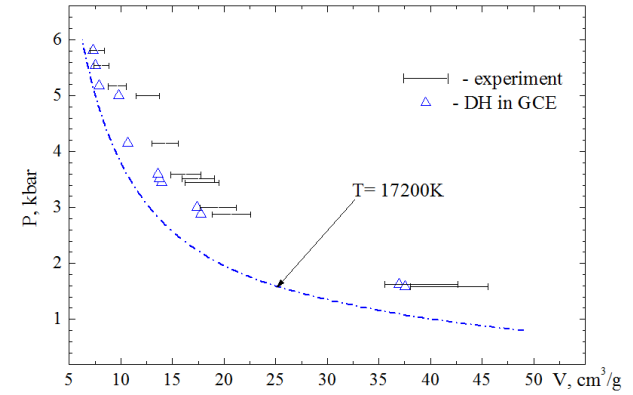
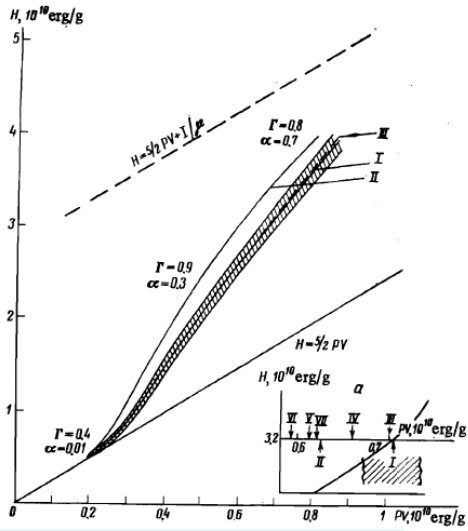
A. V. Bushman, B. N. Lomakin, V. A. Sechenov, V. E. Fortov, O. E. Shchekotov, and I. I. Sharipdzhanov



It is possible that an appreciable decrease of the energy contribution of the bound states to the enthalpy, together with the decrease of the correction for the interaction of the free charges in the equation of state, is due to the deformation and to the distortion of the energy levels at high densities. A quantitative description of this phenomenon calls for complicated self-consistent quantum-mechanical calculations ^[16] with introduction of special assumptions concerning the character of the interparticle interaction in the system.

Argon thermal equation of state





Confined atom model idea

Non-ideal plasma
chemical picture

Hartree-Fock calculation
of atomic structures

1963

РАСЧЕТЫ ЭЛЕКТРОННЫХ ОБОЛОЧЕК НЕКОТОРЫХ АТОМОВ
ПО МЕТОДУ ХАРТРИ—ФОКАА. В. ИВАНОВА, А. Н. ИВАНОВА, А. И. ПРИХОЖЕНКО,
И. И. ПЯТЕЦКИЙ-ШАПИРО, Б. Л. ТАРНОПОЛЬСКИЙ

В связи с задачей расчета поперечных сечений фотоионизации некоторых легких атомов выполнен ряд расчетов волновых функций по методу Хартри—Фока на электронной машине. В статье излагается методика расчета волновых функций в основном и возбужденных состояниях и волновых функций непрерывного спектра.

LIETUVOS
FIZIKOS
RINKINYSЛИТОВСКИЙ
ФИЗИЧЕСКИЙ
СБОРНИК

III

Nr. 1-2
1963Canadian Journal
of PhysicsVolume 41, Number 11
November 1963[← Previous](#) [Next →](#) Canadian
Science
Publishing

NUMERICAL SOLUTION OF THE HARTREE-FOCK EQUATIONS

Charlotte Froese

Vol. 41 • No. 11 • pp. 1895-1910

Procedures for solving the Hartree-Fock equations on an automatic computer such as the IBM 7090 are described. Particular attention is given to the question of numerical accuracy and to the problem of devising automatic procedures.

Calculation of compressed atomic structures by the Hartree-Fock method

The variational principle of quantum mechanics

$$E_{\Psi} = (\Psi, \hat{H}\Psi) = \int \Psi^* \hat{H}\Psi dx_1 \dots dx_N \Rightarrow \min$$

For the Hamiltonian

$$\hat{H} = -\sum_{i=1} \left[\frac{1}{2} \Delta_i + \frac{Z}{r_i} \right] + \sum_{i < j} \frac{1}{|r_i - r_j|}$$

under conditions

$$\int |\Psi|^2 dx_1 \dots dx_N = 1; \quad x_i = (r_i \delta_i)$$

Wave function in the Hartree-Fock approximation (RHF)

$$\Psi = \sum_i C_i \Phi_i$$

$$\hat{L}^2 \Psi = L(L+1)\Psi \quad \Phi_i = \frac{1}{N!} \begin{vmatrix} \varphi_{i_1}(\bar{x}_1) \dots & \varphi_{i_1}(\bar{x}_N) \\ \varphi_{i_2}(\bar{x}_1) \dots & \varphi_{i_2}(\bar{x}_N) \\ \dots & \dots \\ \varphi_{i_N}(\bar{x}_1) \dots & \varphi_{i_N}(\bar{x}_N) \end{vmatrix}$$

$$\hat{S}^2 \Psi = S(S+1)\Psi$$

$$\varphi_i(\bar{x}) = R_{n_i l_i}(r) Y_{l_i}^{m_i}(\theta, \varphi) \chi_i(\delta)$$

$$R_{nl}(r) = \frac{f_{nl}(r)}{r}$$

{nl} = 1s² 2s² 2p⁶ 3s² 3s² 3d² ...

Calculation of compressed atomic structures by the Hartree-Fock method

Hartree-Fock system of integro-differential equations

$$\left[\frac{d^2}{dr^2} + V_{nl}(r) - \lambda_{nl} \right] f_{nl}(r) + x_{nl}(r) - \sum_{n'l' \neq nl} \frac{1}{q_{nl}} \lambda_{nl, n'l'} \delta_{l, l'} f_{n'l'}(r) = 0$$

$$x_{nl}(r) = - \sum_{\substack{n'l' \in f+g \\ n'l' \neq nl}} \frac{2b_k(nl, n'l')}{q_{nl}} f_{n'l'}(r) \int_0^{\infty} U_k(r, r') f_{nl}(r') \hat{f}_{n'l'}(r') dr'$$

λ_{nl} u $\lambda_{nl, n'l'}$ are determined from the orthonormality conditions

$$\int_0^{\infty} f_{nl}(r) f_{n'l'}(r) dr = \delta_{nn'}$$

Solution method - iterative self-consistency procedure

at every step

$$y'' + v(r)y + \int_0^{r_c} g(r, r') y(r') dr' = \lambda y$$

$$y(0) = y(r_c) = 0$$

$$\int_0^{r_c} y^2(r) dr = 1$$



$$y'' + v(r)y + x(r) = \lambda y$$

$$y(0) = y(r_c) = 0$$

$$y(r_1) = y_1 > 0$$

Boundary conditions for radial wave functions

EXISTENCE OF THERMODYNAMICS FOR REAL MATTER WITH COULOMB FORCES

J. L. Lebowitz*

Belfer Graduate School of Science, Yeshiva University, New York, New York 10033
and

Elliott H. Lieb†

Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

VOLUME 22, NUMBER 13 PHYSICAL REVIEW LETTERS 31 MARCH 1969

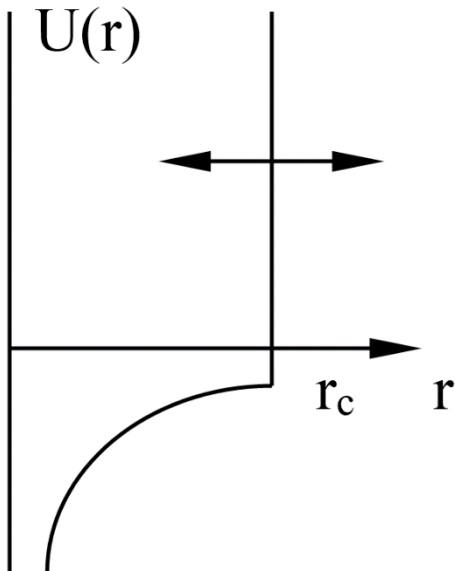
$$Z(N, \Omega) \geq \prod_{i=1}^D Z(N_i, \Omega_i).$$



$$F_{Model}(V, T, \{N_j\}) \geq F(V, T, \{N_j\})$$



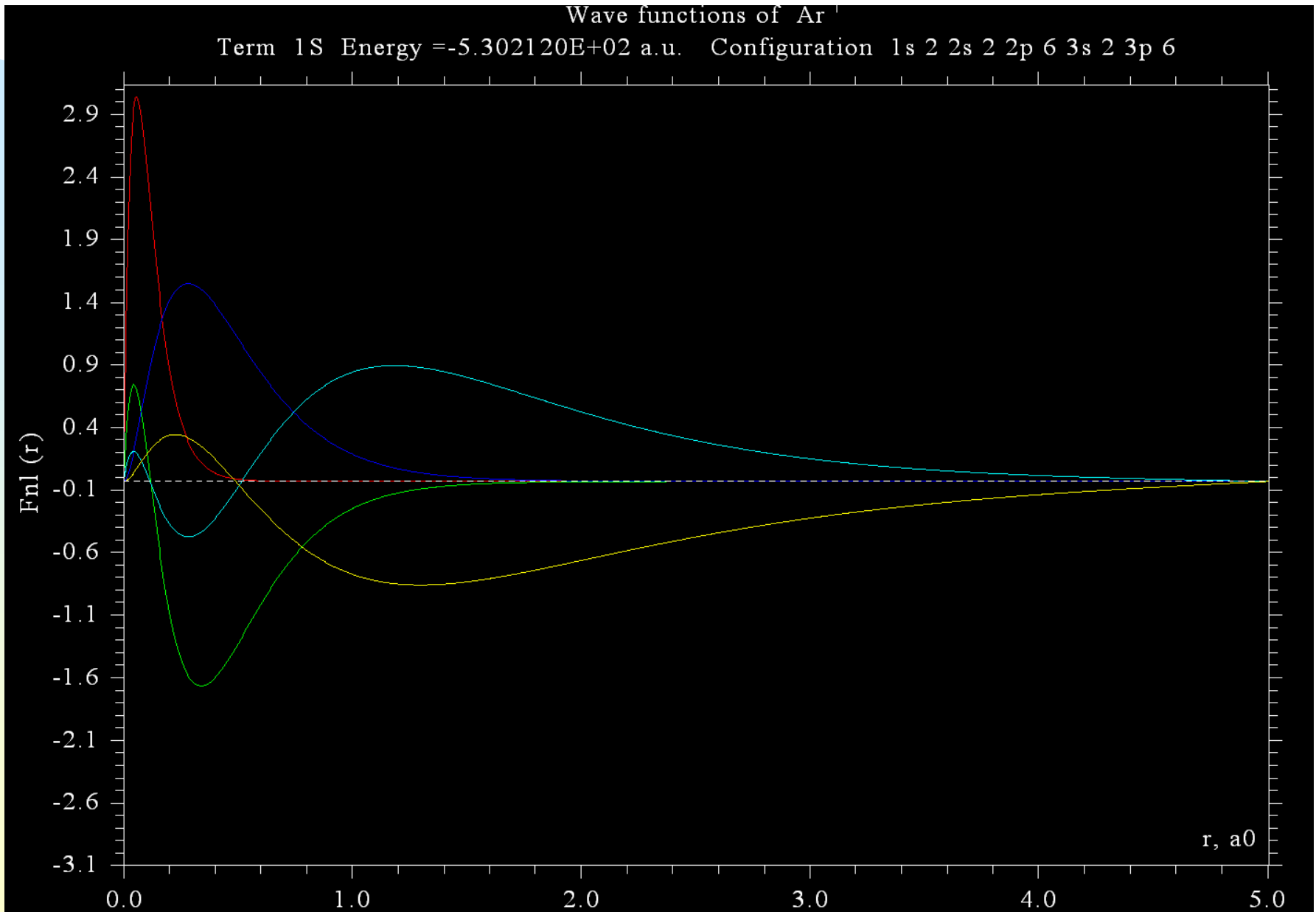
$$f_{nl}(r_c) = 0$$



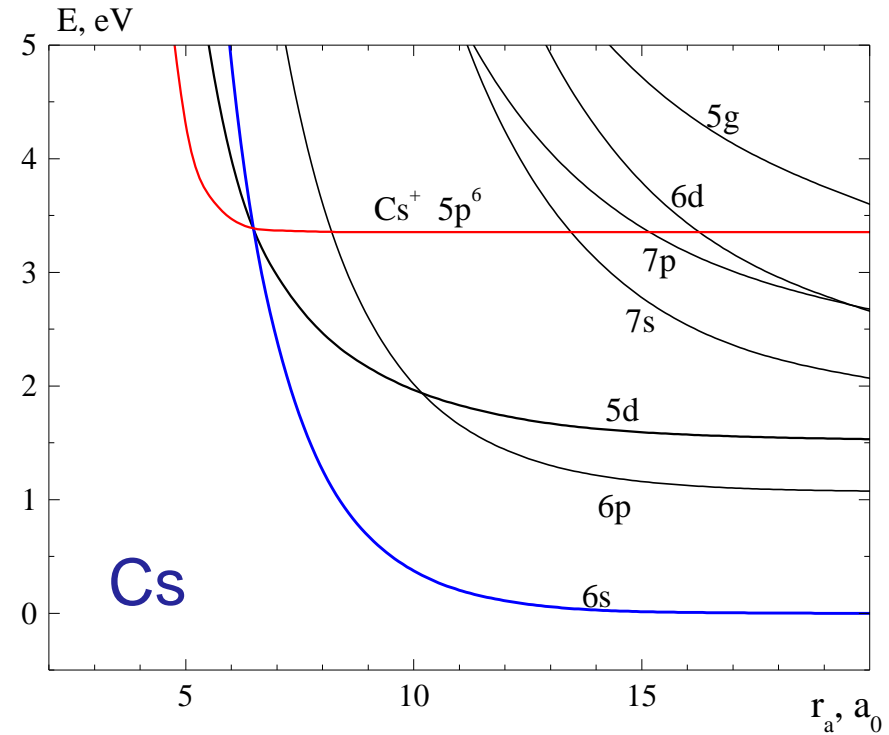
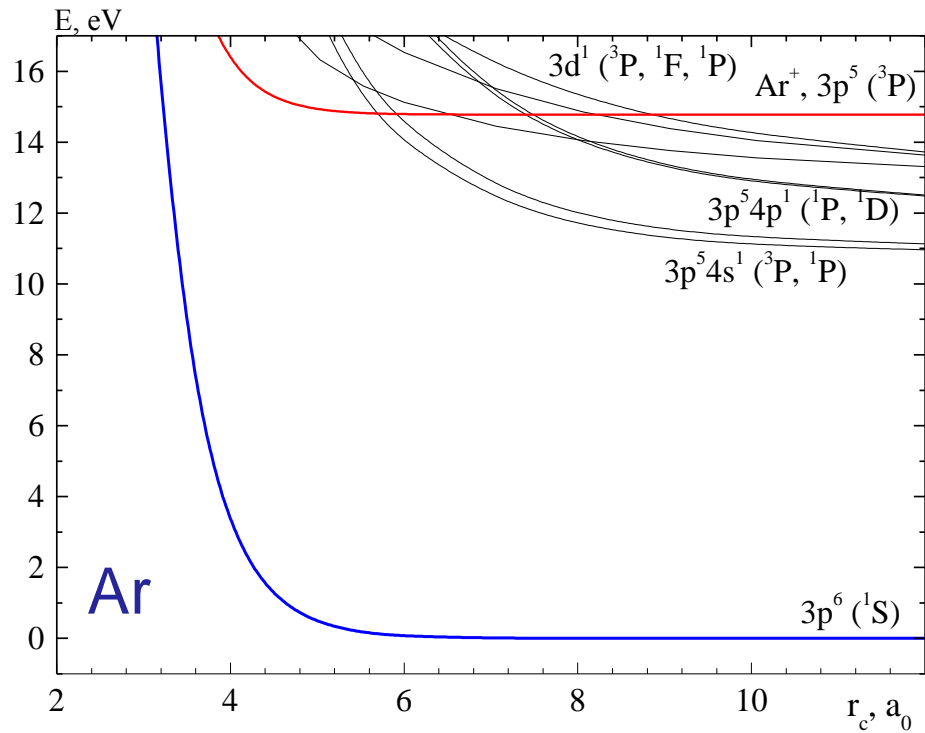
$$f_{nl}(r_c) = 0 \quad f_{nl}(0) = 0$$

$$\int_0^{r_c} f_{nl}(r) f_{n'l}(r) dr = \delta_{nn'}$$

Boundary conditions for radial wave functions

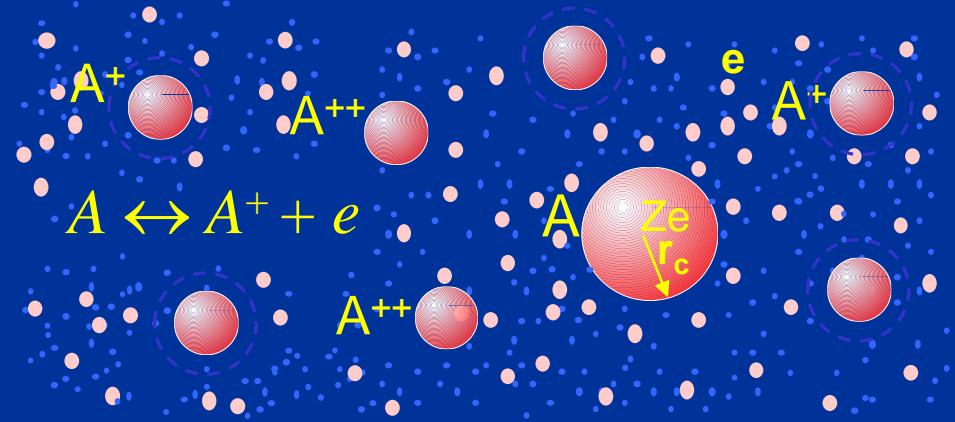


Energy levels of compressed argon and cesium atoms



Thermodynamic model

$$F(\{N_j\}, V, T) = F_{id}(\{N_j\}, V, T) + \Delta F_{HS}(\{N_j\}, V, T) + \Delta F_{Coul}(\{N_j\}, V, T)$$



Atoms, ions and electrons :

$$F_{id} = -k_B T \left[N_a \ln \frac{Q_a(r_c)}{n_a \tilde{\lambda}_a^3} + N_e \ln \frac{2Q_i}{n_e^2 \tilde{\lambda}_i^3 \tilde{\lambda}_e^3} + (N_a + 2N_e) \right]$$

Atomic partition functions:

$$Q_a(r_c) = \sum_i g_i \exp \left[-\frac{\varepsilon_i^{HF}(r_c)}{k_B T} \right]$$



$$\frac{\partial F}{\partial r_c} = 0 \Rightarrow 3r_c y f'(y) = \frac{1}{Q_a} \frac{\partial Q_a}{\partial r_c} \Rightarrow r_c$$

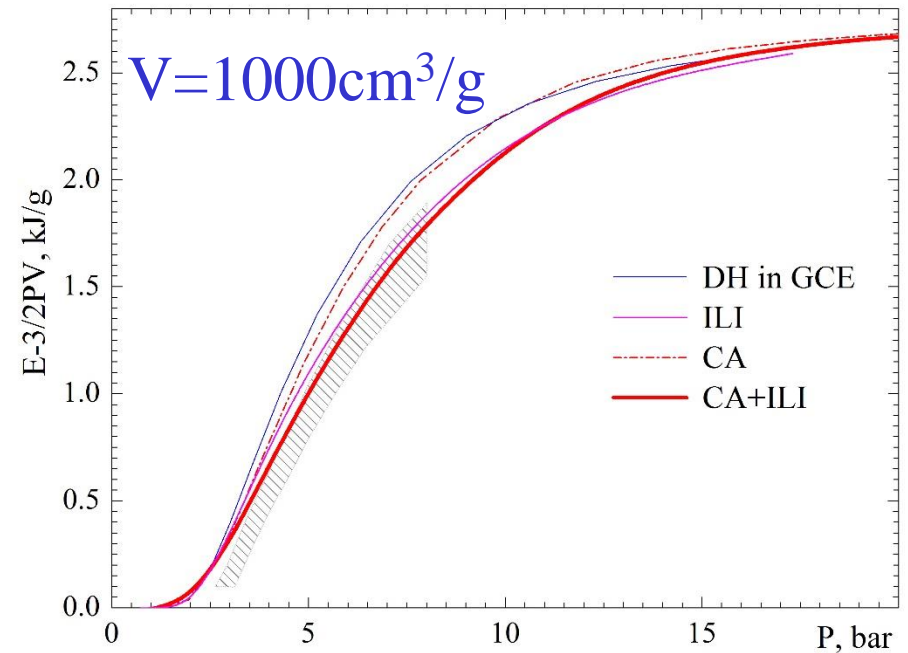
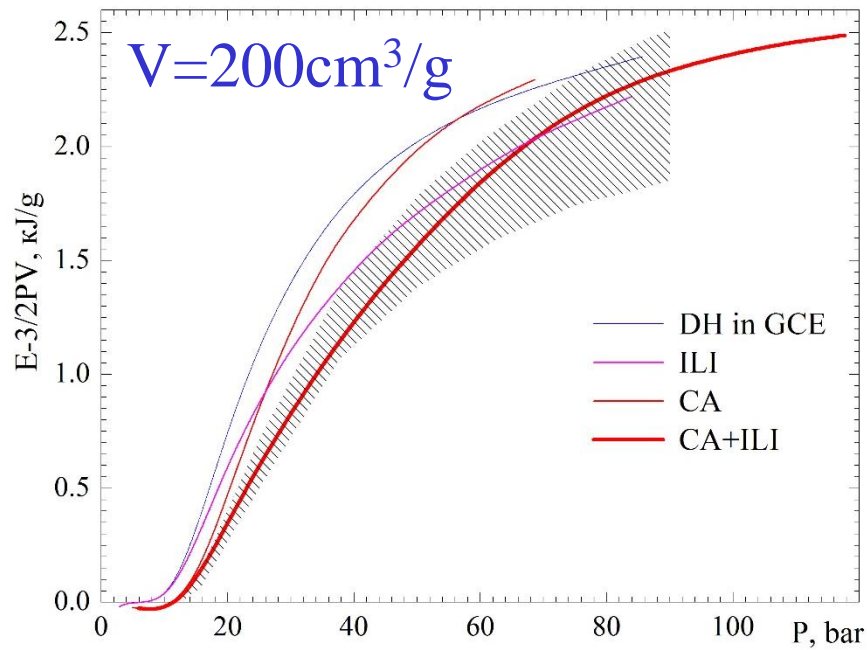
Nonideality effects:

- Coulomb corrections :
Debye approximation in GCE pseudopotential model, ...
- Short-range repulsion :
atoms are hard spheres of finite radius

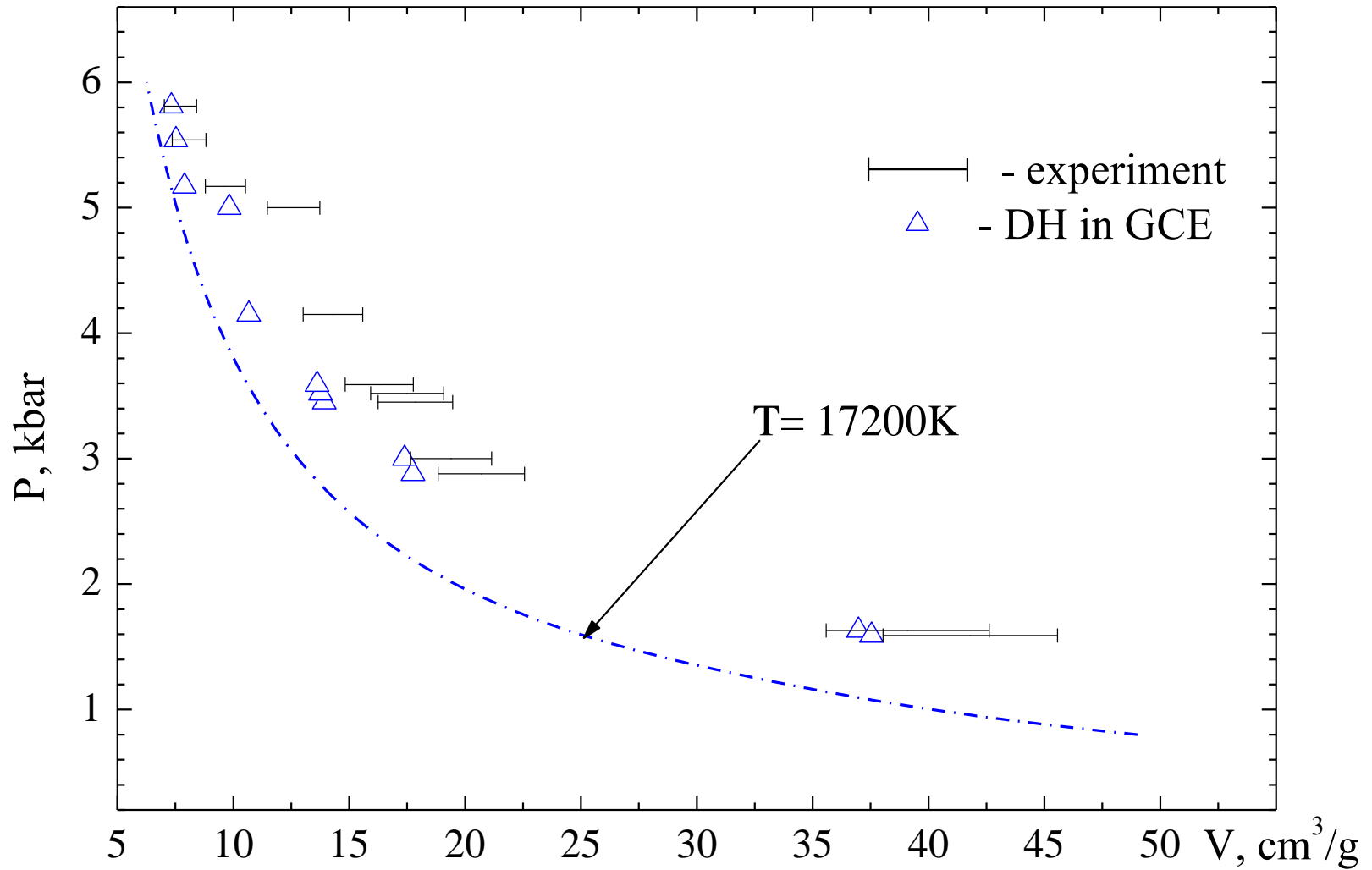
$$\Delta F_{HS} = N_a k_B T y \frac{4 - 3y}{(y - 1)^2}; \quad y = n_a (4\pi r_c^3 / 3)$$



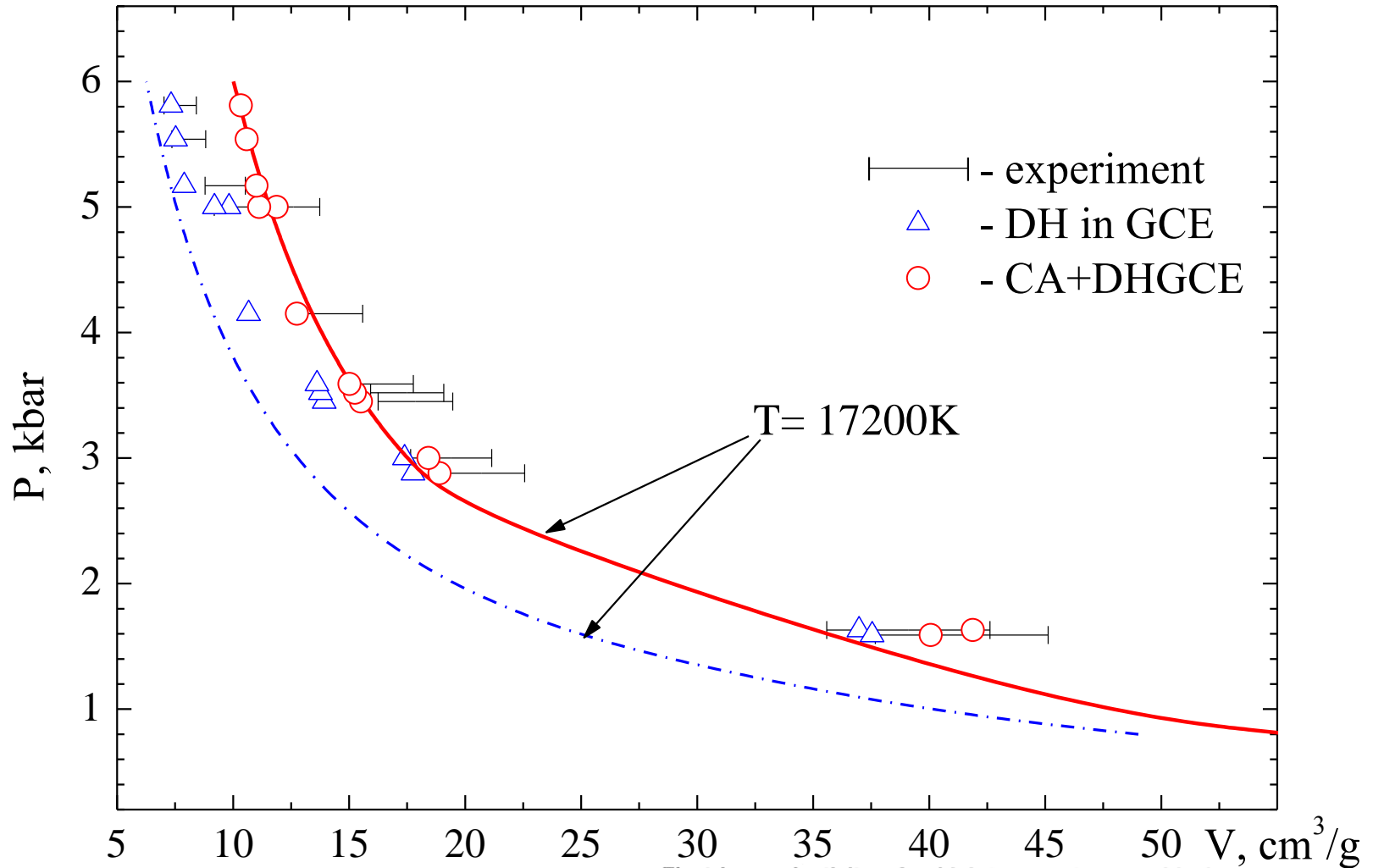
Caloric equation of state for cesium



Thermal equation of state for argon



Thermal equation of state for argon

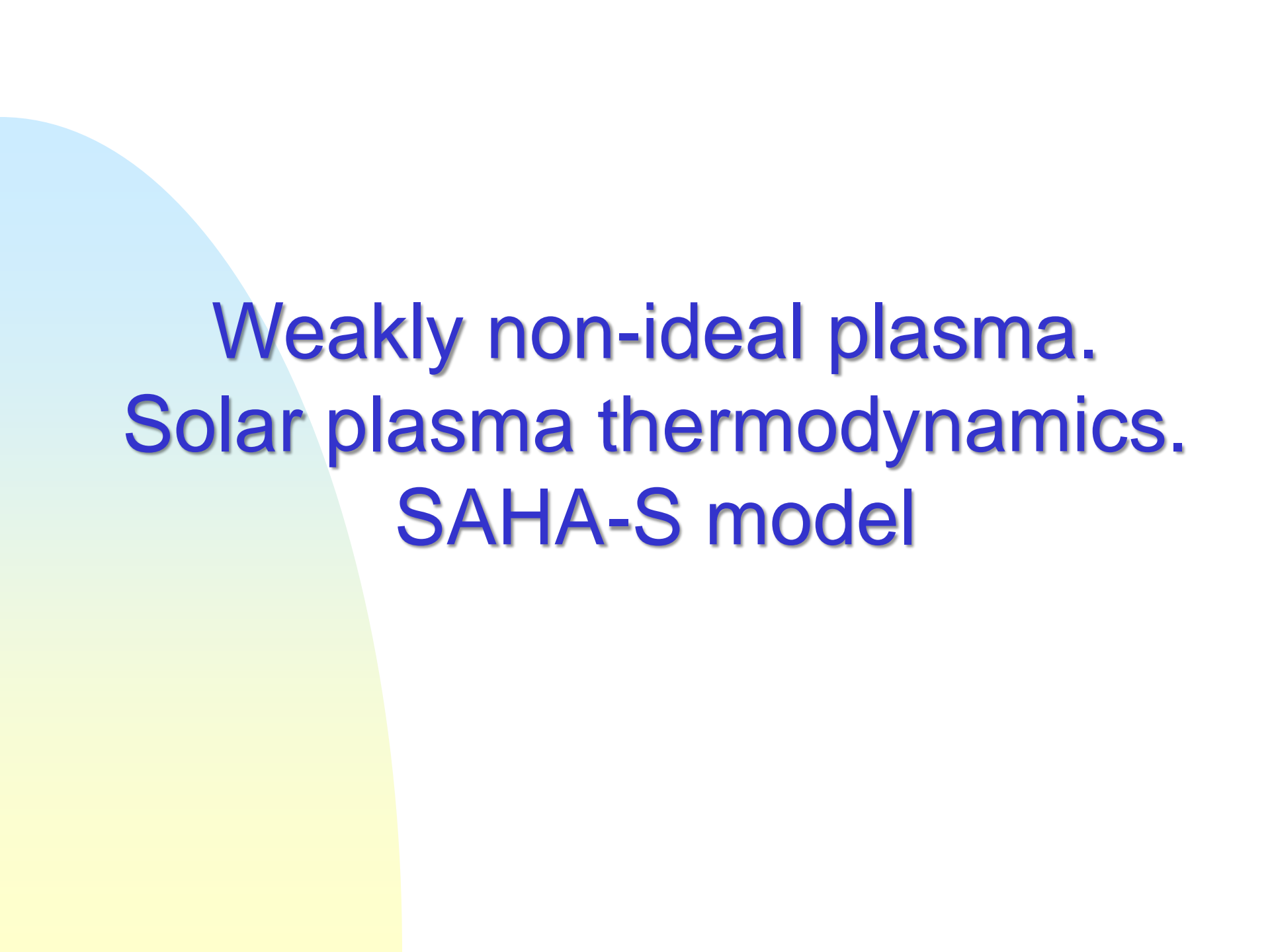


Radiation emitted by a shock-compressed high-pressure argon plasma

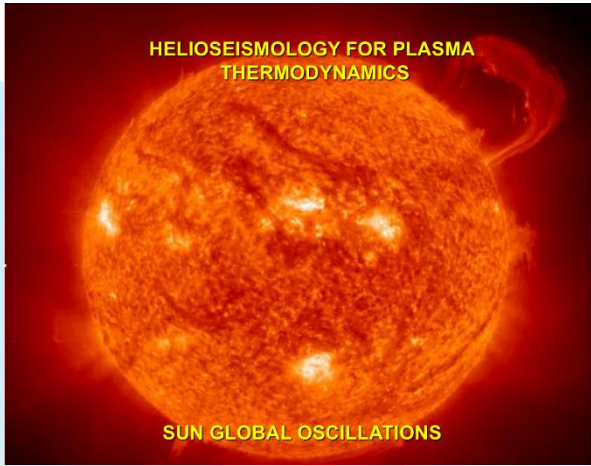
V. E. Bespalov, V. K. Gryaznov, and V. E. Fortov
 Division of Institute of Chemical Physics, USSR Academy of Sciences
 Zh. Eksp. Teor. Fiz. 76, 140-147 (January 1979)

Electric conductivity of a high-temperature nonideal plasma

V. B. Mintsev, V. E. Fortov, and V. K. Gryaznov
 Institute of Chemical Physics, USSR Academy of Sciences
 Zh. Eksp. Teor. Fiz. 79, 116-124 (July 1980)



**Weakly non-ideal plasma.
Solar plasma thermodynamics.
SAHA-S model**



Chemical picture. General approach of SAHA models.

Plasma - mixture of interacting atoms, ions, molecules and electrons

$$F \equiv F_i^{(id)} + F_e^{(id)} + F_{i,ie,ee}^{(int)}$$

Atoms, ions, molecules:

$$F_i^{(id)} = \sum_{j=1}^L N_j k_B T \left[\ln \left(\frac{n_j \lambda_j^3}{Q_j} \right) - 1 + \frac{A_j}{k_B T} \right];$$

$$Q_j = \sum_i g_i W(\sigma_i, n, T) \exp \left[-\frac{\epsilon_i}{k_B T} \right]$$

Electrons:

$$F_e^{(id)} = 4\sqrt{2} T \pi^{-3/2} k_B^{-3/2} \left[\alpha_e I_{3/2}(\alpha_e) - \frac{2}{3} I_{5/2}(\alpha_e) \right]$$

$$\alpha_e = \mu_e / k_B T; \quad n \lambda_e^3 = \frac{\sqrt{2}}{2} I_{3/2}(\alpha_e)$$

Nonideality effects: $F_{i,ie,ee}^{(int)}$

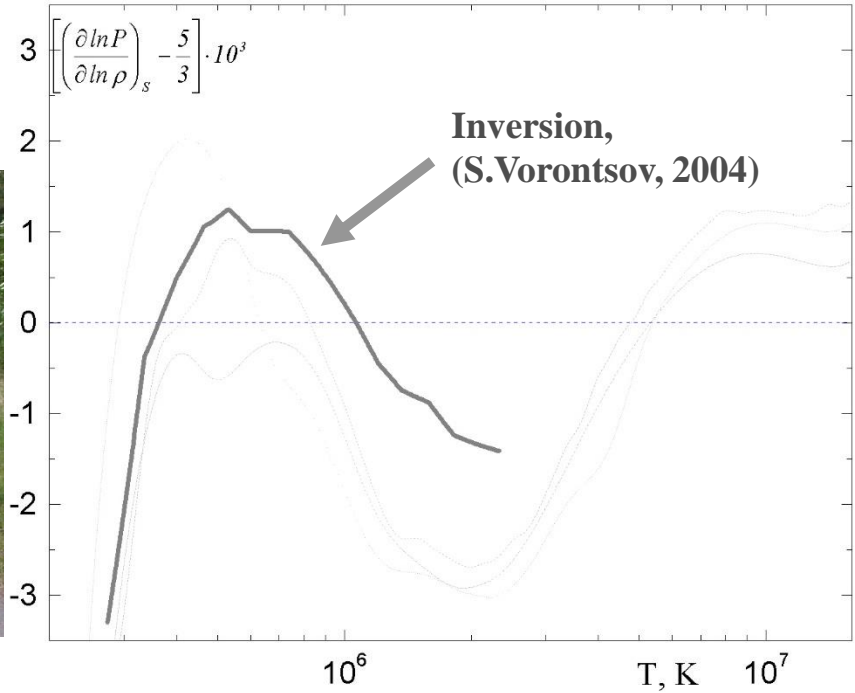
Coulomb corrections: modified Debye approximations, Coulomb pseudopotential model, ...

Strong short range repulsion between all species: atoms, molecules and ions - spheres of nonzero radius...

Neutral-neutral short range attraction

Partition functions: $Q_j = Q_j(\sigma_j, \{n_i\}, T)$

Dependence of PF on density and temperature: $Q_j = B_0, \text{Planck-Larkin, Starostin-Roerich, ...}$



Chemical picture. General approach of SAHA models.

Plasma - mixture of interacting
atoms, ions, molecules and electrons

$$F \equiv F_i^{(id)} + F_e^{(id)} + F_{ii,ie,ee,\dots}^{(int)}$$

Atoms, ions, molecules:

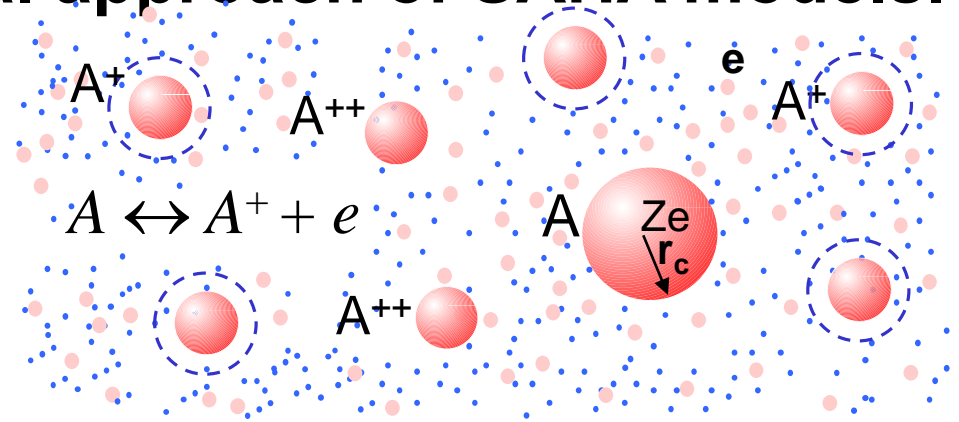
$$F_i^{(id)} = \sum_{j=1}^L N_j k_B T \left[\ln \left(\frac{n_j \tilde{\lambda}_j^3}{Q_j} \right) - 1 + \frac{A_j}{k_B T} \right];$$

$$Q_j = \sum_i g_i W(\varepsilon_i, n, T) \exp \left[-\frac{\varepsilon_i}{k_B T} \right]$$

Electrons:

$$F_e^{(id)} = 4V k_B T \pi^{-1/2} \tilde{\lambda}_e^{-3} \left[\alpha_e I_{1/2}(\alpha_e) - \frac{2}{3} I_{3/2}(\alpha_e) \right]$$

$$\alpha_e = \mu_e / k_B T; \quad \frac{n_e \tilde{\lambda}_e^3}{2} = \frac{\sqrt{\pi}}{2} I_{1/2}(\alpha_e)$$



Nonideality effects : $F_{ii,ie,ee,\dots}^{(int)}$

□ Coulomb corrections:

modified Debye approximations, Coulomb pseudopotential model, ...

□ Strong short range repulsion between all species:
atoms, molecules and ions - spheres of nonzero radius...

□ Neutral-neutral short range attraction

Partition functions: $Q_j = Q_j(\varepsilon_i, \{n_j\}, T)$

□ Dependence of PF on density and temperature:

$Q_j = g_0$, Planck-Larkin, Starostin-Roerich. ...

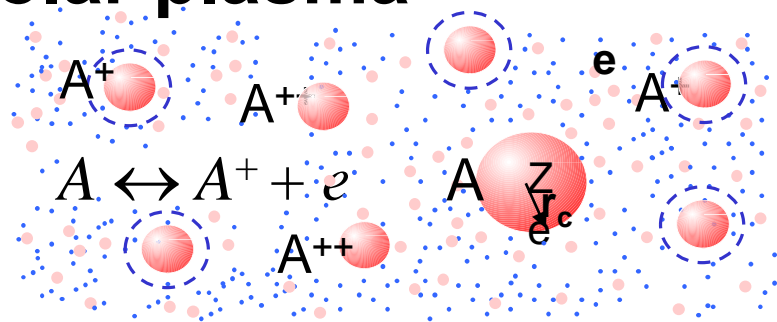
Thermodynamics of solar plasma

Equilibrium composition (**SAHA-S1**)

54 species (H He C N O Ne):

{e, H, H⁺, ..., He, He⁺, He⁺²,
C, C⁺, ..., N, N⁺, ..., O, O⁺, ..., Ne, Ne⁺, ...},

+ **Si Fe** (**SAHA-S2**) > 90 species + **Mg S** (**SAHA-S3**) > 150 species



□ Coulomb interaction:

Debye approximation
in Grand canonical ensemble

$$\frac{\Delta P^{cc}}{k_B T} = -\frac{\tilde{\Gamma}_D^3}{24\pi f^3};$$

$$\frac{\Delta \mu_i}{k_B T} = -\ln \left(1 + Z_i^2 \frac{\tilde{\Gamma}_D}{2} \right);$$

$$\tilde{\Gamma}_D^2 = 4\pi f^3 \sum_{i=1}^L \frac{Z_i^2 n_i}{1 + Z_i^2 \frac{\tilde{\Gamma}_D}{2}}$$

□ Partition functions:

Modification of Planck-Larkin partition
function (A.Starostin, 2002-2004)

$$\Delta \Omega_e = -T \zeta_e \zeta_i \tilde{\lambda}_{ei}^3 \sum_{n=1}^{\infty} n^2 F_n(\beta) \exp \left[\frac{Ry}{n^2 T} \right]$$

$$F_n(\beta) = 1 -$$

$$- e^{-\beta E_n} \left[4 - \frac{6}{\sqrt{\pi}} (\beta E_n)^{1/2} + \frac{4}{\sqrt{\pi}} (\beta E_n)^{3/2} \right] +$$

$$+ \frac{\Gamma(1/2, \beta E_n)}{\sqrt{\pi}} \left[3 - 4\beta E_n + 4(\beta E_n)^2 \right]$$

Thermodynamics of solar plasma

Relativistic corrections:

$$\frac{\Delta P^{rel}}{k_B T} = 0$$

$$\frac{\Delta \mu_e^{rel}}{k_B T} = -\ln \left[1 + \frac{15 k_B T}{8 m_e c^2} \right]$$

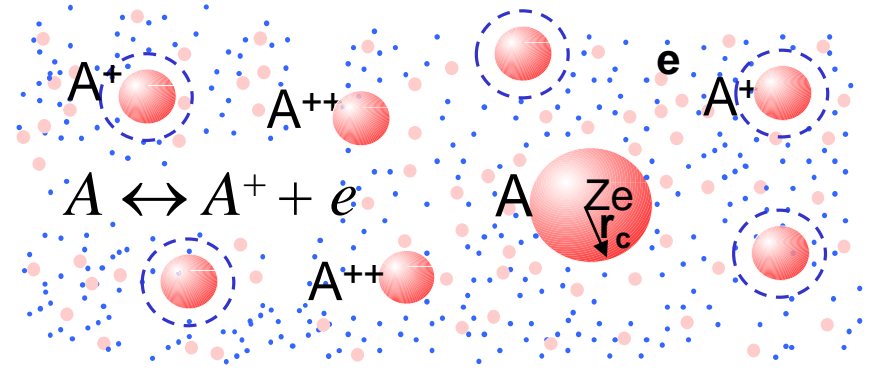
$$\frac{\Delta E^{rel}}{k_B T} = \zeta_e \frac{15 k_B T}{8 m_e c^2}$$

Exchange corrections:

$$\frac{\Delta P^{exch}}{n_e k_B T} = -\frac{\zeta_e \zeta_e \tilde{\lambda}_e^2 f}{n_e 4}$$

$$\frac{\Delta \mu_e^{exch}}{k_B T} = -\ln \left(1 + \frac{1}{2} \zeta_e \tilde{\lambda}_e^2 f \right)$$

$$\frac{\Delta E^{exch}}{n_e k_B T} = \frac{\zeta_e \zeta_e \tilde{\lambda}_e^2 f}{n_e 2} = 2 \frac{\Delta P^{exch}}{n_e k_B T}$$



Diffraction corrections:

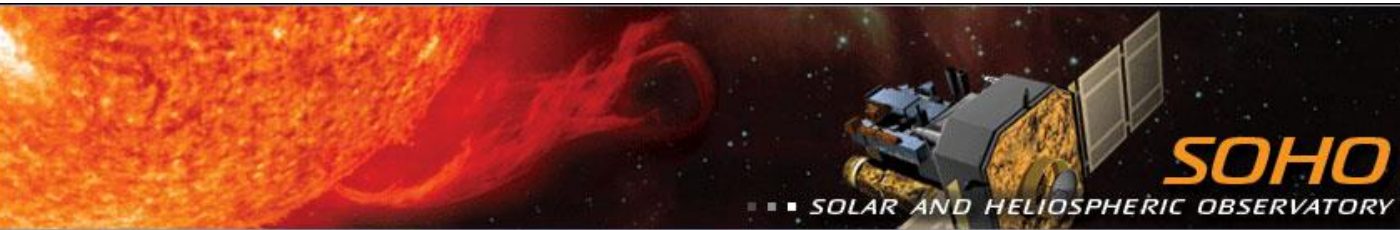
$$\frac{\Delta P^{diff}}{n_e k_B T} = \frac{\tilde{\lambda}_e \zeta_e f^2}{4} \frac{\tilde{\Gamma}^2}{4 n_e f^3} + \frac{\pi \tilde{\lambda}_e f^2 \zeta_e}{4 n_e} \left\{ \frac{(1 - \sqrt{2})}{\sqrt{2}} + \frac{1}{2} \sum_{i=2}^I \sum_{k=2}^I Z_i^2 Z_k^2 \frac{\zeta_i \zeta_k \tilde{\lambda}_{ik}}{\zeta_e \zeta_e \tilde{\lambda}_e} \right\}$$

$$\frac{\Delta \mu_e^{diff}}{k_B T} = \ln \left(1 - \frac{\pi \tilde{\lambda}_e f^2 \zeta_e}{4} \left[\sqrt{2} + \sum_{i=2}^I Z_i^2 \frac{\zeta_i}{\zeta_e} \right] \right)$$

$$\frac{\Delta \mu_i^{diff}}{k_B T} = \ln \left(1 - \frac{\pi \tilde{\lambda}_e f^2 \zeta_e Z_i^2}{4} \left(1 + \sum_{k=2}^I Z_k^2 \frac{\zeta_k \tilde{\lambda}_{ik}}{\zeta_e \tilde{\lambda}_e} \right) \right)$$

$$\frac{\Delta E^{diff}}{n_e k_B T} = \frac{5}{2} \frac{\Delta P^{diff}}{n_e k_B T}$$

Structure of the Sun



Convective Zone

Radiative Zone

Core

□ Core:

$$0 < \frac{r}{R_{\oplus}} < 0.3$$

□ Radiative zone:

$$0.3 < \frac{r}{R_{\oplus}} < 0.7$$

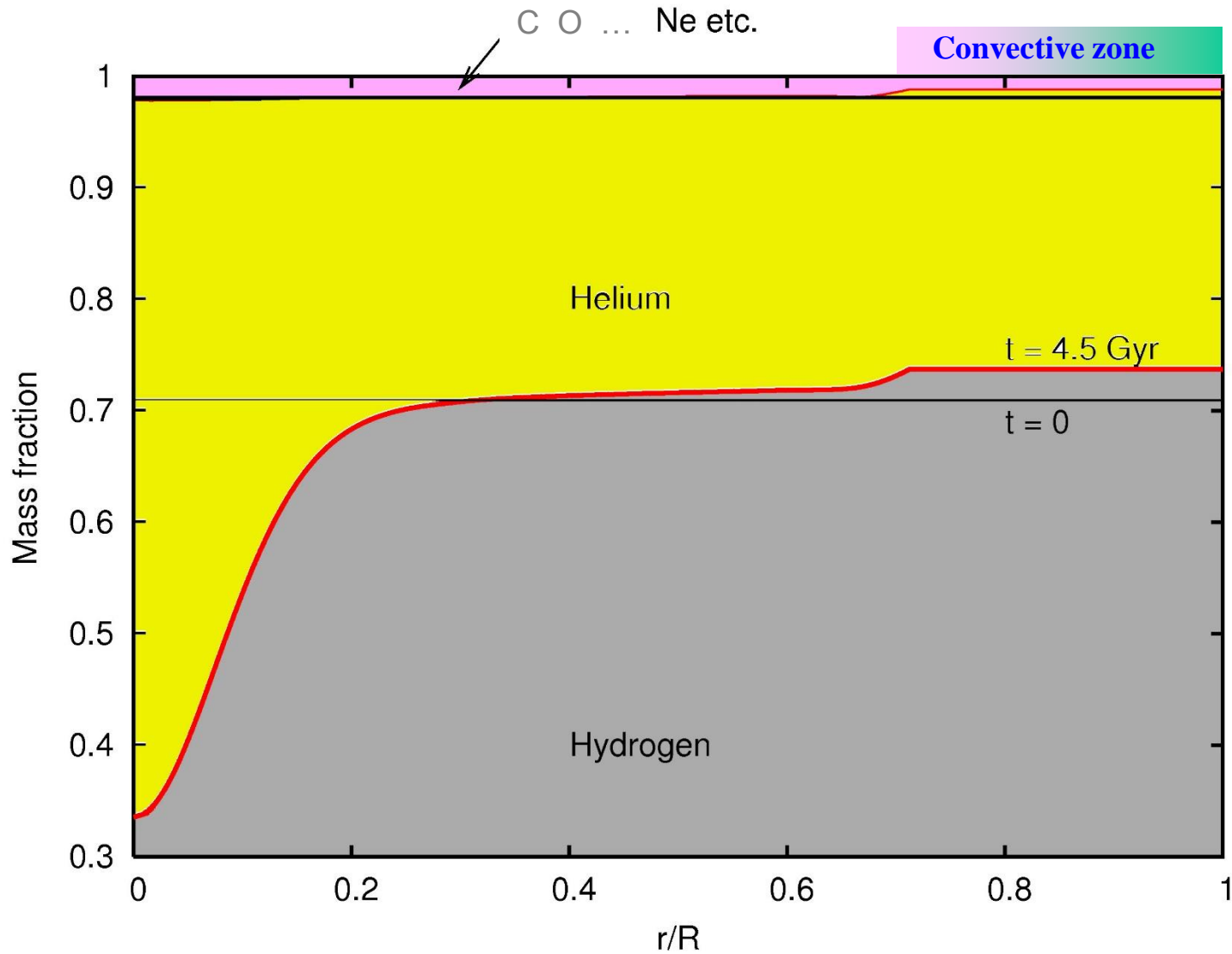
□ Convective zone:

$$0.7 < \frac{r}{R_{\oplus}} < 1$$

Standard solar model

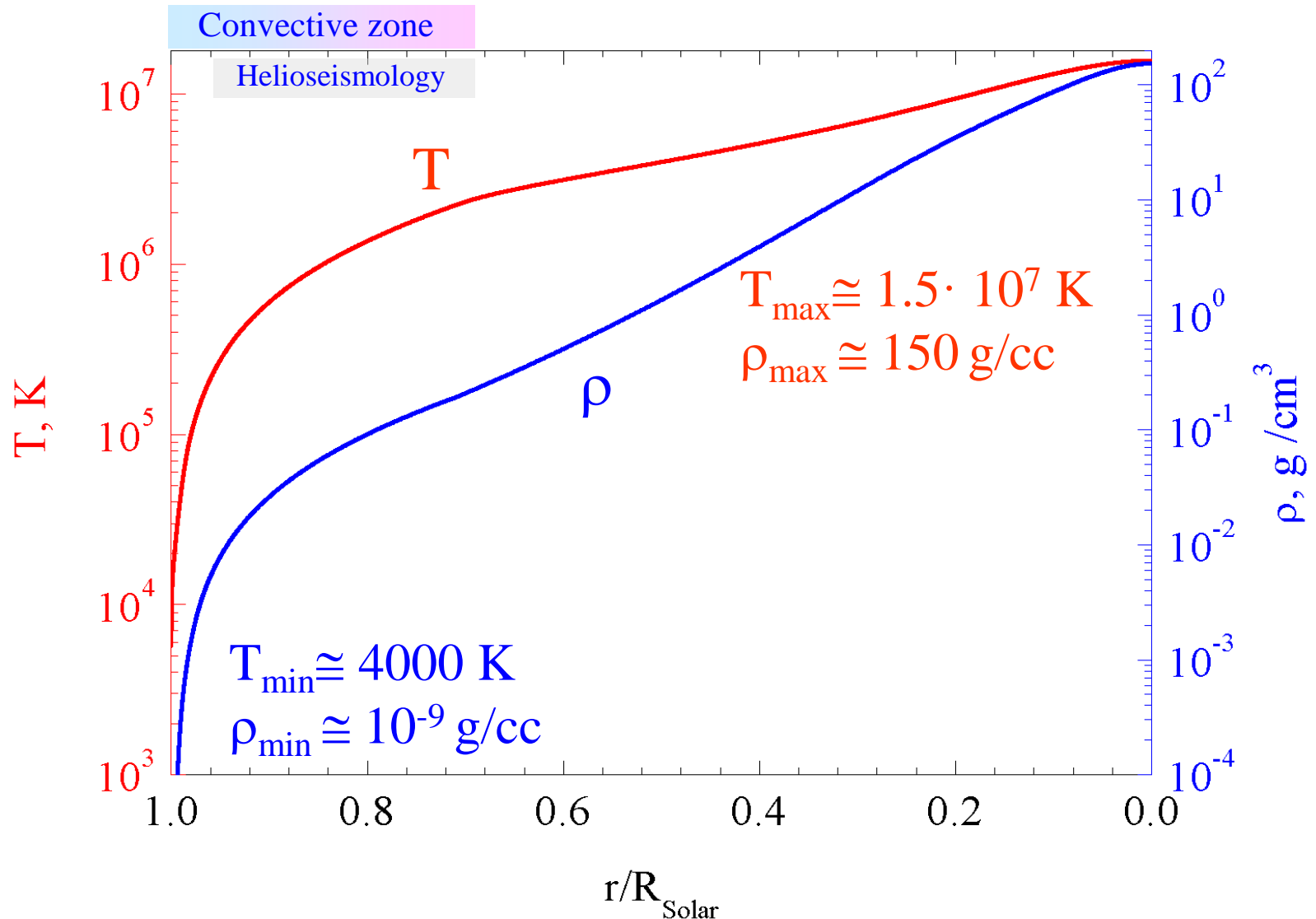
Element composition of solar plasma

H He C O ...

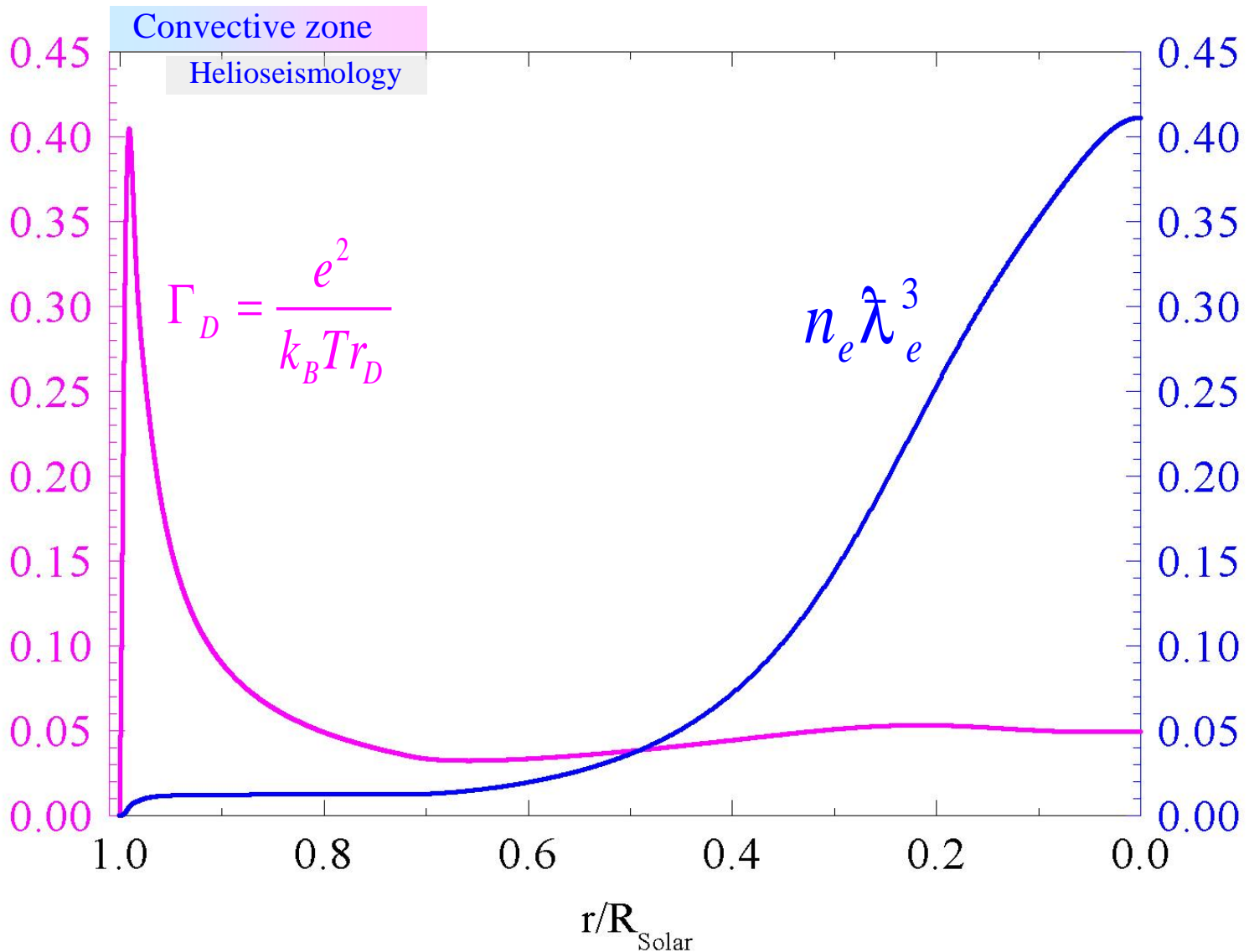


Standard solar model

Density and temperature along solar trajectory

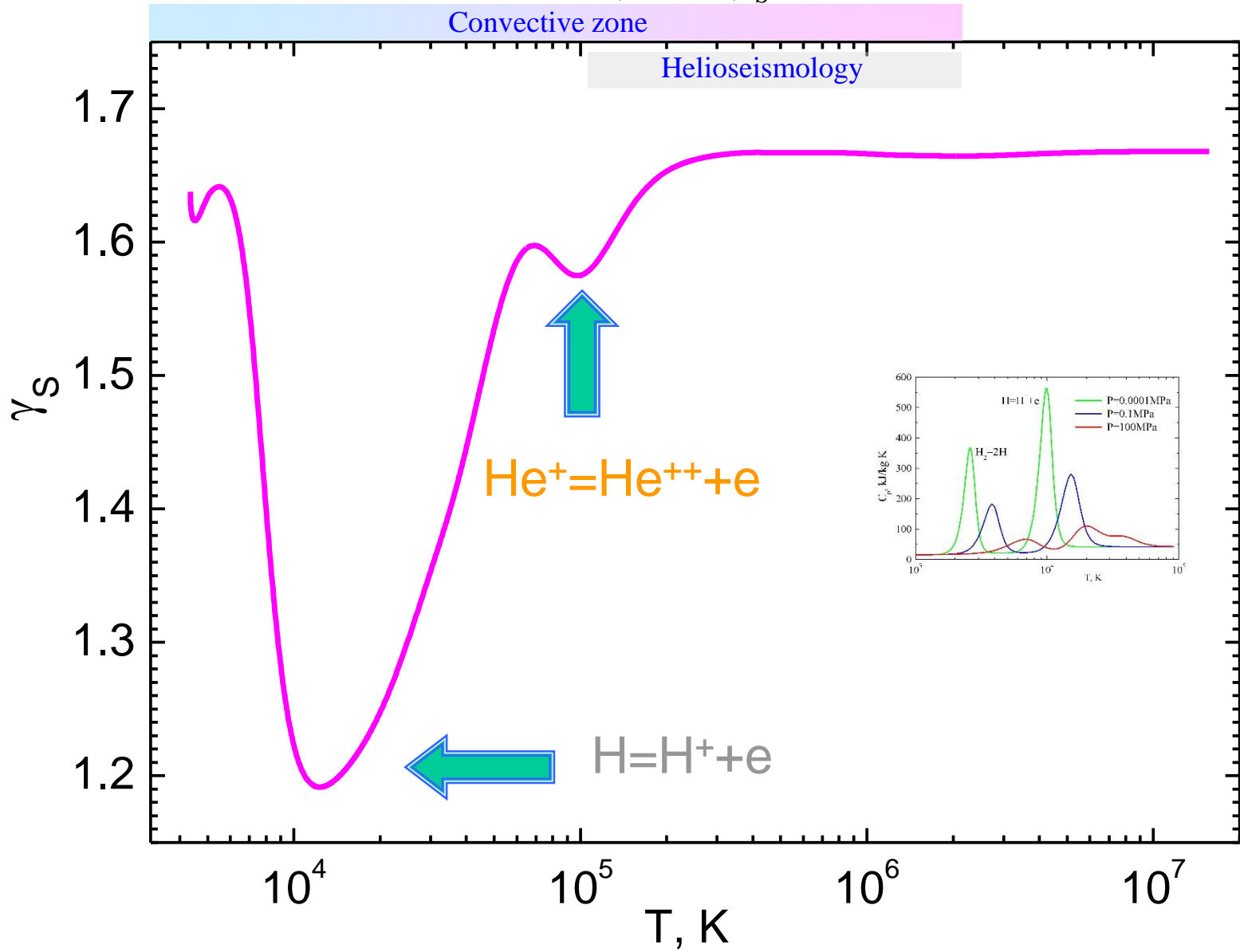


Plasma parameters along solar trajectory

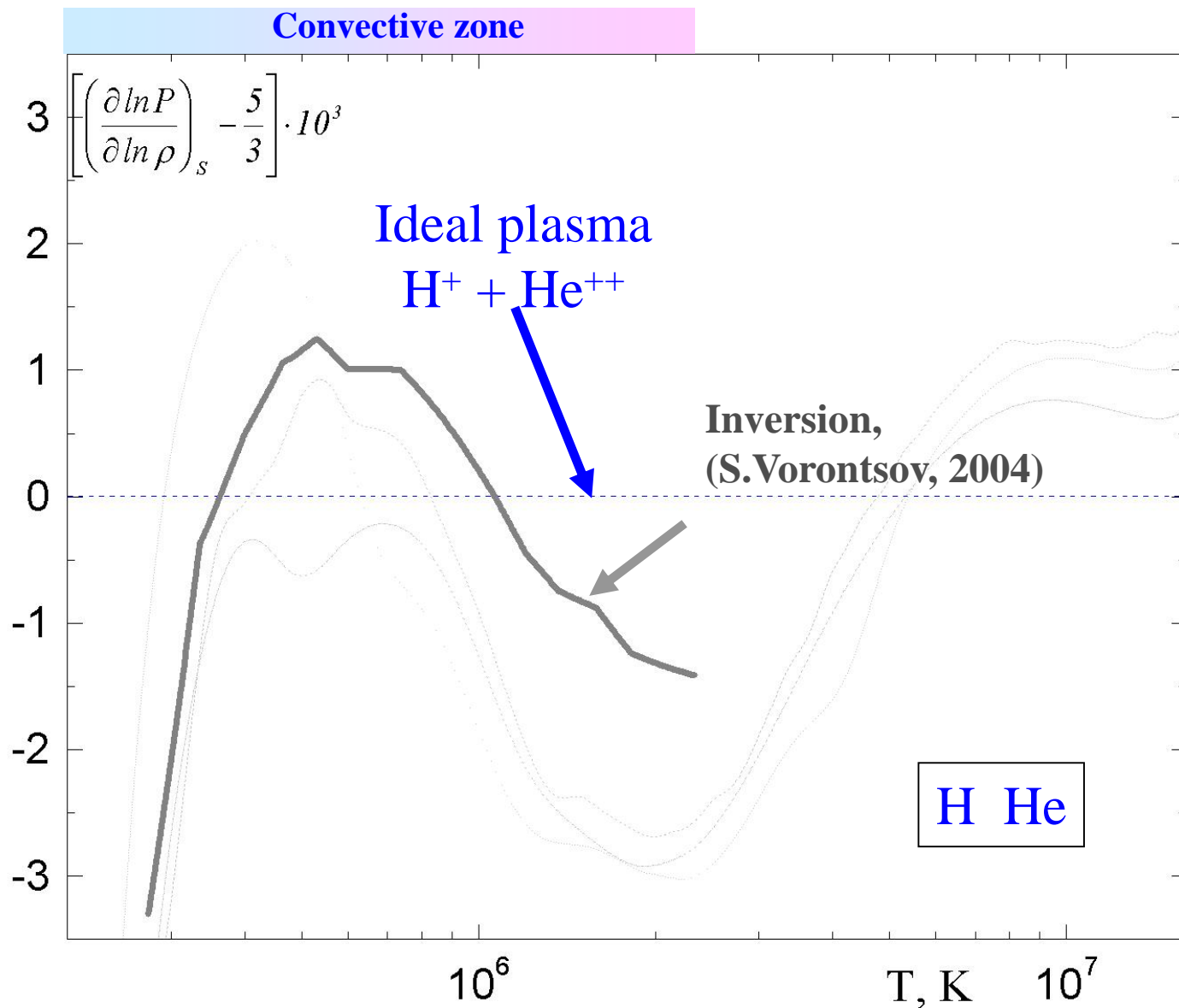


Adiabatic exponent. SAHA-S calculations

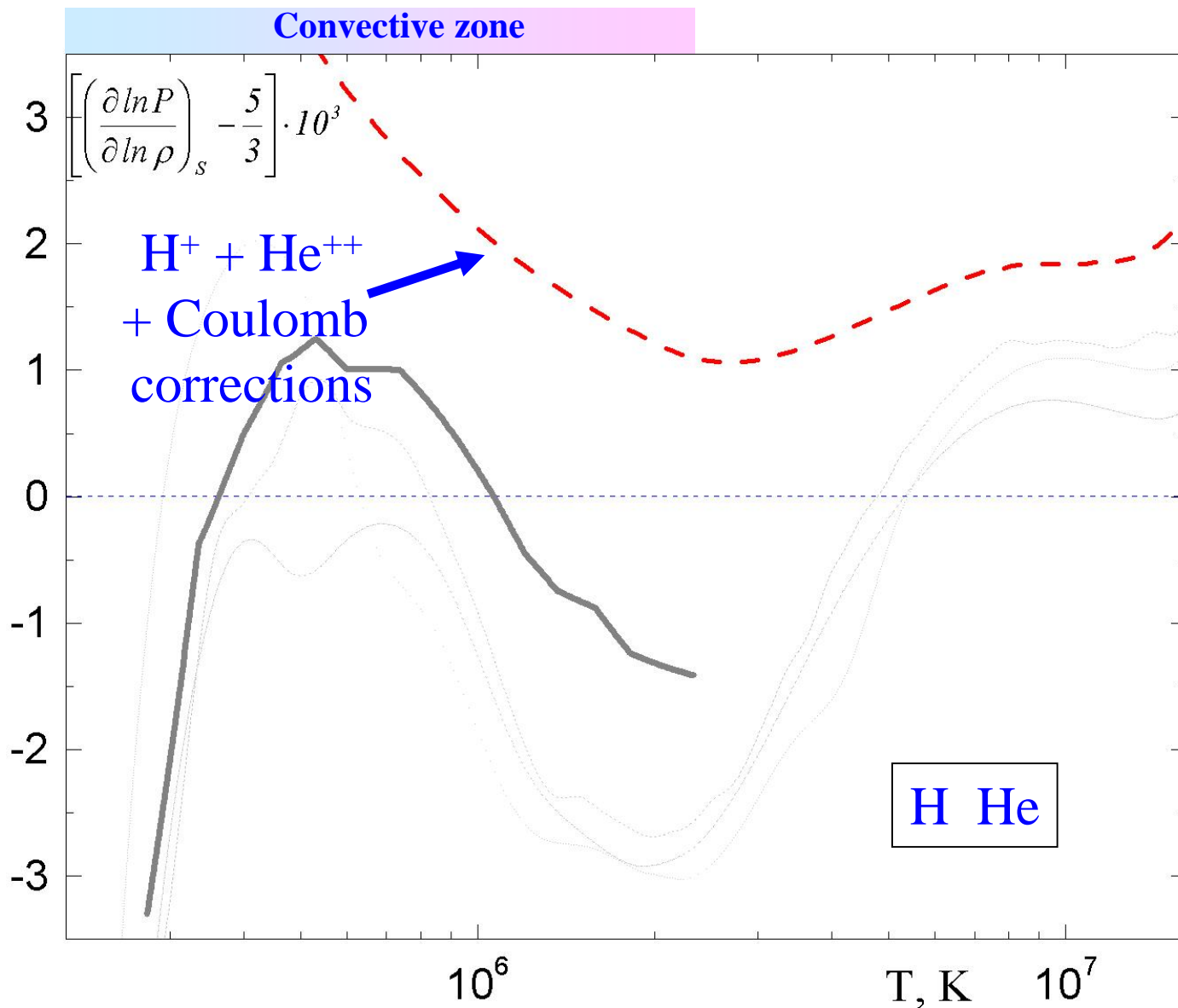
$$\gamma_s \equiv \left(\frac{\partial \ln P}{\partial \ln \rho} \right)_s$$



Adiabatic exponent. Models and inversion results

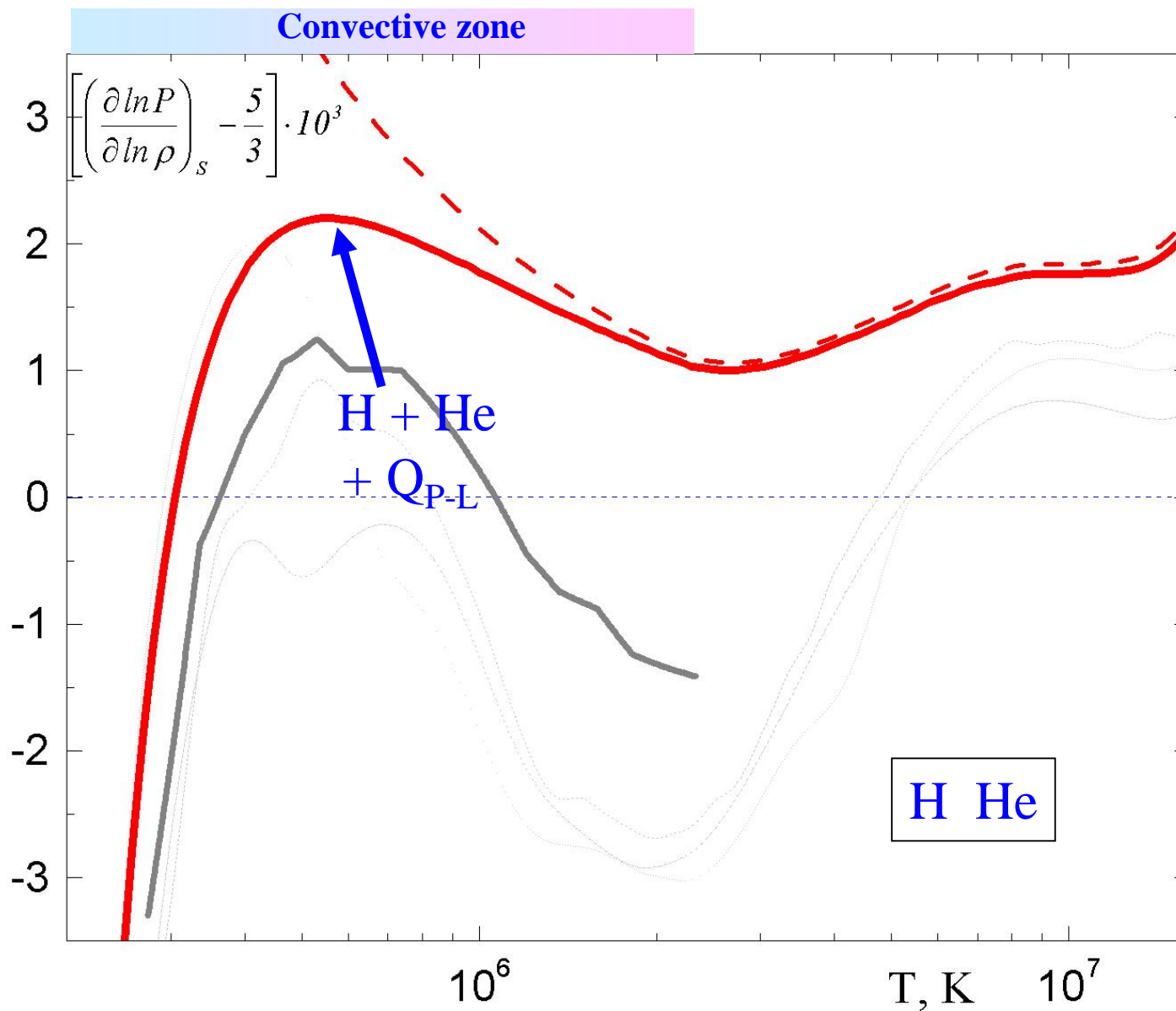


Adiabatic exponent. Models and inversion results



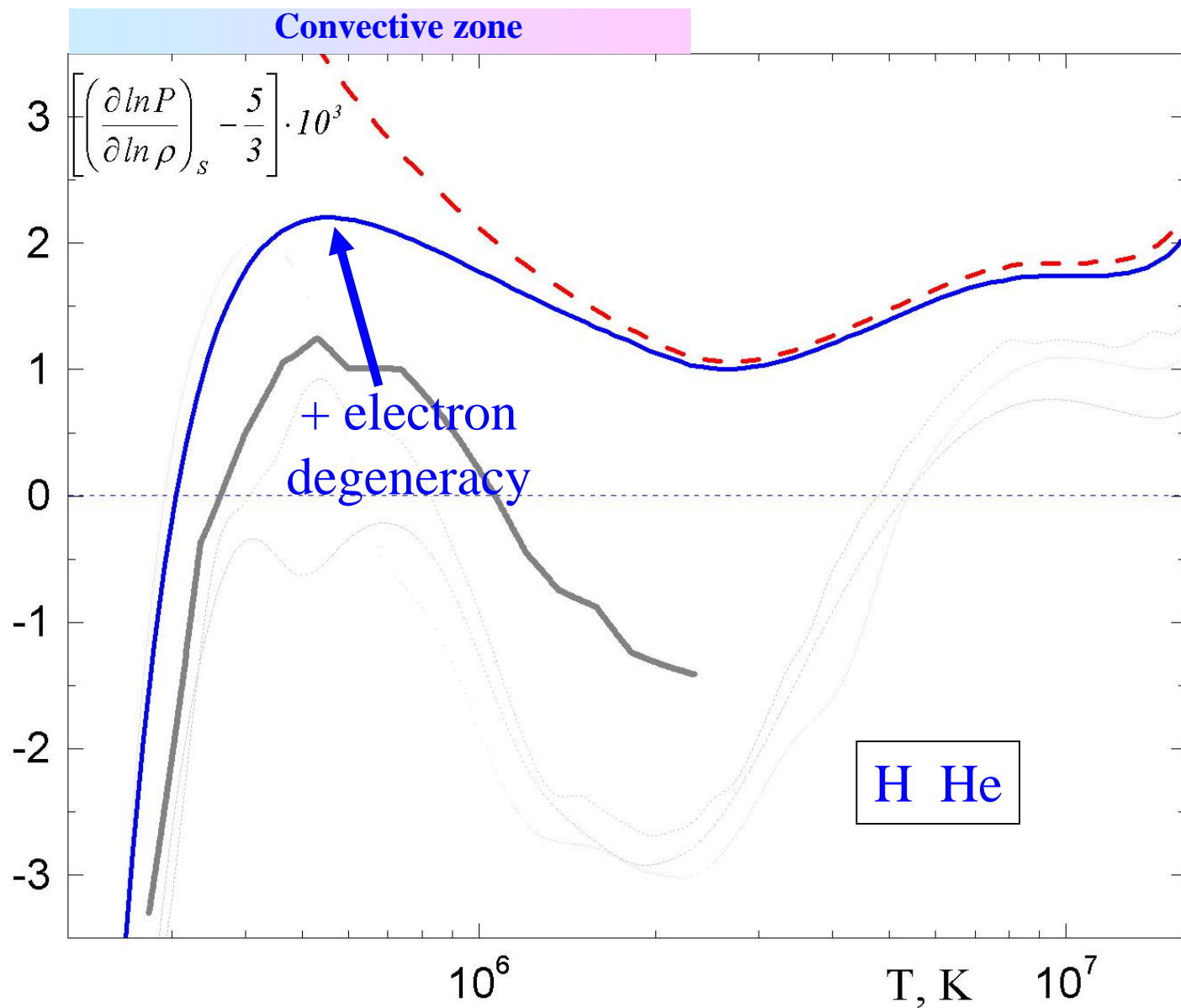
Adiabatic exponent.

Models and inversion results



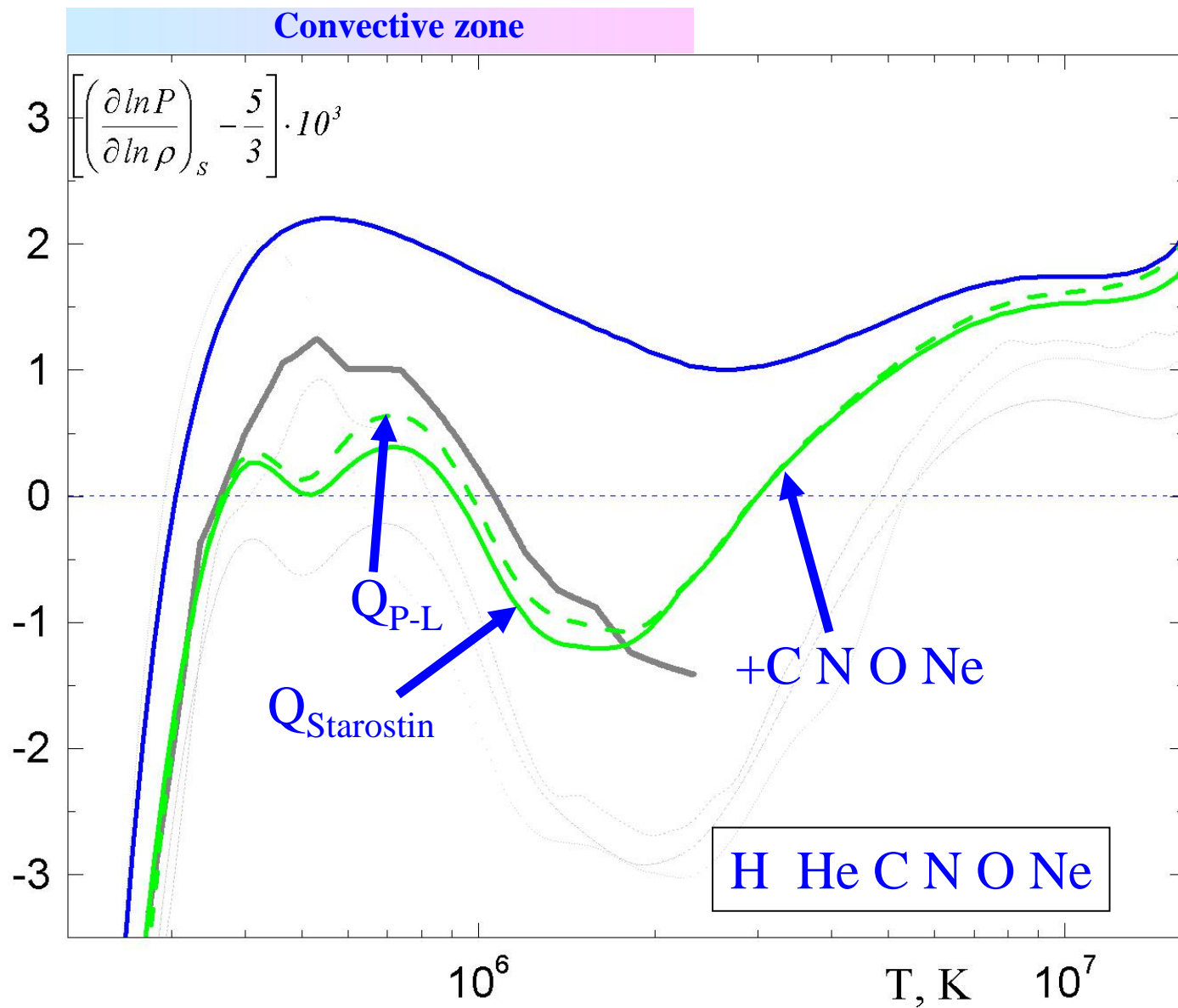
Adiabatic exponent.

Models and inversion results



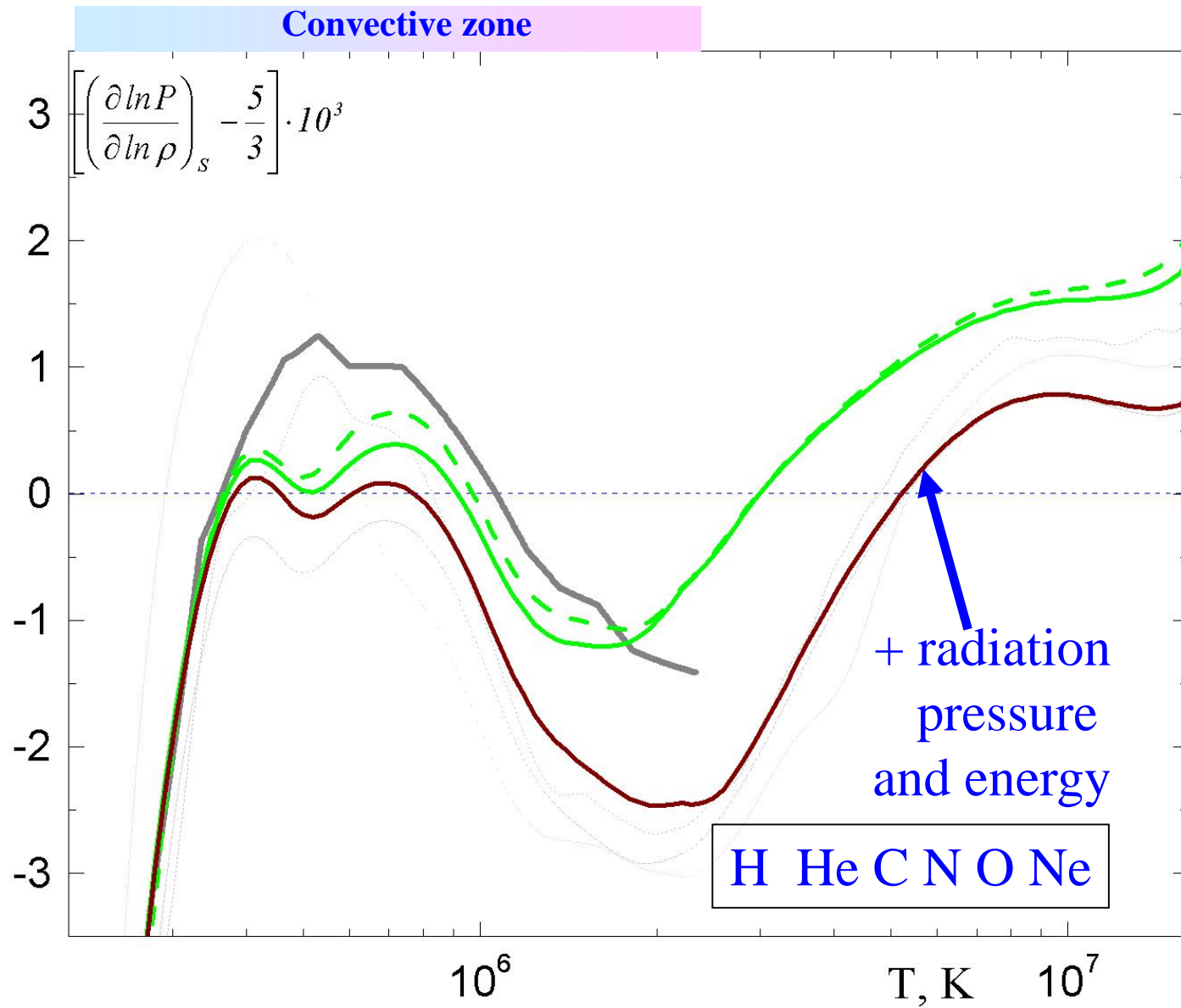
Adiabatic exponent.

Models and inversion results

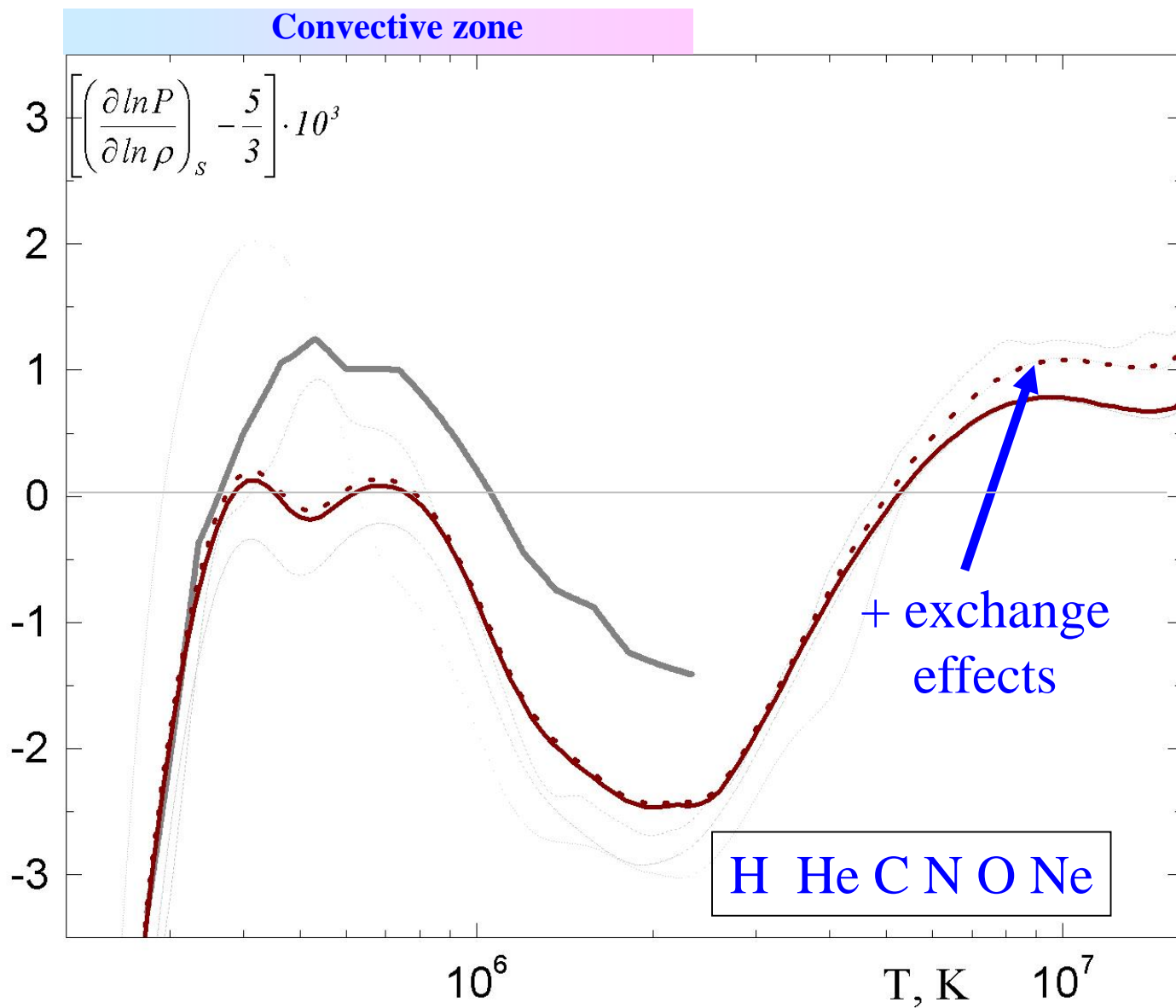


Adiabatic exponent.

Models and inversion results

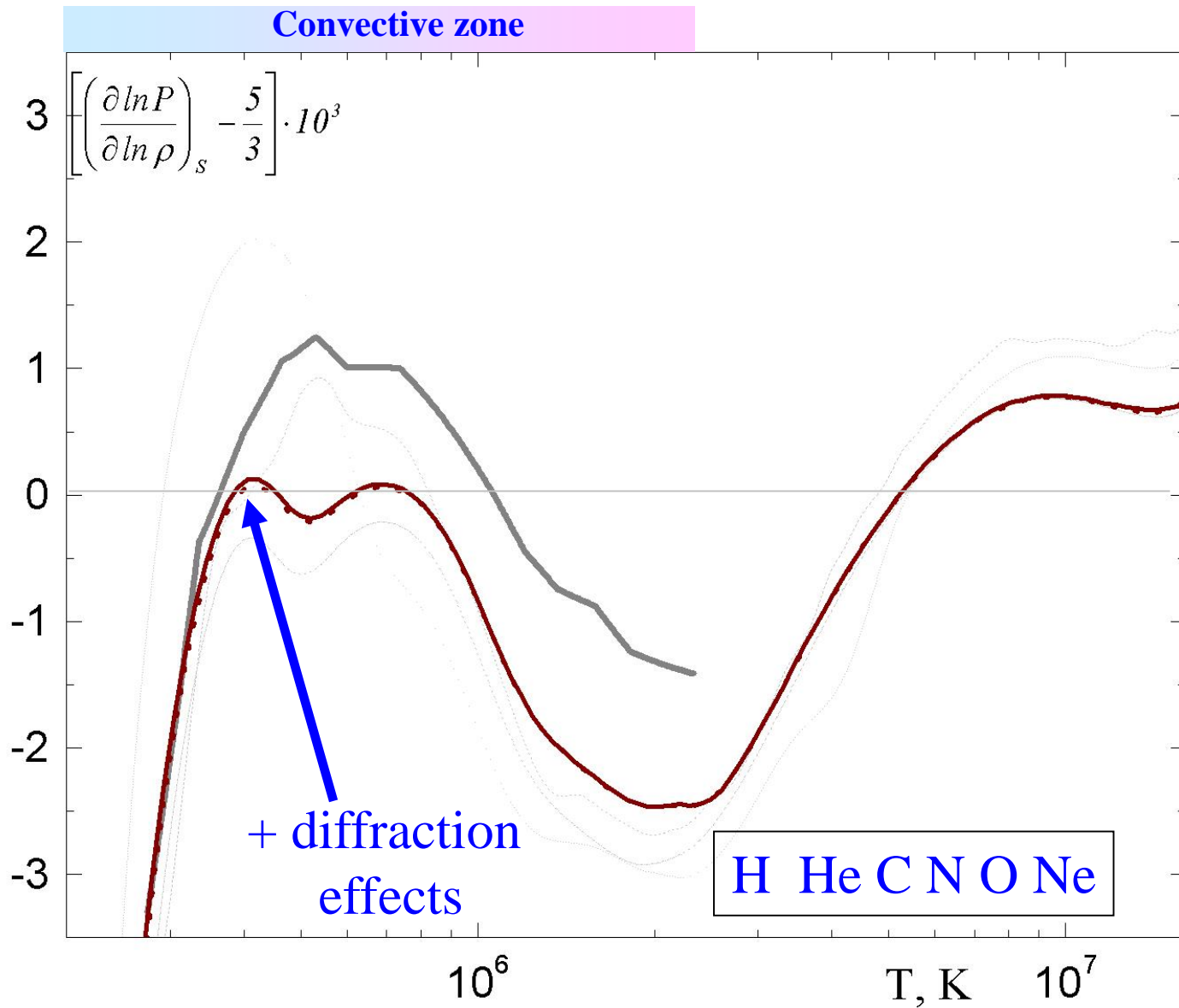


Adiabatic exponent. Models and inversion results

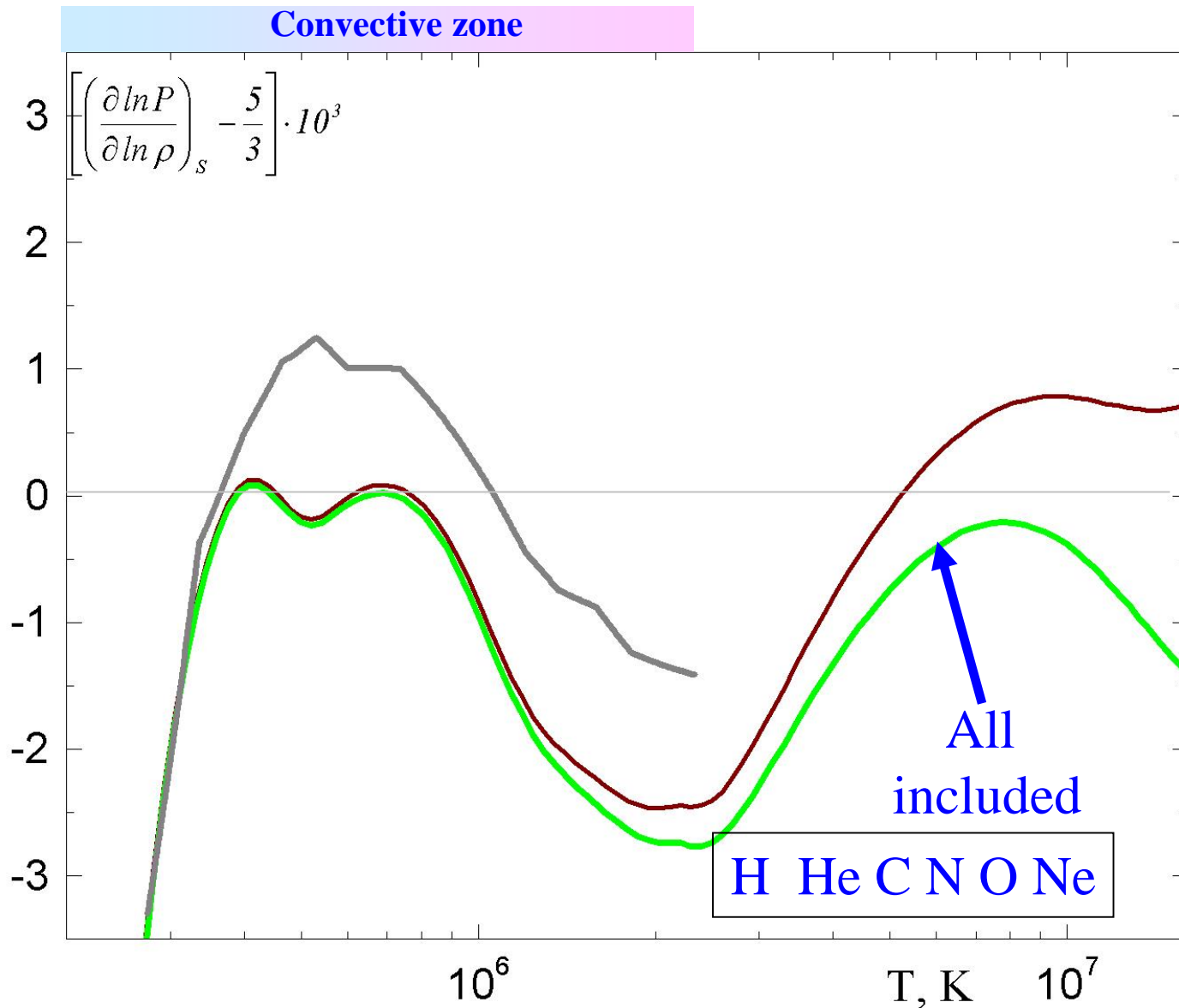


Adiabatic exponent.

Models and inversion results

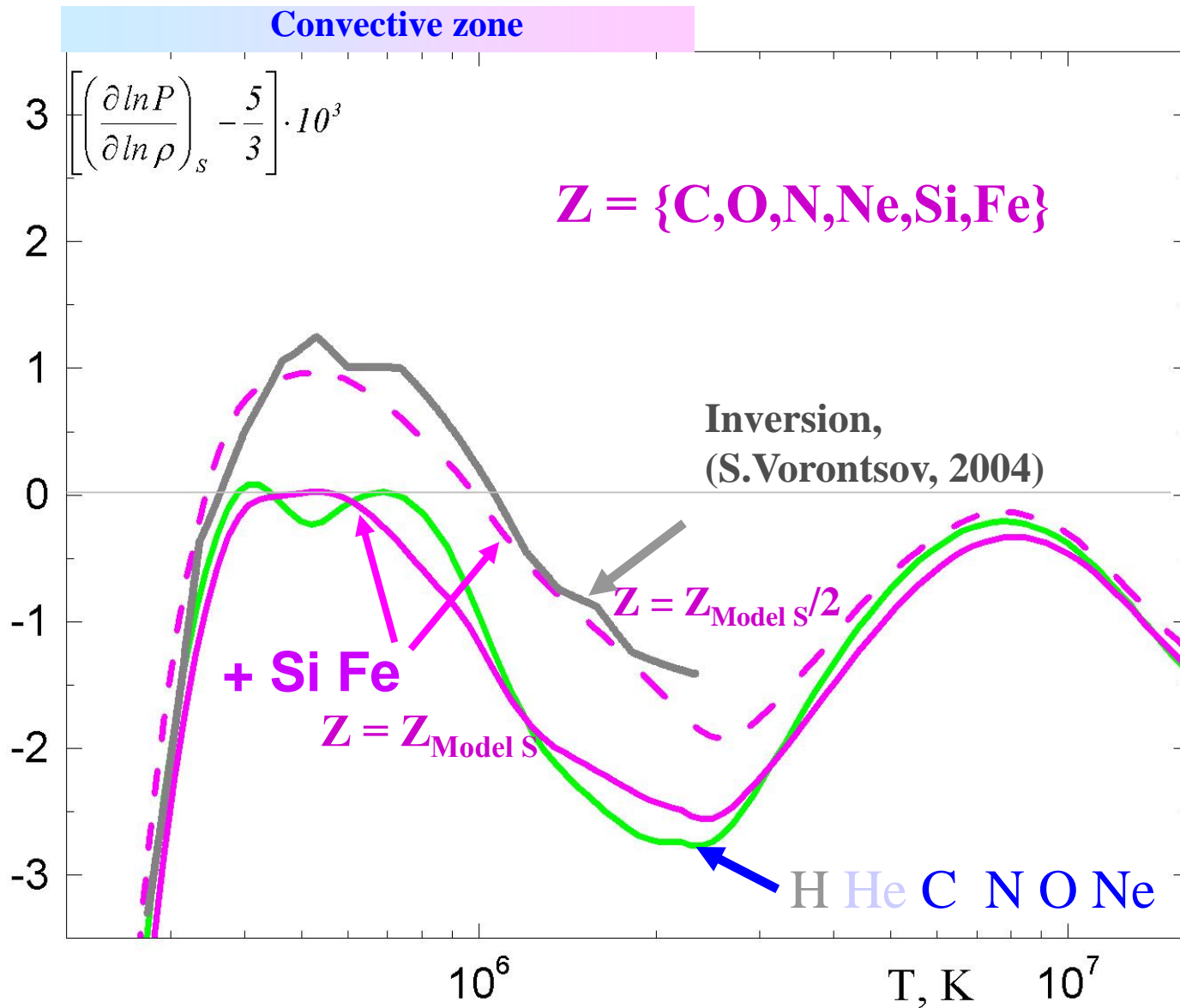


Adiabatic exponent. Models and inversion results



Adiabatic exponent.

Heavy elements contribution



SAHA-S1

Element composition

H He ^{Heavy elements} (C N O Ne)

Heavy element abundance

0.01 ÷ 0.02

50 species of particles**SAHA-S2**

Element composition

H He ^{Heavy elements} (C N O Ne Si Fe)

Heavy element abundance

0.01 ÷ 0.02

95 species of particles, ground states of heavy elements**SAHA-S3****SAHA-S7**

Element composition

H He ^{Heavy elements} (C N O Ne Si Fe Mg S)

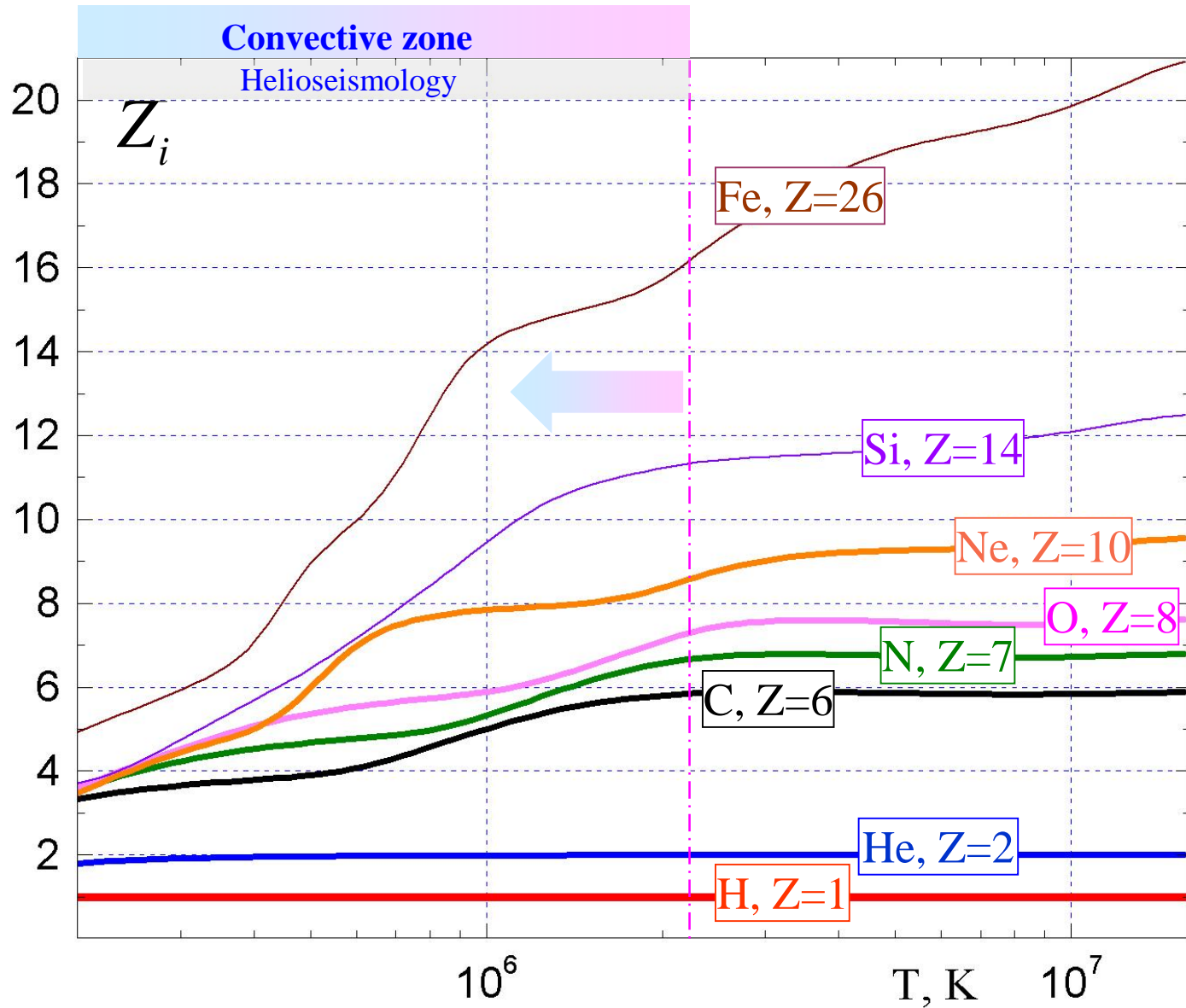
Heavy element abundance

0.005 ÷ 0.02

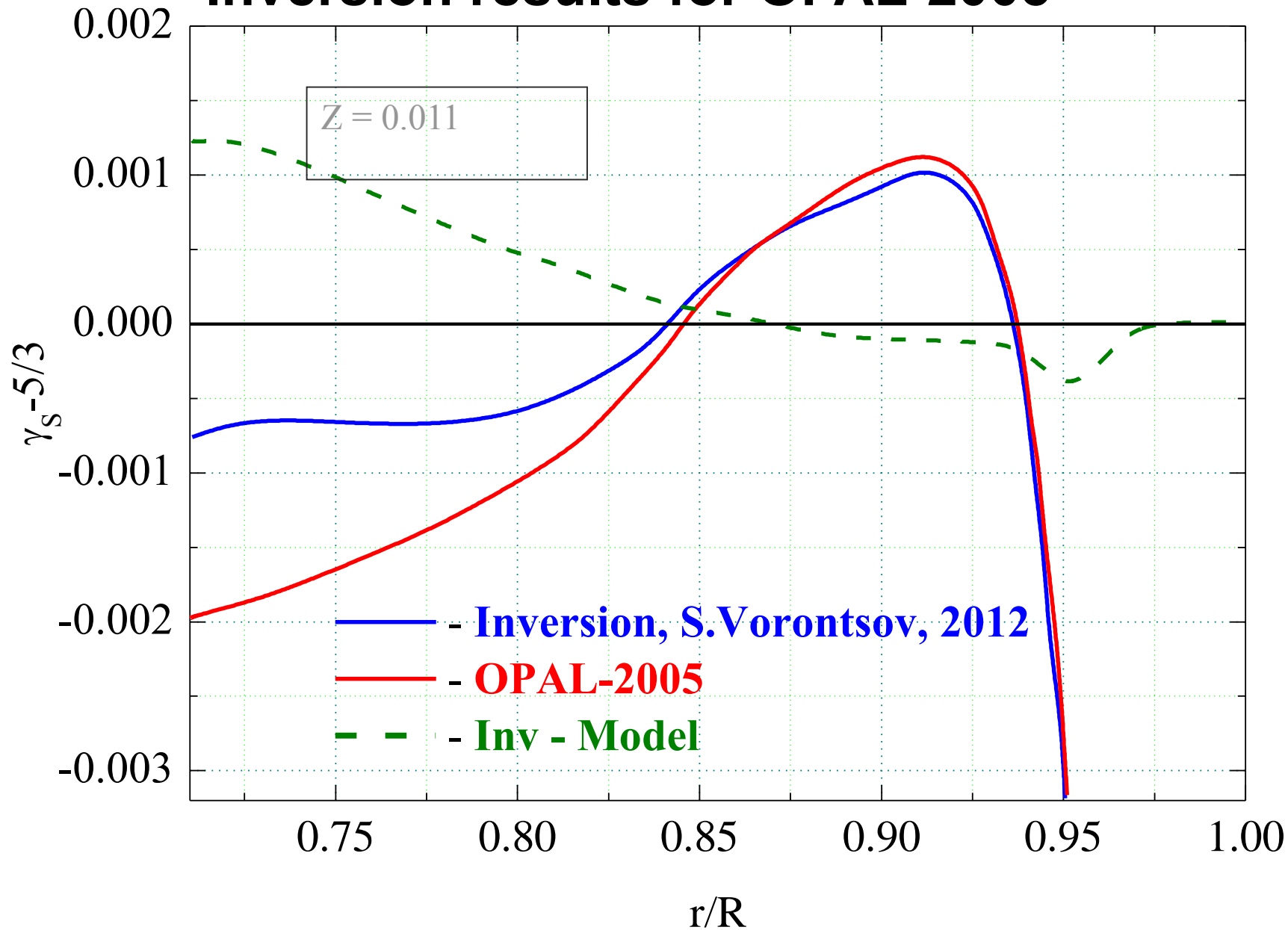
145 species of particles, detailed excitation spectrum of all particles

SAHA-S calculations

Mean charge of ions along solar trajectory

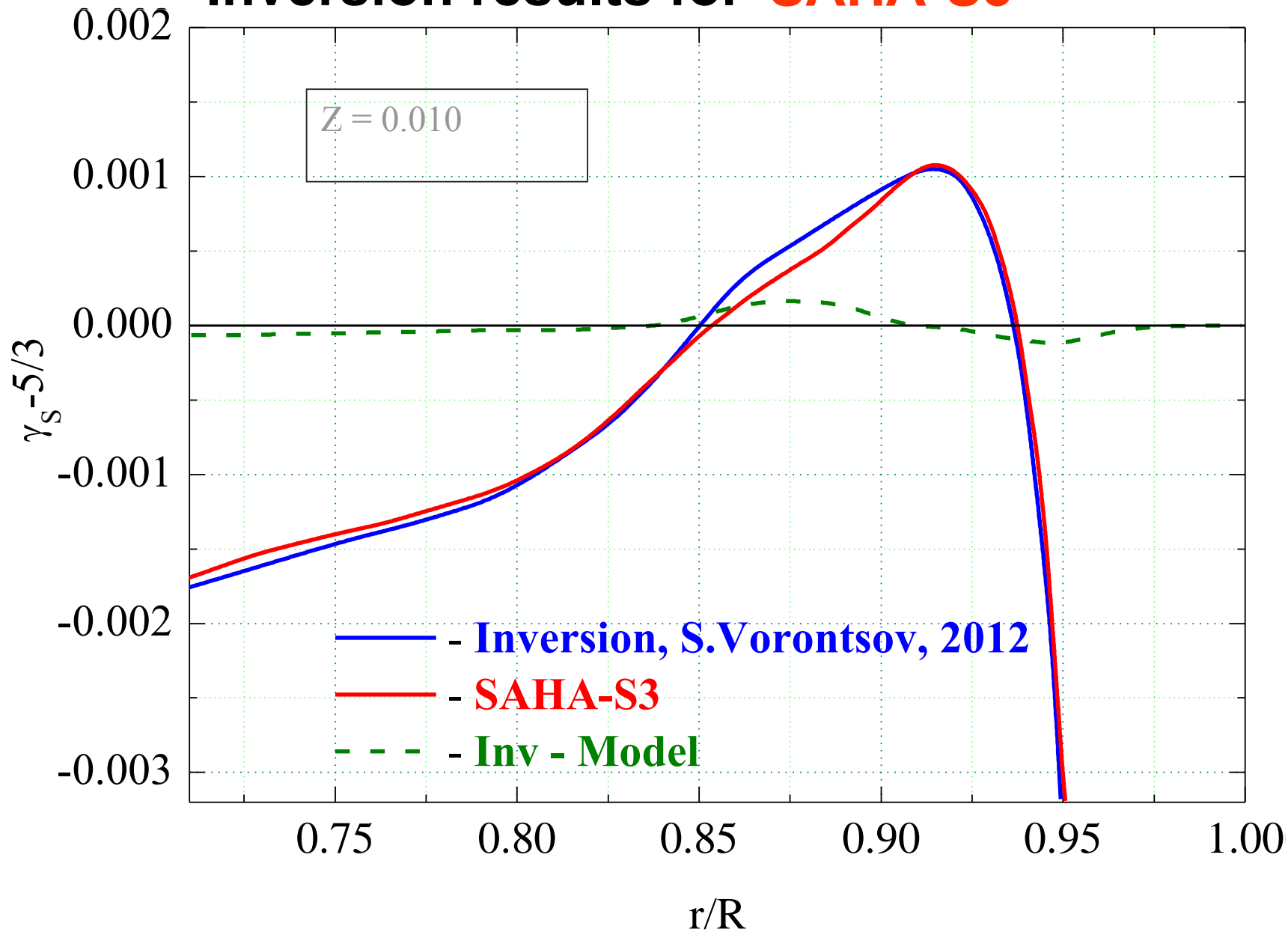


Adiabatic exponent Inversion results for OPAL-2005



Adiabatic exponent

Inversion results for SAHA-S3



Hydrogen. Deviations to the ideal Saha pressure along isochore

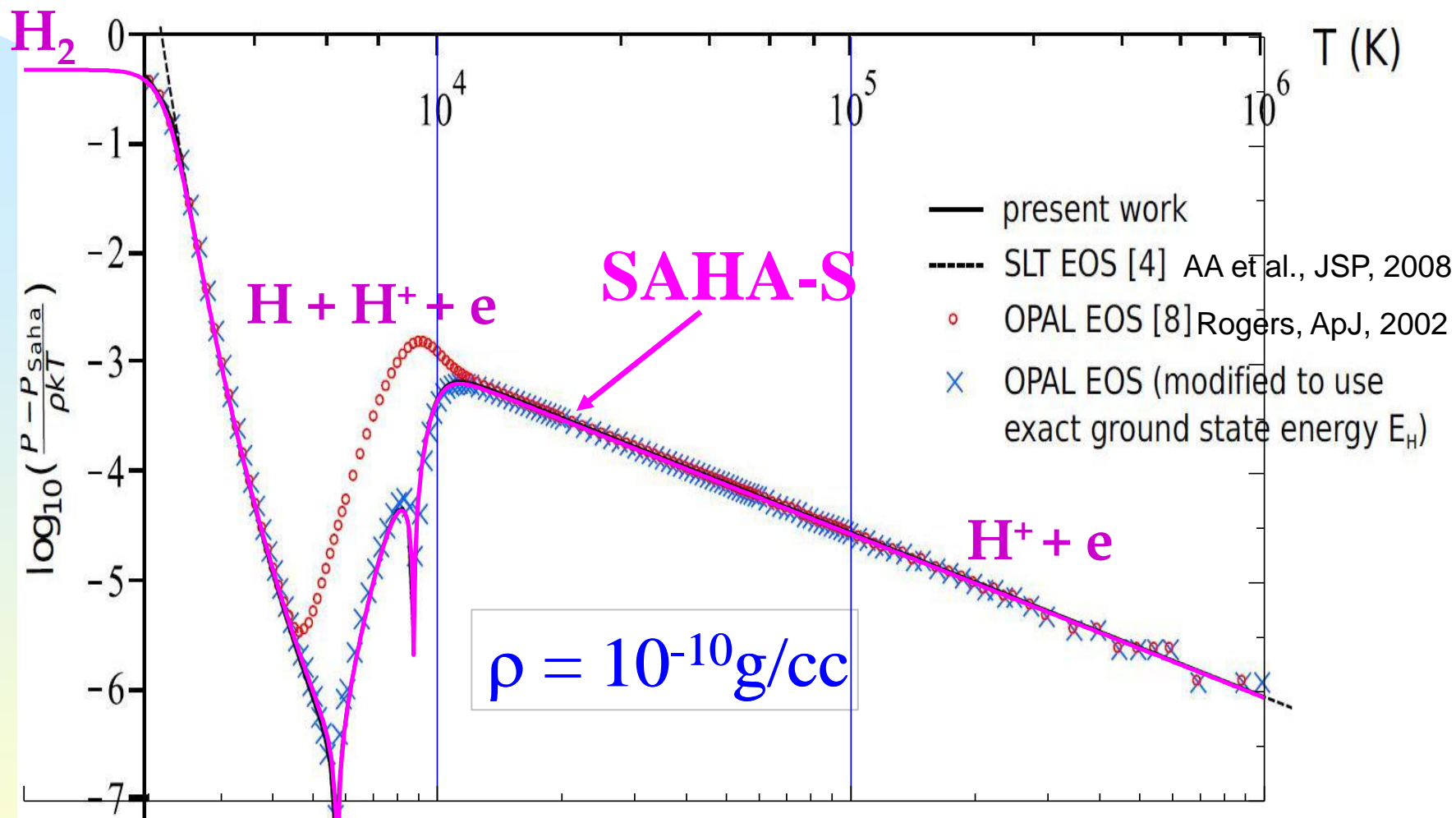


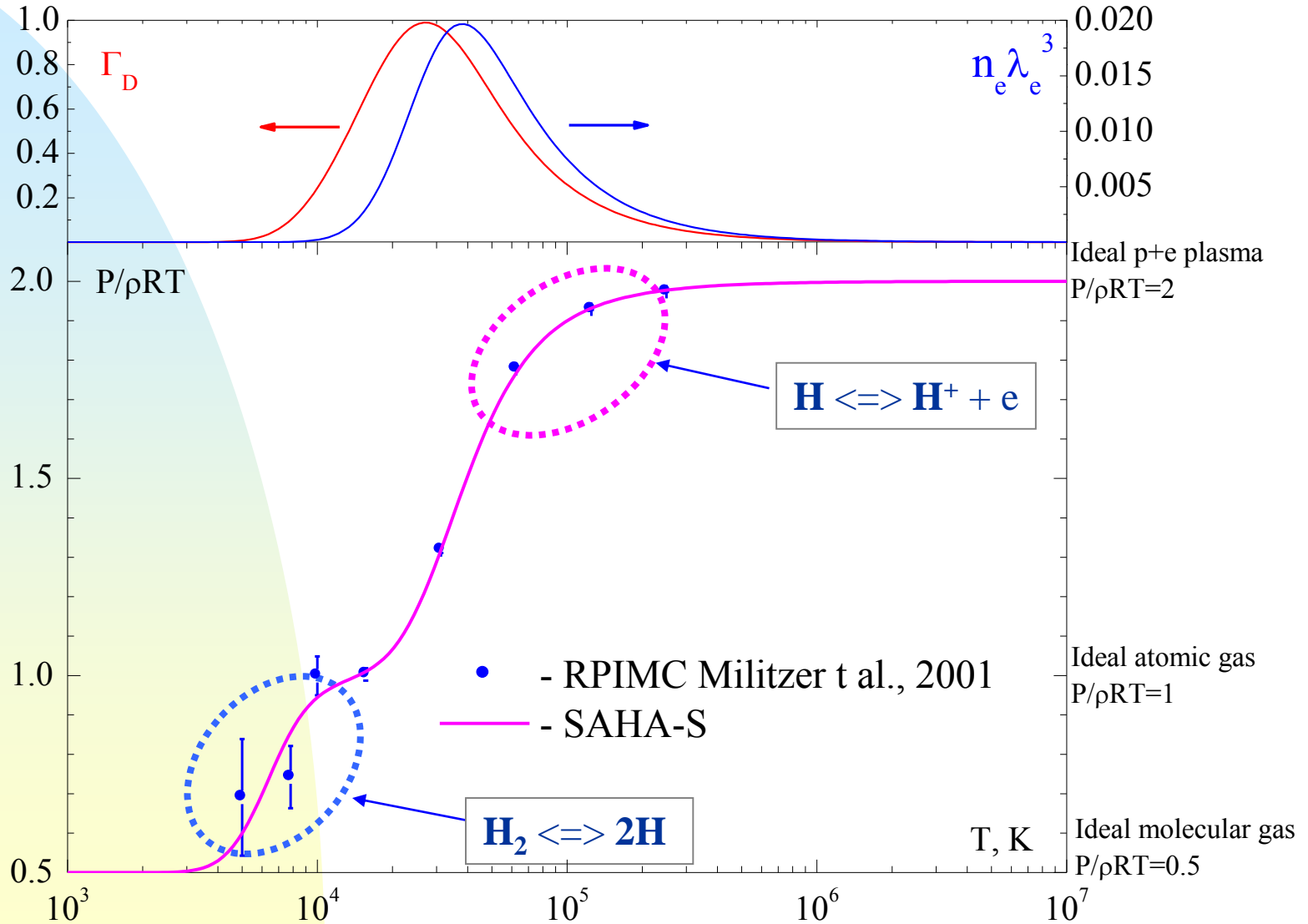
Fig. 2 Log plot of deviations to the ideal Saha pressure along isochore 10^{-10} g/cc . Our predictions (solid line) are compared to the analytical SLT expansion (dashed line) and to the tabulated OPAL equation of state (circles). The crosses correspond to the OPAL EOS modified to account for the finite mass of the proton in the binding energy of the hydrogen atom, i.e. using $E_H = -me^4/(2\hbar^2) \simeq -13.5983 \text{ eV}$ instead of $E_H \simeq 1 \text{ Ry} = -m_e e^4/(2\hbar^2) \simeq -13.65057 \text{ eV}$. We corrected the OPAL values only at the level of the ideal terms: $P_{\text{OPAL, corr}} = P_{\text{OPAL}} + P_{\text{Saha}}[E_H] - P_{\text{Saha}}[1 \text{ Ry}]$.

Fig. from A. Alastuey and V. Ballenegger, Contrib. Plasma Phys. 52, 2012

Thermal EOS of hydrogen along isochore

(low density)

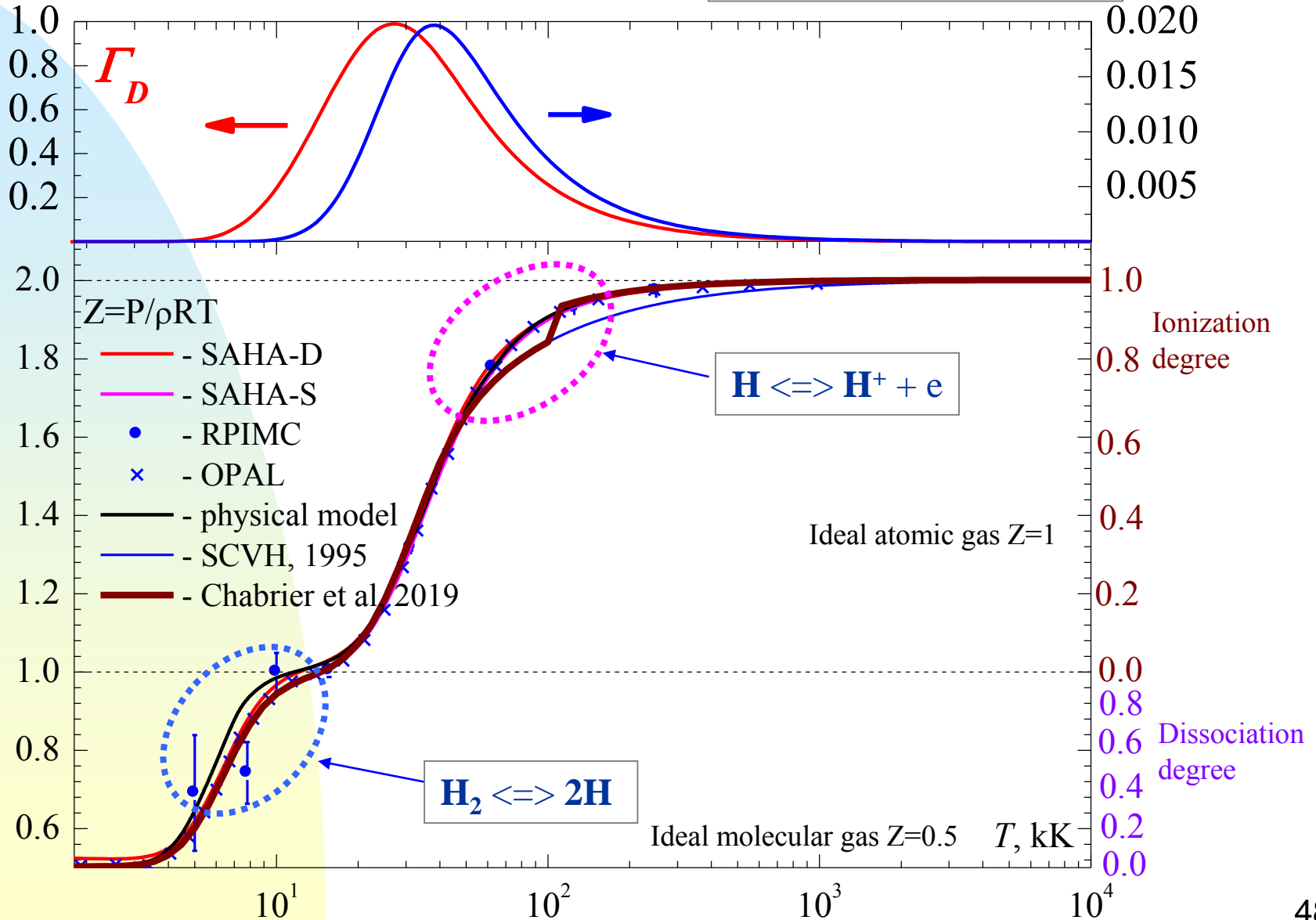
$r_s=14; \rho = 0.001 \text{ g/cm}^3$



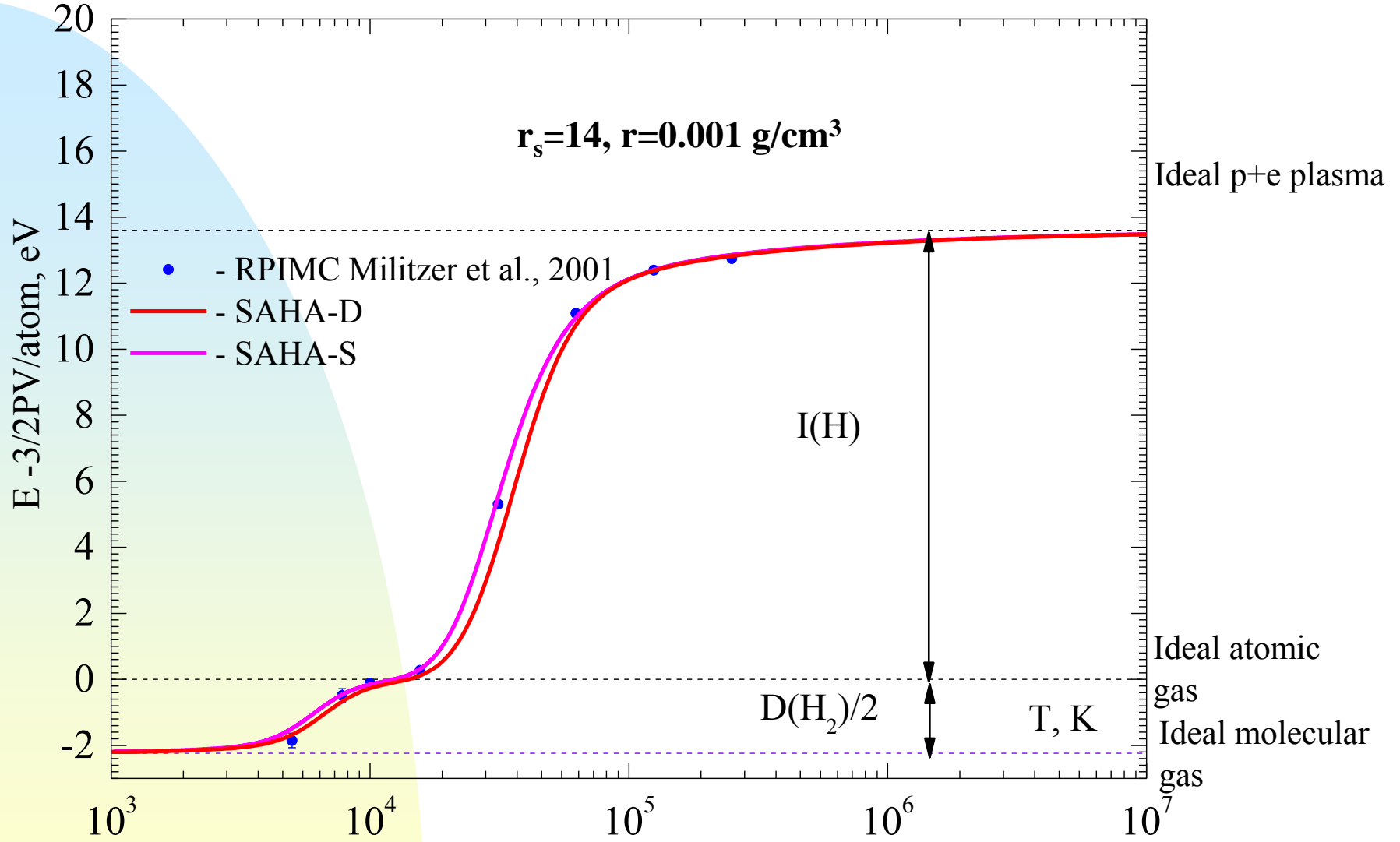
Thermal EOS of hydrogen along isochore

(low density)

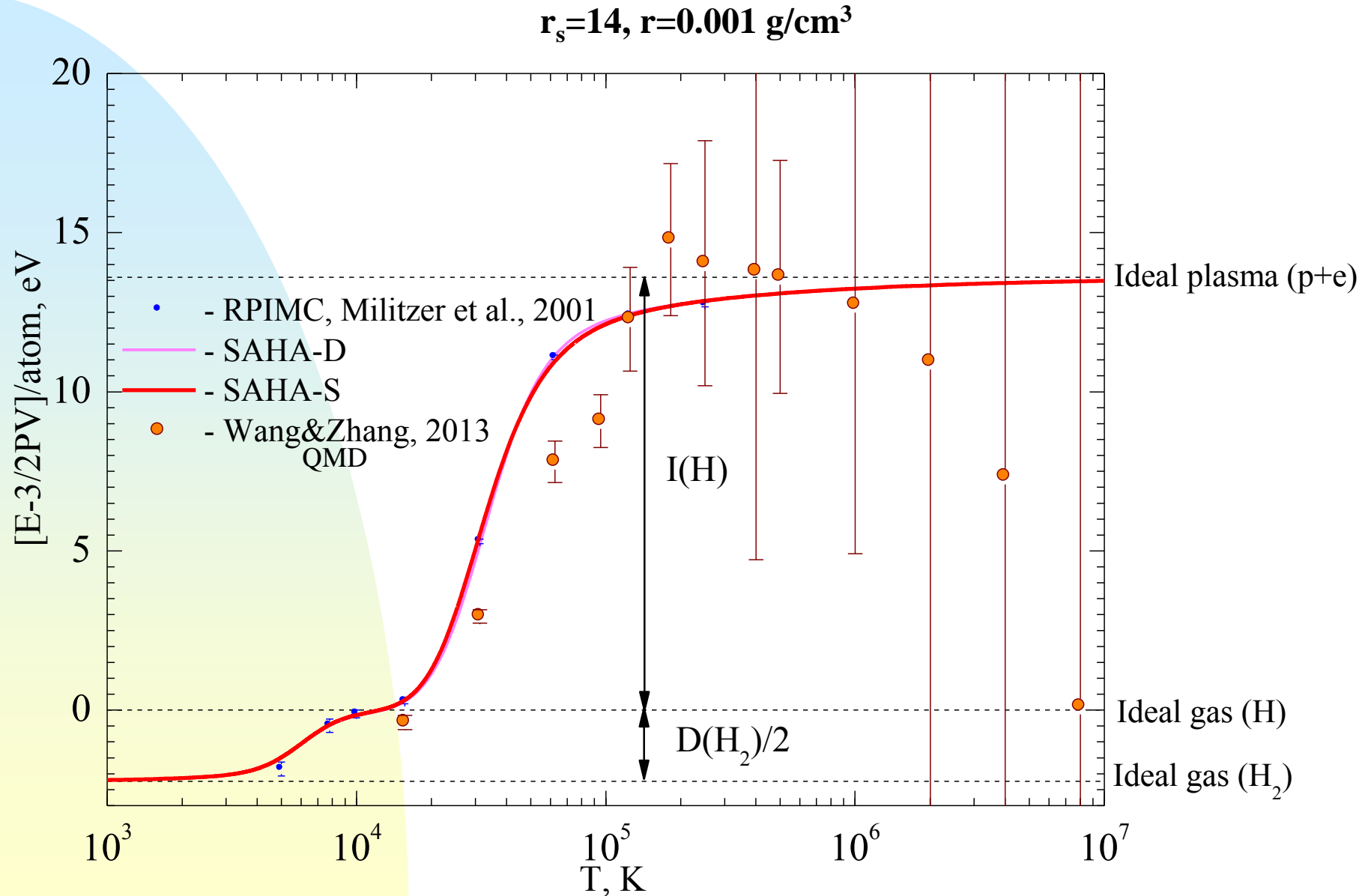
$r_s=14; \rho = 0.001 \text{ g/cm}^3$



Caloric EOS of Hydrogen along isochore

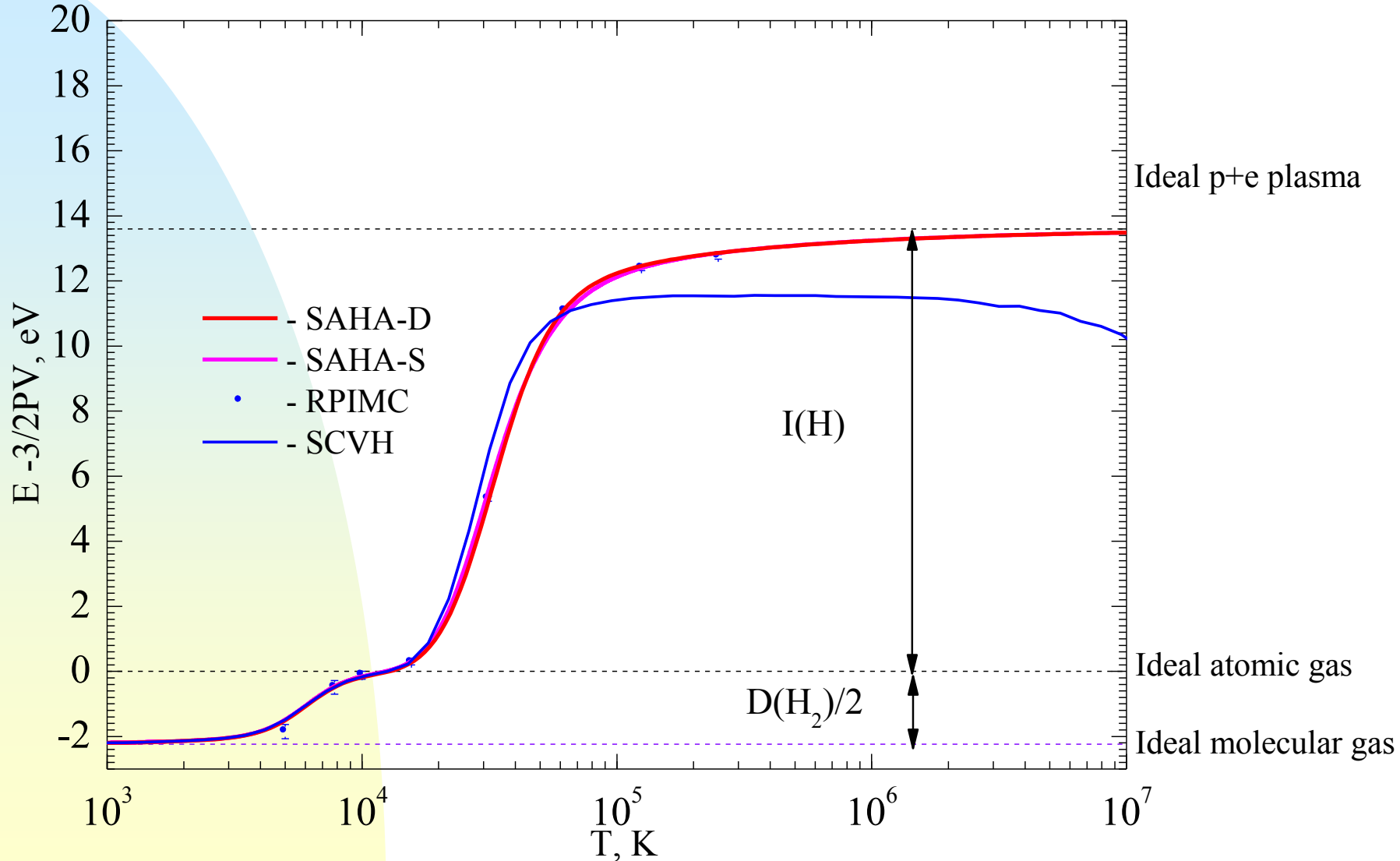


Caloric EOS of Hydrogen along isochore



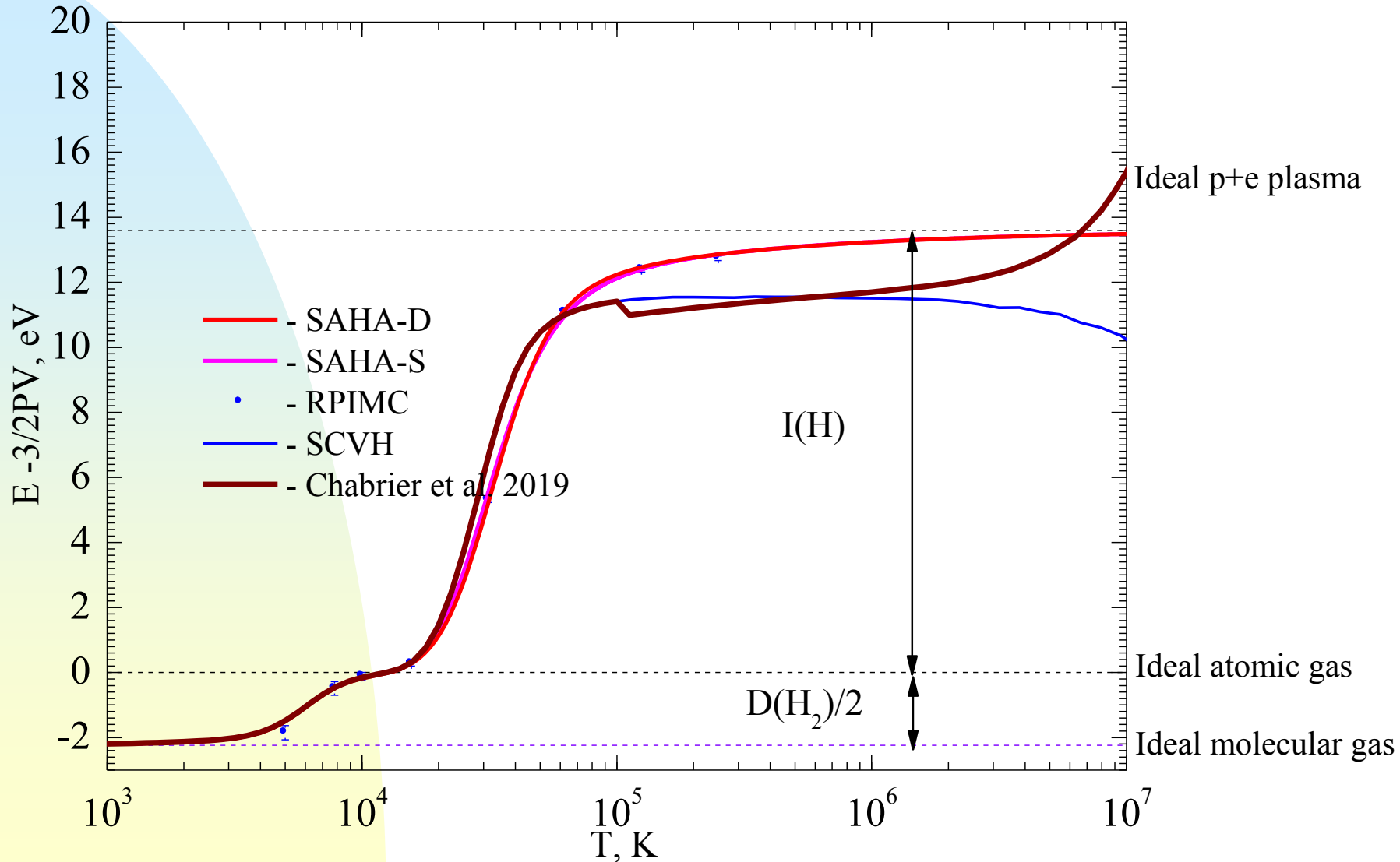
Caloric EOS of Hydrogen along isochore

$r_s=14, r=0.001 \text{ g/cm}^3$



Caloric EOS of Hydrogen along isochore

$r_s=14, r=0.001 \text{ g/cm}^3$

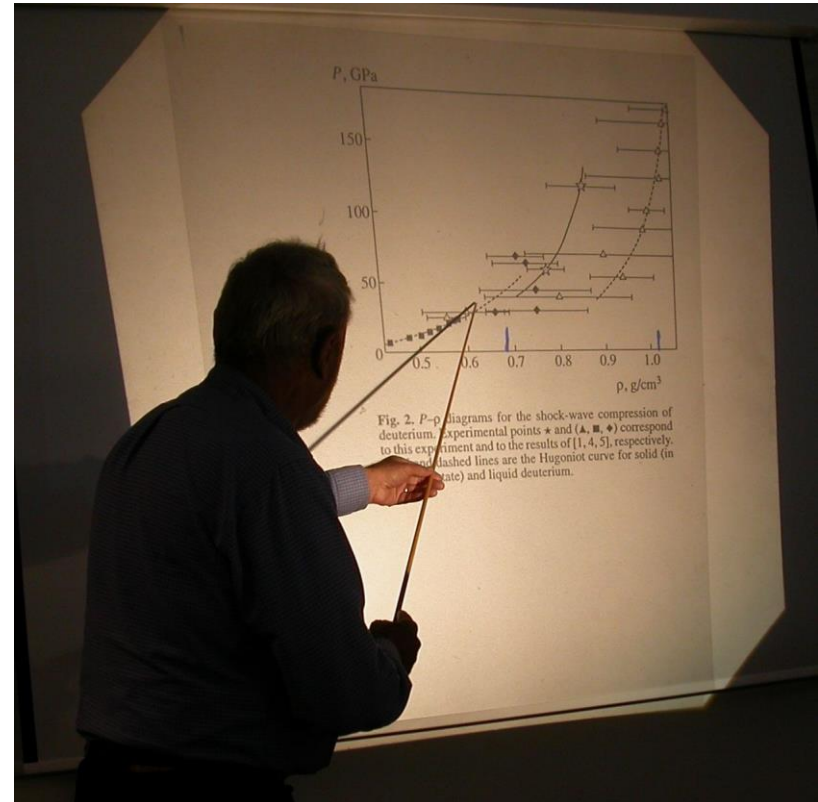


Leiden 2004

Lorentz Center



Equation-of-State and Phase-Transition Issues in Models of Ordinary Astrophysical Matter
from 2 Jun 2004 through 11 Jun 2004







Thank you!