

# Bound states in nonideal plasmas: formulation of the partition function and application to the solar interior

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## Abstract

A detailed independent derivation of the hydrogen weakly nonideal plasma equation of state (EOS) is presented. In our computations relativistic corrections, degeneracy of electrons, radiation pressure in the plasma, Coulomb interaction in the Debye–Hückel approximation together with diffraction and exchange corrections and the contribution of bound and scattering states (SS) are taken into account. In contrast to the Planck–Larkin partition function, a correct separate account of bound and SS allows a natural generalization for the broadening of atomic states.

The essential part of the EOS and adiabatic exponent is connected with the correct account of bound states. In our paper we compare the results of different approaches with the bound states description and for the first time consider the influence of atomic states broadening on the bound states contribution.

## 1. Introduction

Helioseismology reveals a unique possibility of checking within an accuracy of better than  $10^{-4}$  the equation of state (EOS) of weakly nonideal plasmas due to the inversion of local sound velocity from optical observations [1]. The comparison of different theoretical models with experiment permits checking the existing ways to account for the bound and scattering states (SS) contributions, which are presented in the physical literature for the second virial coefficient (SVC) [2–4].

The contribution of the bound states is usually described by the Planck–Larkin (P–L) partition function [5, 6]. An expression different from the P–L formula was published in [7] and was later confirmed in [8–10]. This partition function contains the pure contribution of the bound states in contrast to the P–L one which includes some terms due to the continuum spectrum. The Baym–Kadanoff formalism permits generalizing the bound states contribution in a natural way to account for the broadening effects. In our work this generalization is presented together with the preliminary results in the calculation of thermodynamic properties of weakly nonideal hydrogen plasma for atomic states broadening.

## 2. Thermodynamic perturbation theory

According to [10] we can calculate plasma pressure  $P$ , using corrections to the pressure  $P_0$  of ideal gas that consists of electrons and protons:

$$P = P_0 + P_H + P_{\text{exch}} + P_{\text{D-H}} + \delta P, \quad (1)$$

where we include the corrections discussed below:  $P_H$  is the Hartree correction,  $P_{\text{exch}}$  is due to the electron–electron exchange interaction,  $P_{\text{D-H}}$  is the plasma Coulomb interaction in the Debye–Hückel approximation and  $\delta P$  is a higher order correction, which takes into account the contribution from ladder diagrams.

We shall consider protons as non-degenerate particles; their ideal gas activity  $\zeta_p$  is connected in grand canonical ensemble with their chemical potential  $\mu_p$  and temperature  $T$  ( $\beta = T^{-1}$ ):

$$\zeta_p = 2\lambda_p^{-3} e^{\beta\mu_p}, \quad (2)$$

where  $\lambda_p = \sqrt{(2\pi\hbar^2)/(m_p T)}$  is the thermal de Broglie wavelength for protons. The pressure of an ideal gas of protons is

$$P_{0p} = T\zeta_p. \quad (3)$$

Electrons may be degenerate (e.g. at the centre of the Sun a parameter  $n_e \lambda_e^3 \approx 0.6$ ), so we shall express their activity  $\zeta_e$  [11] via ideal gas concentration  $n_e^0$ , for the general case of degenerate particles, taking into account the relativistic correction:

$$n_e^0(\mu_e) \equiv \zeta_e = \frac{2}{\sqrt{\pi}} \frac{2}{\lambda_e^3} \int_0^\infty \frac{x^{1/2} (1 + (5/4)(T/mc^2)x)}{e^{x-y} + 1} dx. \quad (4)$$

Here  $x = \varepsilon/T$ ,  $y = \mu_e/T$ . For electron gas pressure we have

$$P_{0e} = \frac{4T}{3\sqrt{\pi}} \frac{2}{\lambda_e^3} \int_0^\infty \frac{x^{3/2} (1 + (3/4)(T/mc^2)x)}{e^{x-y} + 1} dx. \quad (5)$$

In this approximation the electroneutrality condition is written in the form

$$\zeta_p = \zeta_e. \quad (6)$$

The Hartree correction has the following presentation [6, 11, 12] for the Helmholtz thermodynamic potential  $\Omega = -PV$  ( $V$  is the system volume)

$$\delta\Omega_H V^{-1} = \tilde{V}(0) \cdot (\zeta_e - \zeta_p)^2 = -P_H(\kappa). \quad (7)$$

Here  $\tilde{V}(0)$  is the Fourier transform of the Coulomb potential at zero transferred momentum. Using the regularization of the integral by means of  $e^{-\kappa r}$ ,  $\kappa \rightarrow 0$  being an infinitesimal parameter, we shall obtain ( $\mathbf{r} = (r_1, r_2, r_3)$ ,  $|\mathbf{r}| = r$ ,  $d\mathbf{r} = dr_1 dr_2 dr_3$ )

$$\begin{aligned} \tilde{V}(\mathbf{q}) &= \lim_{\kappa \rightarrow 0} \int \frac{e^2}{r} e^{i\mathbf{q}\mathbf{r} - \kappa r} d\mathbf{r} = \frac{4\pi e^2}{q^2 + \kappa^2}, \\ \tilde{V}(0) &= 4\pi e^2 \kappa^{-2}. \end{aligned} \quad (8)$$

This method of regularization of the Fourier component of the Coulomb potential gives zero result for expression (7), due to neutrality condition (6). For the general case of multicomponent plasma, neutrality condition (6) has the form ( $z_k$  is a particle of  $k$ -kind charge in units of electron charge  $e$ )

$$\zeta_e = \sum_k z_k \zeta_k \quad (9)$$

and (7) is generalized in an obvious way

$$\frac{\delta\Omega_H}{V} = \tilde{V}(0) \cdot \left( \zeta_e - \sum_k z_k \zeta_k \right)^2. \quad (10)$$

In the next Hartree–Fock approximation we obtain the well-known convergent result [11, 13, 14] for the electron–electron exchange interaction (see below).

Next-order terms in the interaction potential called ring diagrams [15] correspond to the Debye–Hückel contribution (see, for example, [5, 6, 12, 16–19])

$$\frac{\delta\Omega_{D-H}}{V} = -T \frac{\kappa_D^3}{12\pi}. \quad (11)$$

Here  $\kappa_D$  is the inverse Debye radius [19] (the sum over  $m$  includes ions and electrons):

$$\kappa_D^2 = 4\pi e^2 \sum_m z_m^2 \left( \frac{\partial n_m}{\partial \mu_m} \right)_T. \quad (12)$$

We must recall that the physical concentrations are usually connected with chemical potentials by relation [11]:

$$n_m = - \left( \frac{\partial(\Omega/V)}{\partial \mu_m} \right)_T. \quad (13)$$

For physical concentrations the standard electrical neutrality condition takes place:

$$n_e = \sum_k z_k n_k. \quad (14)$$

Since condition (9) is necessary for cancelling the divergence of the Hartree term (10), when parameter  $\kappa$  tends to zero, we shall use the following method to adjust (9) and (14). We determine the physical concentrations from condition (13), taking into account bounds, which follow from (9), when calculating derivatives of thermodynamic potential over chemical potentials. Let us find the value of  $n_e$  from (14) and  $\zeta_e$  from (9):

$$n_e + \sum_k n_k = \sum_k (z_k + 1) n_k = -\beta \sum_k \left( \frac{\partial(\Omega/V)}{\partial \zeta_k} \right)_T \zeta_k. \quad (15)$$

In expression (15) all derivations and summations are performed over ionic activities only, and  $\zeta_e$  in potential  $\Omega$  is expressed using (9).

For the non-degenerate case we can obtain in the first approximation over the  $\lambda\kappa$  parameter [17] the so-called diffraction corrections to the Debye–Hückel term:

$$\begin{aligned} \frac{\delta\Omega_{\text{diff}}}{V} &= \frac{\pi}{8} T \left( \frac{e^2}{T} \right)^2 \left( \lambda_{ee} \zeta_e^2 + 2\zeta_e \sum_k \zeta_k z_k^2 \lambda_{ek} \right. \\ &\quad \left. + \sum_{kj} \zeta_k \zeta_j z_k^2 z_j^2 \lambda_{kj} \right). \end{aligned} \quad (16)$$

Here  $\lambda_{kj} = \sqrt{(2\pi\hbar^2)/(\mu_{kj}T)}$ ,  $\mu_{kj} = (m_k m_j)/(m_k + m_j)$  is the reduced mass.

### 3. Ladder approximation for SVC calculation

Let us consider the contribution  $\delta P$  in (1). From the Matsubara technique (see [10] and references therein) for  $\delta\Omega/V = -\delta P$  we have

$$\frac{\delta\Omega_L}{V} = \frac{2}{\beta} \sum_{i,\omega} \int_0^1 \frac{d\lambda}{2\lambda} \int \frac{d\mathbf{p}}{(2\pi)^3} G_i(\hbar\mathbf{p}, \hbar\omega) \Sigma_i(\hbar\mathbf{p}, \hbar\omega). \quad (17)$$

Here the subscript ‘L’ stands for ‘ladder’, the integration over parameter  $\lambda$  corresponds to charge integration  $e^2 \mapsto e^2\lambda$ , the summation is performed over particle kinds  $i$  and energies  $\hbar\omega$  (or  $\hbar p_4$ )—for fermions  $\hbar\omega = \pi T(2n+1)$ ,  $\hbar\mathbf{p}$  is the particle momentum and  $G_i(\hbar\mathbf{p}, \hbar\omega)$  is Green’s function of a particle in the Matsubara technique. The self-energy operator  $\Sigma_i(\hbar\mathbf{p}, \hbar\omega)$  can be expressed via a two-particle vertex part  $\Gamma_{ij}$ , obtained in the ladder approximation [14]:

$$\begin{aligned} \Sigma_i(\mathbf{p}) &= \frac{2}{\beta} \sum_{j,k_4} \int \frac{d\mathbf{k}}{(2\pi)^3} G_j(\mathbf{k}) \\ &\quad \times \Gamma_{ij} \left( \frac{m_j \mathbf{p} - m_i \mathbf{k}}{m_i + m_j}, \frac{m_j \mathbf{p} - m_i \mathbf{k}}{m_i + m_j}; \mathbf{p} + \mathbf{k} \right). \end{aligned} \quad (18)$$

For example, for electron–proton interaction  $m_i = m_e$ ,  $m_j = m_p$ ,  $\mathbf{p} = (\hbar\mathbf{p}, \hbar p_4) \equiv (\hbar\mathbf{p}, \hbar\omega)$  is the 4-vector for electrons and  $\mathbf{k} = (\hbar\mathbf{k}, \hbar k_4)$ —correspondingly for protons. The quantity  $\Gamma_{ij}(\mathbf{q}, \mathbf{q}'; \mathfrak{P})$  may be written in the following form:

$$\Gamma_{ep}(\mathbf{q}, \mathbf{q}'; \mathfrak{P}) = \tilde{V}_{ep}(\mathbf{q} - \mathbf{q}') + (2\pi)^3 \sum_n \frac{\tilde{\Psi}_n(\mathbf{q})\tilde{\Psi}_n^*(\mathbf{q}')(E_n - (\hbar^2 q^2)/(2\mu))(E_n - (\hbar^2 q'^2)/(2\mu))}{i\hbar P_4 - (\hbar^2 P^2)/(2M) - E_n + \mu_e + \mu_p}, \quad (19)$$

where  $\mathbf{q}, \mathbf{q}'$  are relative motion momenta before and after scattering,  $\mathfrak{P} = \mathbf{p} + \mathbf{k} = (\hbar\mathbf{P}, \hbar P_4)$  is the 4-vector for total momentum and  $\mu = \mu_{ep}$  is the reduced mass. From (17) and (18) we obtain  $\delta\Omega$  in the form, using the electrical neutrality condition in terms of activities (6),

$$\frac{\delta\Omega_L}{V} = \sum_{i,j} \zeta_i \zeta_j \tilde{\lambda}_{ij}^3 \int_0^1 \frac{d\lambda}{2\lambda} \int \frac{d\mathbf{q}}{(2\pi)^3} \sum_{\{n\}_k} \times \left( E_{\{n\}_k} - \frac{\hbar^2 q^2}{2\mu} \right) \left| \tilde{\Psi}_{\{n\}_k}(\mathbf{q}) \right|^2 \left( e^{-\beta E_{\{n\}_k}} - e^{-\beta \varepsilon_q} \right). \quad (20)$$

In (20) for the ‘e–p’ interaction it is necessary to sum over the discrete spectrum (bound states) as well as to integrate over SS, described by index  $\mathbf{k}$ . For ‘e–e’ and ‘p–p’ interactions only the last action is not unreasonable.

#### 4. Contribution to the SVC from SS

To calculate the contribution of continuum states to expressions such as (20) one needs to evaluate Fourier components of the wave functions that describe the mutual scattering of charged particles. Taking into account subtraction in the factor  $(e^{-\beta E_k} - e^{-\beta \varepsilon_q})$  in formula (20), we can transform expression (20) for the continual spectrum (of SS) to (e.g. for the ‘e–p’ interaction  $\tilde{\xi}_{ep} = (\lambda \alpha_{ep})/\sqrt{y}$ ,  $\alpha = \alpha_{ep} = \sqrt{\mathcal{R}y}/T$ ,  $\tilde{\eta}_{ep}^2 = (\hbar^2 \varkappa^2)/(8\mu T)$ )

$$\begin{aligned} \frac{\delta\Omega_{ep}^{SS}}{V} &= -\frac{\tilde{\lambda}_{ep}}{\pi} \zeta_e \zeta_p T \left( \frac{e^2}{T} \right)^2 \int_0^1 \lambda d\lambda \int_0^\infty \int_0^\infty dx dy \\ &\times \frac{\pi \tilde{\xi}_{ep}}{\text{sh } \pi \tilde{\xi}_{ep}} \exp(\pi \tilde{\xi}_{ep}) \frac{e^{-y} - e^{-x}}{x - y} \\ &\times \left( \frac{1}{(\sqrt{x} - \sqrt{y})^2 + \tilde{\eta}_{ep}^2} - \frac{1}{(\sqrt{x} + \sqrt{y})^2 + \tilde{\eta}_{ep}^2} \right) \\ &\times \exp \left[ -2\tilde{\xi}_{ep} \text{Im} \ln \left( x - y + \tilde{\eta}_{ep}^2 + i2\sqrt{y\tilde{\eta}_{ep}^2} \right) \right]. \quad (21) \end{aligned}$$

The 3D numerical integration results in the following asymptotics as  $\varkappa \rightarrow 0$  ( $a = e, p$ ):

$$\begin{aligned} \frac{\delta\Omega_{aa}^{SS}}{V} - \frac{\delta\Omega_{aa}^{(2)}}{V} &\rightarrow -\zeta_a^2 \left\{ \frac{e^6}{T^2} \left[ \frac{\pi}{3} \ln \frac{\varkappa \tilde{\lambda}_{aa}}{2\sqrt{\pi}} - \frac{\pi}{6} (1 - C) \right] \right. \\ &\left. + \frac{\tilde{\lambda}_{aa}^3 T}{2} \Sigma_Q \left( -\frac{\alpha_a}{2} \right) \right\}, \quad (22) \end{aligned}$$

where  $\delta\Omega_{aa}^{(2)}$  is a part of a ladder with two steps, already included in the Debye–Hückel approximation,  $\alpha_a = \sqrt{(m_a e^4)/(\hbar^2 T)}$  and  $C$  is the Euler constant,  $C = 0.5772\dots$ :

$$\begin{aligned} \frac{\delta\Omega_{ep}^{SS}}{V} - \frac{\delta\Omega_{ep}^{(2)}}{V} &\rightarrow 2\zeta_e \zeta_p \left\{ \frac{e^6}{T^2} \left[ \frac{\pi}{3} \ln \frac{\varkappa \tilde{\lambda}_{ep}}{2\sqrt{\pi}} - \frac{\pi}{6} (1 - C) \right] \right. \\ &\left. + \frac{\tilde{\lambda}_{ep}^3 T}{2} \left[ \Sigma_{SRM}^{BS} - \Sigma_Q(\alpha) \right] \right\}. \quad (23) \end{aligned}$$

An expression for  $\Sigma_{SRM}^{BS}$  is adduced in the following section (44), and

$$\begin{aligned} \Sigma_Q(x) &= \frac{1}{2} \sum_{n=4}^{\infty} \frac{\zeta(n-2)}{\Gamma((n/2)+1)} x^n = - \left( \ln |2x| + \frac{3C}{2} - \frac{4}{3} \right) \\ &\times \frac{2x^3}{3\sqrt{\pi}} + o(|x|^3) \text{ as } x \rightarrow -\infty. \end{aligned}$$

In [6] in expressions that are similar to (22) and (23) the second item inside brackets contains an excess term with  $\ln 3$  in parentheses  $(1 - C - 2 \ln 3)$  as a mistake.

Note that this result is also confirmed by a detailed comparison with numerical integration.

Summation of expressions such as (23) for ‘p–p’, ‘e–e’ and ‘e–p’ interactions taking into account that  $\zeta_e = \zeta_p$  will result in an expression independent of  $\varkappa$  for a classical part of the SVC:

$$\frac{\delta\Omega^{cl}}{V} = \zeta_e^2 T \left( \frac{e^2}{T} \right)^3 \cdot \frac{\pi}{6} \ln \frac{m_p}{4m_e}. \quad (24)$$

For the exchange contribution  $\delta\Omega_{ee}^{\text{exch}}$  we obtain a convergent expression:

$$\frac{\delta\Omega_{ee}^{\text{exch}}}{V} = \frac{1}{8\sqrt{\pi}} \zeta_e^2 \tilde{\lambda}_{ee}^3 T E(\alpha_{ee}). \quad (25)$$

For  $E(\alpha_{ee})$  one can get an explicit expression ( $\alpha_{ee} = -\alpha_e/2$ ):

$$\begin{aligned} E(x) &= x + \sqrt{\pi} \ln 2 \cdot x^2 + \frac{\pi^2}{9} x^3 + \sum_{n=4}^{\infty} \frac{\sqrt{\pi}(1 - 2^{2-n})}{\Gamma((n/2)+1)} \\ &\times \zeta(n-1) x^n. \quad (26) \end{aligned}$$

Expression (26) is just the same as in [6] for exchange contribution and is confirmed by numerical integration.

#### 5. Contribution to the SVC from bound states

The bound states contribution may be written in the form

$$\delta\Omega^{BS} V^{-1} = -\delta P_{BS} = -\zeta_e \zeta_p T \tilde{\lambda}_{ep}^3 \Sigma^{BS}. \quad (27)$$

Note that expressions such as (20) are obtained using the Keldysh technique [10]:

$$\begin{aligned} \delta P &= \sum_a (2S_a + 1) \hbar \int_0^1 \frac{d\lambda}{2\lambda} \int \frac{d\mathbf{p}}{(2\pi)^3} \\ &\times \int \frac{d\omega d\omega'}{(2\pi)^2} \frac{\Sigma_a^>(\hbar\mathbf{p}, \hbar\omega) G_a^<(\hbar\mathbf{p}, \hbar\omega')}{\omega - \omega'} (1 - e^{-\beta\hbar(\omega - \omega')}). \quad (28) \end{aligned}$$

From (28) we can obtain for the general form of the bound states contribution (we use parametrization on charge  $\lambda$ :  $e^2 \mapsto e^2 \lambda$ )

$$\begin{aligned} \Sigma^{BS} &= \beta \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d\mathbf{q}}{(2\pi)^3} \int d\omega \sum_{n=1}^{\infty} (E_n - \varepsilon_q)^2 |\tilde{\Psi}_n(\mathbf{q})|^2 \\ &\times \frac{e^{-\beta\hbar\omega} - e^{-\beta\varepsilon_q}}{\varepsilon_q - \hbar\omega} a_n(\omega - E_n/\hbar), \quad (29) \end{aligned}$$

where  $\mathbf{q}$  is the wave vector of the relative motion of the particles,  $q = |\mathbf{q}|$  and  $a_n(\omega)$  is the profile of the atomic state  $n$ , broadened by plasma ions and electrons [20].

To obtain the contribution of bound states to the SVC as in [9] we use the exact Fock [21] result for the wave functions of non-relativistic hydrogen atoms in momentum representation

$$\frac{1}{(2\pi)^3} \sum_{l,m} |\tilde{\Psi}_{nlm}(\mathbf{q})|^2 = \frac{8}{\pi^2 a_0^5 n^3 (q^2 + p_n^2)^4}. \quad (30)$$

Here  $p_n = (a_0 n)^{-1}$ ;  $a_0 = \hbar^2 / (\mu e^2 \lambda)$  is the Bohr 'radius' for current charge  $e^2 \lambda$ .

Taking into account that

$$\begin{aligned} E_n &= -\frac{\hbar^2 p_n^2}{2\mu}, & E_n - \varepsilon_q &= -\frac{\hbar^2}{2\mu} (q^2 + p_n^2), \\ \varepsilon_q &= \frac{\hbar^2 q^2}{2\mu}, & \int d\mathbf{q} &= 4\pi \int_0^\infty q^2 dq \end{aligned} \quad (31)$$

and using dimensionless variables

$$\begin{aligned} x &= \frac{\hbar^2 q^2}{2\mu T}, & y &= \beta \hbar \omega, \\ z &= \frac{\hbar^2 p_n^2}{2\mu T} = -\beta E_n = u_n \lambda^2, \end{aligned} \quad (32)$$

where

$$u_n = \frac{\alpha^2}{n^2}, \quad \alpha = \alpha_{\text{ep}} = \sqrt{\frac{\mu e^4}{2\hbar^2 T}} = \sqrt{\beta R_Y}, \quad (33)$$

finally we obtain

$$\begin{aligned} \Sigma^{\text{BS}} &= \sum_{n=1}^{\infty} G_n = \sum_{n=1}^{\infty} n^2 \int_0^{u_n} \frac{8}{\pi} z^{3/2} dz \int_{-\infty}^{\infty} dy \cdot \tilde{a}_n(y+z) \\ &\times \int_0^\infty \frac{\sqrt{x}(e^{-y} - e^{-x}) dx}{(x+z)^2(x-y)}. \end{aligned} \quad (34)$$

The integral over  $x$  in (34) may be calculated explicitly:

$$\begin{aligned} \mathcal{I} &= -\frac{\sqrt{\pi} - \pi \tilde{F}(z)(1 + (1/2z))}{z+y} \\ &+ \begin{cases} \frac{\pi e^{-y}(z-y)}{2\sqrt{z}(z+y)^2} - \frac{\pi(\tilde{F}(z) - \tilde{G}(y))}{(z+y)^2}, & y > 0, \\ \frac{\pi e^{-y}(\sqrt{z} - \sqrt{-y})^2}{2\sqrt{z}(z+y)^2} - \frac{\pi(\tilde{F}(z) - \tilde{F}(-y))}{(z+y)^2}, & y < 0, \end{cases} \end{aligned} \quad (35)$$

where

$$\tilde{F}(x) = e^x \sqrt{x} \operatorname{erfc} \sqrt{x}, \quad \tilde{G}(x) = \sqrt{x} \operatorname{Im} w(\sqrt{x}), \quad (36)$$

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt,$$

$$w(z) = e^{-z^2} \left( 1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} dt \right) = e^{-z^2} \operatorname{erfc}(-iz) \quad (37)$$

and both branches represent one and the same analytic expression.

If broadening is not taken into account then  $\tilde{a}_n(y) = \delta(y)$  and the integral over  $y$  in (34) is

$$\begin{aligned} I_\omega|_{a_n \equiv \delta} &= I_{\delta\omega} = \left\{ \int_0^\infty \frac{\sqrt{x}(e^{-y} - e^{-x}) dx}{(x+z)^2(x-y)} \right\} \Big|_{y=-z} \\ &= \int_0^\infty \frac{\sqrt{x}(e^z - e^{-x})}{(x+z)^3} dx. \end{aligned} \quad (38)$$

Analytic integration over  $x$  results in

$$\begin{aligned} \Sigma^{\text{BS}}|_{a_n \equiv \delta} &= \sum_{n=1}^{\infty} n^2 \int_0^{u_n} dz \left( e^z - \frac{2}{\sqrt{\pi}} \sqrt{z}(1+2z) - e^z \operatorname{erfc} \sqrt{z} \right. \\ &\times \left. (1 - 4z - 4z^2) \right). \end{aligned} \quad (39)$$

After integration in (39) (see [10]),

$$\Sigma^{\text{BS}} = \Sigma_{\text{SRM}}^{\text{BS}} = \sum_{n=1}^{\infty} n^2 e^{u_n} F(u_n), \quad (40)$$

$$\begin{aligned} F(u) &= 1 - e^{-u} \left( 4 - \frac{6}{\sqrt{\pi}} u^{1/2} + \frac{4}{\sqrt{\pi}} u^{3/2} \right) + \operatorname{erfc} \sqrt{u} \\ &\times (3 - 4u + 4u^2). \end{aligned} \quad (41)$$

Asymptotically for  $u \rightarrow 0$  ( $n \gg 1$  or for large  $T$ ) from (41) it follows that

$$F(u) \sim 2u^2. \quad (42)$$

This is four times more than the similar expression shown in the P-L expression

$$F_{\text{P-L}}(u) = 1 - e^{-u} - u e^{-u} \sim \frac{u^2}{2} \text{ as } u \rightarrow 0. \quad (43)$$

Finally, the partition function of non-broadened bound states may be written in the form

$$\begin{aligned} \Sigma_{\text{SRM}}^{\text{BS}} &= \sum_{k=4}^{\infty} \zeta(k-2) \frac{(-\alpha)^k}{\Gamma((k/2)+1)} (k-2)^2 \\ &+ \sum_{k=1}^{\infty} \zeta(2k+1) \frac{\alpha^{2k+3}}{\Gamma(k+(5/2))}. \end{aligned} \quad (44)$$

Here  $\zeta(n)$  is the Riemann  $\zeta$ -function. The corresponding P-L formula looks as follows:

$$\begin{aligned} \Sigma_{\text{P-L}}^{\text{BS}} &= \sum_{k=2}^{\infty} \zeta(2k-2) \frac{\alpha^{2k}}{\Gamma(k+1)} \\ &= \sum_{n=4,6,8,\dots} \zeta(n-2) \frac{\alpha^n}{\Gamma((n/2)+1)}. \end{aligned} \quad (45)$$

## 6. Atomic states broadening by electronic collisions in an ion field

For an atomic state with the principal quantum number  $n$  ( $n \geq 2$ ) the following formula is used for collisional broadening ([20], section 22):

$$a_n(\omega) = \frac{1}{\pi} \int \frac{\mathcal{H}(x) \gamma_n(\omega) dx}{(B_n \mathcal{E}_0 x - \omega)^2 + \gamma_n^2(\omega)}, \quad x = \frac{\mathcal{E}}{\mathcal{E}_0}, \quad (46)$$

$$\mathcal{E}_0 = 2\pi \left( \frac{4}{15} \right)^{2/3} Z e N^{2/3}, \quad B_n = \left( \frac{3}{8} \right)^{2/3} \frac{\hbar}{Z m_e e} (n^2 - n'^2), \quad (47)$$

$$\gamma_n(\omega) = \gamma_{en} \begin{cases} 1, & \omega > 0 \\ e^{-\beta \hbar |\omega|}, & \omega < 0 \end{cases}, \quad (48)$$

$$\gamma_{en} = \frac{32}{3} N(v)^{-1} \frac{\hbar^2}{m_e^2} \left( \max \left( 1, \ln \frac{R_D}{\rho_0} \right) + 0.215 \right) I(n, n'). \quad (49)$$

Here  $\mathcal{H}(x)$  is the Holtmark function (see below),  $\mathcal{E}$  is the ion field,  $\mathcal{E}_0$  is its characteristic value,  $B_n$  is the effective Stark constant for the state,  $n' = 1$ ,  $N = N_A \rho$ ,  $\gamma_{en}$  is the effective constant of broadening by electronic collisions,  $\langle v \rangle$  is the average velocity,  $\rho_0$  is the Weisskopf radius and  $R_D = \kappa_D^{-1}$  is the Debye radius. The lowest state ( $n = 1$ ) may be considered as non-broadened:  $\gamma_1 \rightarrow 0$ .

$$\langle v \rangle = \frac{2}{\sqrt{\pi}} \sqrt{\frac{2T}{m_e}}, \quad I(n, n') = \frac{1}{2}(n^4 + n'^4). \quad (50)$$

We use the Weisskopf radius as defined in [20] (equation (22.33), p 298):

$$\rho_0^2 = \frac{2}{3} \left( \frac{e^2}{\hbar \langle v \rangle} \right)^2 I(n, n') a_0^2. \quad (51)$$

Taking into account the parametrization  $e^2 \mapsto e^2 \lambda$ , we use

$$\rho_0 = \frac{1}{\sqrt{3}} \frac{\hbar}{\mu \langle v \rangle} \sqrt{n^4 + 1}. \quad (52)$$

The Holtmark function used in (46) is defined as

$$\mathcal{H}(x) = \frac{2}{\pi x} \int_0^\infty t \sin t \exp \left[ - \left( \frac{t}{x} \right)^{3/2} \right] dt. \quad (53)$$

The integral in (46) is calculated by a separate analytic integration of the polynomial approximations of the Holtmark function on finite intervals or of the semi-integer power approximations for large  $x$ . In some cases a direct Gauss–Kronrod quadrature with adaptive grid refinement was used instead of the analytic expressions with arctg and ln functions. Special care was taken to avoid a loss in accuracy.

For the partition function represented in form (34) for the case of non-broadening

$$G_n \equiv G_n^{\text{N-B}} = n^2 e^{u_n} F(u_n) \sim \frac{2\alpha^4}{n^2} \text{ as } n \rightarrow \infty. \quad (54)$$

The ratio of the broadened term to the non-broadened one,  $G_n^{\text{B}}/G_n^{\text{N-B}}$ , decreases with  $n$  for low and moderate principal quantum numbers, then grows linearly, and the broadened partition function seems to be divergent. Nevertheless, estimates and calculations show that asymptotically

$$G_n^{\text{B}}/G_n^{\text{N-B}} \sim \ln n \text{ as } n \rightarrow \infty, \quad (55)$$

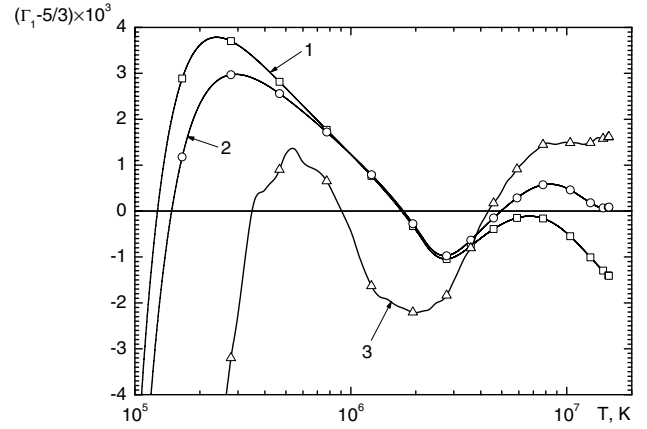
which guarantees convergence of the partition function with account of broadening.

In fact, the partition function  $\Sigma^{\text{BS}}$  must be limited to the first  $n_l$  states with the dimensionless ionization potential  $u_n = \alpha^2/n^2$  being greater than a similar characteristic energy  $B = \beta \hbar B_n \mathcal{E}_0$ . In the calculations we used a smooth limitation of the number of states by a state weight factor  $w_n$ :

$$\Sigma_s^{\text{BS}} = \sum_n w_n G_n, \quad w_n = \min(1, e^{-\tau}),$$

$$\tau = \frac{B - u_n}{u_n}. \quad (56)$$

Note that more correct ways of treating the microfield distribution function exist (see, for example, the adjustable parameter exponential (APEX) approximation [22]). For our application—the solar interior—the Holtmark distribution is enough, since the nonideality parameter  $\Gamma_D = \kappa_D e^2/T \ll 1$ .



**Figure 1.** Adiabatic exponent along the solar trajectory: 1—the chemical picture with  $\Sigma^{\text{BS}} = \Sigma_{\text{P-L}}^{\text{BS}}$ , 2—the chemical picture with  $\Sigma^{\text{BS}} = \Sigma_{\text{SRM}}^{\text{BS}}$  and 3—the S-model [1].

## 7. Application to the solar interior

In the physical picture we consider the total contribution of the expressions (3), (5), (11), (16), (22)–(25), (27) to describe the EOS of hydrogen weakly nonideal plasmas in application to helioseismological problems. The bound states contribution (27) is calculated with (44) for the non-broadened states or (34) to account for broadening. To the plasma EOS (value of pressure  $P(\rho, T)$  and other thermodynamic functions) a contribution of equilibrium thermal radiation in plasma should be added [10].

A chemical picture includes terms (3), (5), (11), (27) with (45) and also the contribution of radiation.

We calculated the hydrogen weakly nonideal plasmas EOS that is characterized by the dependence of the total pressure  $P(\rho, T)$  on  $T$  ‘the solar trajectory’ (the function  $\rho = \rho(T)$  in the S-model [1] for the interior of the Sun).

Two main parameters used in helioseismological problems are the adiabatic exponent and the sound velocity. They are calculated as follows:

$$\Gamma_1 = \frac{\rho}{P} c_s^2, \quad c_s^2 = \left( \frac{\partial P}{\partial \rho} \right)_T \left[ 1 + \frac{T(\partial P/\partial T)_\rho^2}{C_V \rho (\partial P/\partial \rho)_T} \right]. \quad (57)$$

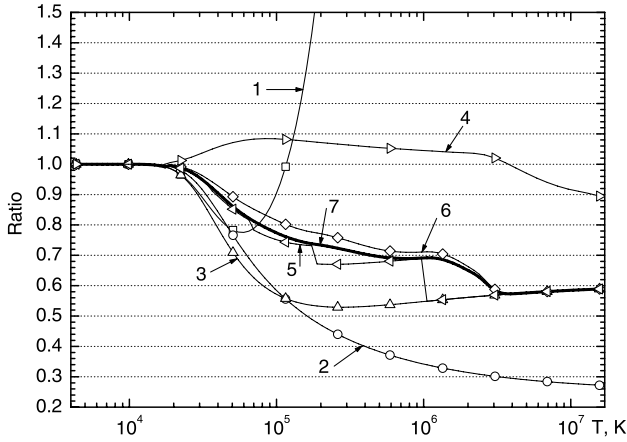
In figure 1 the adiabatic exponent along the solar trajectory with the non-broadened bound states is plotted for the chemical picture with the P–L partition function and with  $\Sigma^{\text{BS}} = \Sigma_{\text{SRM}}^{\text{BS}}$  together with the data obtained in the S-model calculations [1].

In figure 2 variants of partition functions are presented. According to (34), (54), (55) the following notations are used:

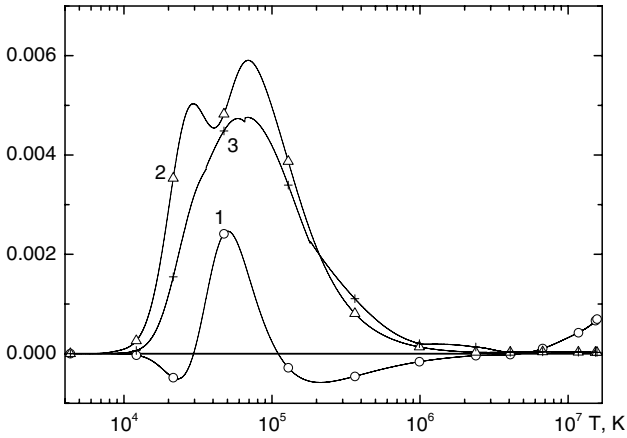
$$\Sigma_k^{\text{N-B}} = \sum_{n=1}^k G_n^{\text{N-B}}, \quad \Sigma_k^{\text{B}} = \sum_{n=1}^k G_n^{\text{B}},$$

$$\Sigma_\infty^{\text{N-B}} \equiv \Sigma_{\text{SRM}}^{\text{BS}}. \quad (58)$$

In figure 3 the relative differences  $(c_s/c_{s,\text{ph}} - 1)$  for the sound velocity  $c_s$  with respect to the sound velocity in the physical picture  $c_{s,\text{ph}}$  with  $\Sigma^{\text{BS}} = \Sigma_{\text{SRM}}^{\text{BS}}$  for the variants of partition functions are presented.



**Figure 2.** Ratio  $\Sigma^{BS}/\Sigma_{SRM}^{BS}$  along the solar trajectory for different  $\Sigma^{BS}$ : 1— $\Sigma^{BS} = e^{\beta R_V}$  (Saha), 2— $\Sigma_{P-L}^{BS}$  (Planck–Larkin), 3— $G_1$  (ground state term), 4— $\Sigma_{\infty}^B$  (broadened, infinite), 5— $\Sigma_{n_l}^B$  (broadened, limited), 6— $\Sigma_s^{N-B}$  (non-broadened, smooth restriction on  $n$ ) and 7— $\Sigma_s^B$  (broadened, smooth restriction on  $n$ ).



**Figure 3.** Relative differences  $(c_s/c_{s,ph} - 1)$  of the sound velocity along the solar trajectory for different models: 1—chemical picture  $\Sigma^{BS} = \Sigma_{P-L}^{BS}$  (Planck–Larkin), 2—physical picture  $\Sigma^{BS} = G_1$  (ground state term) and 3—physical picture  $\Sigma^{BS} = \Sigma_{n_l}^{N-B}$  (non-broadened, limited).

## 8. Conclusion

The new expressions for the bound states contribution to the EOS of weakly nonideal plasmas are presented. The broadening of atomic states by electron collisions and Stark microfields are taken into account.

In our opinion the account of broadening effects (see (29) and [9]) is more promising for the spectral lines description as well as for the weakly nonideal dense plasma thermodynamics.

The account of broadening effects for the bound states can be considered as an influence of pressure ionization with increasing plasma density.

In principle this approach combines the problems of the radiational gas dynamics and the collisional–radiative kinetics, where ‘atoms’ are represented in a different way for the calculation of pressure and radiation [9].

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