

# Coulomb corrections to the equation of state for a weakly-coupled plasma

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**Abstract.** Coulomb corrections to the equation of state of degenerate matter are usually described by Debye-Hückel theory; however, recent studies have considered modifications of thermodynamic quantities which are caused by the interactions of charged particles beyond the Debye-Hückel approximation. Based on the weakly-coupled plasma limit, the formulae for the physical properties of non-ideal effects on the equation of state are derived. The treatment of the non-ideal effects due to Coulomb coupling combines the results of quantum-statistic calculations for the electrons,  $N$ -body semianalytic theory for ions, and the extended Debye-Hückel theory with hard-core correction for the electron-ion interaction. The leading Coulomb correction not only can be applied to the weak-coupling region, but also preserves the well-known Debye-Hückel limit at  $\Gamma \ll 1$ . We examine the Coulomb correction to the thermodynamic quantities of a weakly coupled and fully ionized plasma. The result reveals that the contribution is quite significant, and hence modifies the thermodynamic properties of the plasma substantially.

**Key words:** equation of state – Sun: general – stars: interiors

## 1. Introduction

The equation of state (EOS) is one of the most important physical inputs for the study of stellar envelopes and interiors. Although a simple ideal-gas model of the plasma of the solar interior, the so-called EFF equation of state (Eggleton et al. 1973), was adequate before the advent of helioseismology, the use of high-quality helioseismic data requires much greater accuracy in the EOS (Christensen-Dalsgaard & Däppen 1992). The calculation of the EOS of a multicomponent quantum plasma, consisting of charged particles interacting via the Coulomb potential, is of theoretical and practical interest.

The gas in the solar interior is only weakly coupled and weakly degenerate; however, non-ideal effects, especially Coulomb corrections, significantly influence the structure of the solar interior. The Coulomb correction due to the sum of

all pair interactions between charged particles (electrons, nuclei and compound ions), is conventionally described in the Debye-Hückel approximation. The simplest improved EOS is the so-called CEFF equation of state, obtained by adding Debye-Hückel terms to the EFF model (Christensen-Dalsgaard et al. 1988; Stix & Skaley 1990; Christensen-Dalsgaard & Däppen 1992). To estimate the possible deficiencies of this approximation, a more realistic expression for the higher-order corrections is required. The specific form of  $\tau$  correction based on the assumption of a constant ion radius to the Debye-Hückel term was adopted in the MHD equation of state (Hummer & Mihalas 1988; Mihalas et al. 1988; Däppen et al. 1988; Gabriel 1994). However, the influence of this  $\tau$  correction is too large to be realistic for a stellar plasma. Recent studies have addressed specific non-ideal effects beyond the Debye-Hückel approximation (Pols et al. 1995; Christensen-Dalsgaard et al. 1996; Stolzmann & Blöcker 1996; Däppen 1998; Nayfonov & Däppen 1998), and there is clearly a strong interest in further development of the EOS.

The EOS presented in this paper is formulated for a hydrogen-helium mixture and takes into account the physical processes of electron degeneracy and Coulomb coupling based on the free energy minimization method in the chemical picture (Harris et al. 1960; Graboske et al. 1969). A simple thermodynamic model of the hydrogen-helium mixture is presented in Sect. 2. In Sect. 3, we establish the detailed processes of Coulomb coupling, and propose simple approximations for the non-ideal free energies of the plasma. The calculated results and comparisons are presented in Sect. 4. A brief summary is given in Sect. 5.

## 2. Theoretical schemes

### 2.1. Parameters of plasma for a H-He mixture

To describe non-ideal effects of the plasma, it is convenient to introduce several dimensionless parameters to characterize the plasma. We consider a H-He plasma mixture consisting of electrons and ions of species  $\{H^+, He^{++}\}$ , which we label with the index  $j = 1, 2$ , with charges  $Z_j e$ , masses  $m_j$  in a volume  $V$ . If the abundances by mass are  $X$  and  $Y$  for H and He with

density  $\rho$  and temperature  $T$ , the number of nuclei for H and He are given by

$$N_{\text{H}} = \frac{N_{\text{A}}\rho V X}{A_{\text{H}}}, \quad N_{\text{He}} = \frac{N_{\text{A}}\rho V Y}{A_{\text{He}}}, \quad (1)$$

where  $N_{\text{A}}$  is Avogadro's number, and  $A_{\text{H}} = 1.0079$  and  $A_{\text{He}} = 4.0026$  are the atomic weights. The averaged nuclear charge  $\langle Z \rangle$  is defined as

$$\langle Z \rangle = \frac{N_{\text{H}} + 2N_{\text{He}}}{N_{\text{H}} + N_{\text{He}}}. \quad (2)$$

For the ion system, the Wigner-Seitz radius defined as

$$a = \left( \frac{3V}{4\pi N_{\text{ion}}} \right)^{1/3} \quad (3)$$

is the so-called ion-sphere radius which measures the mean interionic distance; here the total number of ions  $N_{\text{ion}} = N_{\text{e}} / \langle Z \rangle$  is determined by the electroneutrality condition, and  $N_{\text{e}}$  is the number of free electrons.

The averaged Coulomb coupling constant of the ions, which describes the strength of the Coulomb coupling, is given by (Ichimaru et al. 1987):

$$\begin{aligned} \Gamma_{\text{ion}} &= \frac{(\langle Z \rangle e)^2}{k_{\text{B}} T a} = \frac{(\langle Z \rangle e)^2}{k_{\text{B}} T} \left( \frac{4\pi N_{\text{e}}}{3 \langle Z \rangle V} \right)^{1/3} \\ &= \langle Z \rangle^{5/3} \Gamma_{\text{e}}, \end{aligned} \quad (4)$$

where  $\Gamma_{\text{e}}$  denotes the classical Coulomb coupling constant of the electrons, which is written as

$$\Gamma_{\text{e}} = \frac{e^2}{k_{\text{B}} T} \left[ \frac{4\pi N_{\text{e}}}{3V} \right]^{1/3}, \quad (5)$$

where  $k_{\text{B}}$  is the Boltzmann constant.

A typical dimensionless density parameter characterizing the system of electrons is:

$$r_{\text{s}} \equiv \frac{a_{\text{e}}}{a_{\text{B}}} = \left( \frac{3V}{4\pi N_{\text{e}}} \right)^{1/3} \frac{m_{\text{e}} e^2}{\hbar^2}, \quad (6)$$

where  $m_{\text{e}}$  is the mass of an electron. The parameter  $r_{\text{s}}$  is the Wigner-Seitz radius  $a_{\text{e}}$  of the electrons in units of the Bohr radius  $a_{\text{B}} = \hbar^2 / m_{\text{e}} e^2$  and depends only on the number of electrons  $N_{\text{e}}$ .

The most evident quantum-mechanical characteristic length is the thermal de-Broglie wavelength of particles

$$\lambda_j = \left( \frac{2\pi\hbar^2}{k_{\text{B}} T m_j} \right)^{1/2}. \quad (7)$$

The degree of Fermi degeneracy of electrons, which is measured by the ratio of the temperature  $T$  to the Fermi temperature  $T_{\text{F}} = \hbar^2 (3\pi^2 n_{\text{e}})^{2/3} / 2k_{\text{B}} m_{\text{e}}$  (Iyetomi & Ichimaru 1986), is described as

$$\theta = \frac{T}{T_{\text{F}}} = 2 \left( \frac{4}{9\pi} \right)^{2/3} \frac{r_{\text{s}}}{\Gamma_{\text{e}}}. \quad (8)$$

Another important quantity is the Debye shielding length  $r_{\text{D}}$  for a mixture of ions and electrons, which is defined as

$$\begin{aligned} r_{\text{D}}^{-1} &= k_{\text{D}} = \left[ \frac{4\pi e^2 \left( \sum_j Z_j^2 N_j + N_{\text{e}} \right)}{V k_{\text{B}} T} \right]^{1/2} \\ &= \left[ \frac{4\pi e^2 N_{\text{e}} \left( 1 + \langle Z^2 \rangle / \langle Z \rangle \right)}{V k_{\text{B}} T} \right]^{1/2}, \end{aligned} \quad (9)$$

with the charge average

$$\langle Z^2 \rangle = \frac{\sum_j Z_j^2 N_j}{\sum_j N_j}, \quad (10)$$

where  $k_{\text{D}}$  is the reciprocal of the Debye shielding length  $r_{\text{D}}$ , and  $j$  runs over all ion species in the plasma, so that  $N_j$  denotes the number of ions of species  $j$ .

For a classical system of charged particles the potential energy is of the order of  $e^2 n^{1/3}$ , and the weakly non-ideal condition is reduced to the inequality

$$e^2 n^{1/3} \ll k_{\text{B}} T. \quad (11)$$

It will be useful to evaluate the number of charged particles within the Debye sphere. This number is equal to

$$N_{\text{D}} = \frac{4\pi}{3} r_{\text{D}}^3 n = \frac{1}{12\sqrt{2\pi}} \left( \frac{k_{\text{B}} T}{e^2 n^{1/3}} \right)^{3/2} \gg 1, \quad (12)$$

where  $n$  is the total number density of the plasma (note that full ionization is assumed). This extremely important inequality says that there is more than one charged particle within the Debye sphere. The closer to being ideal is the plasma, the greater is the number of particles within the Debye sphere. In the Debye sphere each charged particle is in a self-consistent plasma field. This means that the long-range character of Coulomb interactions makes particles interact with each other simultaneously even in a weakly non-ideal plasma. Thus, the Debye-Hückel theory is valid under solar interior conditions. However, the simple Debye-Hückel theory does not include any quantum-statistical effect on the electrons.

## 2.2. Free energy model for a H-He mixture

The total free energy  $F$  of a fully ionized H-He mixture consisting of ions and electrons can be written as (Chabrier & Potekhin 1998):

$$F(T, V, \{N_j\}, N_{\text{e}}) = F_{\text{id}}^{(\text{ion})} + F_{\text{id}}^{(\text{e})} + F_{\text{Coul}}, \quad (13)$$

where  $F_{\text{id}}^{(\text{i,e})}$  denote the ideal free energy of ions and electrons respectively, and  $F_{\text{Coul}}$  denotes the excess free energy due to Coulomb coupling.

The pressure  $P$ , the entropy  $S$  and the chemical potentials  $\mu$  can be obtained by differentiation of the free energy  $F$  with respect to either  $V$  and  $T$ , at fixed  $\{N_{\text{e}}, N_j\}$ , or with respect to  $N_{\text{e}}$  and  $N_j$ , at fixed  $V$  and  $T$ , respectively:

$$P = - \left( \frac{\partial F}{\partial V} \right)_{T, \{N_{\text{e}}, N_j\}}, \quad S = - \left( \frac{\partial F}{\partial T} \right)_{V, \{N_{\text{e}}, N_j\}} \quad (14)$$

$$\mu_j = \left( \frac{\partial F}{\partial N_j} \right)_{T,V,N_e}, \quad \mu_e = \left( \frac{\partial F}{\partial N_e} \right)_{T,V,N_j}. \quad (15)$$

Here we restrict ourselves to conditions where the ions are regarded as point charges while the electrons are assumed to form a uniform background of neutralizing space charges. Thus  $F_{\text{id}}^{(i)}$  and  $F_{\text{id}}^{(e)}$  are given by Maxwell-Boltzmann statistics and Fermi-Dirac integrals. The ideal free energy of classical ions, neglecting their spin statistics, can be written as

$$F_{\text{id}}^{(i)} = k_B T \sum_j N_j \left[ \ln \left( \frac{N_j}{V} \lambda_j^3 \right) - 1 \right]. \quad (16)$$

For partially degenerate electrons, the ideal free energy of the quantum electron is

$$F_{\text{id}}^{(e)} = N_e \mu_e - P_e V, \quad (17)$$

where  $P_e$  is the pressure of the ideal electron Fermi gas. The pressure  $P_e$  and electron density  $n_e$ , in turn, are functions of the chemical potential  $\mu_e$  and temperature  $T$ , given by:

$$P_e = \frac{8}{3\sqrt{\pi}} \frac{k_B T}{\lambda_e^3} I_{3/2}(\eta_e), \quad (18)$$

and

$$n_e = \frac{4}{\sqrt{\pi} \lambda_e^3} I_{1/2}(\eta_e). \quad (19)$$

(For simplicity, we assumed that the electrons can be treated as non-relativistic.) Here  $\eta_e \equiv \mu_e (k_B T)^{-1}$ , and the Fermi-Dirac integrals are defined by

$$I_n(\eta_e) = \int_0^\infty \frac{x^n dx}{e^{x-\eta_e} + 1}, \quad n > -1. \quad (20)$$

The chemical potential is related to the Fermi-degeneracy parameter  $\theta$

$$I_{1/2}(\eta_e) = \frac{2}{3} \theta^{-3/2}. \quad (21)$$

### 3. Coulomb coupling

The accuracy of the physical description demands a large range of applicability of the formalism for the EOS. Thus the formalism should be valid, e.g., from the central part of the Sun, with a temperature  $T \sim 10^7$  K and a density  $\rho \sim 10^2$  g cm $^{-3}$ , to the solar surface with  $T \sim 10^3$  K and  $\rho \sim 10^{-7}$  g cm $^{-3}$ . Since  $\Gamma_e \sim 0.05$  at the centre and  $\Gamma_e \sim 0.2$  near the surface, the solar plasma cannot strictly be regarded as being in the weakly coupled state; the polarization and quantum effects of the electrons play significant roles in determining the plasma properties. Although the Debye-Hückel approximation provides the correct limit for  $\Gamma_e \ll 1$ , it overestimates the Coulomb effects when the coupling becomes significant at moderately small  $\Gamma_e$ . An accurate representation of the excess free energy due to Coulomb coupling may be obtained by going beyond the Debye-Hückel approximation, including the following three modifications:

- effects of exchange and correlation interactions between electrons,
- electron finite-temperature (finite- $\theta$ ) effects,
- screening effects of the degenerate electrons.

For a weakly coupled plasma, the local-field effects between particles can be neglected (Ichimaru 1982). The Coulomb interactions can be treated within the linear screening theory. Under this condition, the total Hamiltonian  $H$  of the two-component plasma can be separated into (Ichimaru et al. 1987):

$$H = F_e + K_i + \frac{1}{2V} \sum_{\mathbf{k} \neq 0} \frac{4\pi e^2}{k^2} \left[ \frac{\rho_{Z\mathbf{k}} \rho_{Z\mathbf{k}}^*}{\epsilon(k)} - N_{\text{ion}} \langle Z^2 \rangle \right], \quad (22)$$

where  $F_e$  and  $K_i$  represent the Helmholtz free energy of the uniform electron background and the kinetic energy of the ions;  $\rho_{Z\mathbf{k}} \equiv \sum_j Z_j \rho_{j\mathbf{k}}$  is the Fourier component of the ion charge number fluctuations; and the dielectric function  $\epsilon(k)$  ( $k = |\mathbf{k}|$ ) is the static screening function of the electron fluid. For the ionic mixture in a rigid electron background,  $\epsilon(k) = 1$ . Thus, the Coulomb term of the free energy can be written as

$$F_{\text{Coul}} = F_{ee} + F_{ii} + F_{ie}, \quad (23)$$

where the quantities labeled ee, ii and ie refer to the contributions corresponding to the electron-electron interaction, ion-ion interaction, and ion-electron interaction, respectively. It is convenient to introduce dimensionless quantities for the free energy

$$f_{ee} = \frac{F_{ee}}{N_e k_B T}, \quad f_{ie} = \frac{F_{ie}}{N_{\text{ion}} k_B T}, \quad f_{ii} = \frac{F_{ii}}{N_{\text{ion}} k_B T}, \quad (24)$$

and for the internal energy

$$u_{ee} = \frac{U_{ee}}{N_e k_B T}, \quad u_{ie} = \frac{U_{ie}}{N_{\text{ion}} k_B T}, \quad u_{ii} = \frac{U_{ii}}{N_{\text{ion}} k_B T}. \quad (25)$$

The Coulomb free energy can be obtained from integration of the internal energy with respect to the coupling constant (Tanaka et al. 1985a; Ichimaru et al. 1987)

$$f_{\text{Coul}} = \int_0^\Gamma \frac{d\Gamma'}{\Gamma'} [u_{\text{Coul}}(\Gamma')]_\theta. \quad (26)$$

By using dimensionless form defined above, Eq.(25) is expressed as

$$F_{\text{Coul}} = N_e k_B T f_{ee} + N_{\text{ion}} k_B T (f_{ii} + f_{ie}), \quad (27)$$

or

$$f_{\text{Coul}} = x_e f_{ee} + x_{\text{ion}} (f_{ii} + f_{ie}), \quad (28)$$

where  $x_{\text{ion},e} \equiv N_{\text{ion},e}/N$  denote the number fraction of ions and electrons, respectively, and  $N = N_{\text{ion}} + N_e$  is the total number of charged particles.

A model for the H-He mixture requires a knowledge of the interaction between the charged hydrogen and helium species; however, the non-ideal free energy of the mixture can be expressed with high accuracy by the so-called linear mixing rule in terms of the free energy of the pure phases (Hansen et al.

1977). Taking hydrogen as “1” and helium as “2”, the excess free energy due to Coulomb coupling is written as

$$\begin{aligned} f_{ee}(N_1, N_2, N_e) &= f_{ee}(\Gamma_e, \theta), \\ f_{ii}(N_1, N_2, N_e) &= \sum_{j=1}^2 \zeta_j f_{ii}(N_j, N_e), \\ f_{ie}(N_1, N_2, N_e) &= \sum_{j=1}^2 \zeta_j f_{ie}(N_j, N_e). \end{aligned} \quad (29)$$

where  $\zeta_j \equiv N_j/N_{\text{ion}}$  represents the number fraction of ions of species  $j$  in the total ionic configurations. The electron-electron interaction term  $f_{ee}$  is a function of  $\Gamma_e$  and  $\theta$ , which are related to the number of the degenerate electrons.

The contributions to  $F_{\text{Coul}}$ , have been studied by various procedures by solving a set hypernetted-chain (HNC) or Monte Carlo simulations (Brami et al. 1979; Tanaka et al. 1985a, 1985b; Ichimaru et al. 1987; Ebeling 1990; DeWitt et al. 1996; Stolzmann & Blöcker 1996; Chabrier & Potekhin 1998). In this paper, we make use of fitting formulae for dealing with the weakly coupled plasmas.

### 3.1. Electron-electron interaction

For the sake of simplicity, we describe an interacting electron system in terms of an effective single-particle problem. Considering the contribution from the sum of ring-diagrams to the free energy, the exchange-correlation free energy of electrons  $f_{ee}$  is calculated numerically according to (Fetter & Walecka 1971; Tanaka et al. 1985a):

$$f_{ee} = \frac{3}{4} \sum_{l=-\infty}^{l=\infty} \int_0^{\infty} y^2 \{ \ln [1 + \Psi_l(y)] - \Psi_l(y) \} dy, \quad (30)$$

where

$$\begin{aligned} \Psi_l(y) &= \left( \frac{9\pi}{4} \right)^{1/3} \frac{\Gamma\theta}{\pi y^3} \times \\ &\times \int_0^{\infty} x n_0(k_F x) dx \ln \left[ \frac{(2\pi l\theta)^2 + (y^2 + 2xy)^2}{(2\pi l\theta)^2 + (y^2 - 2xy)^2} \right], \end{aligned} \quad (31)$$

and  $n_0(k_F x)$  is the quantum-mechanical Fermi-Dirac distribution

$$n_0(k_F x) = \frac{1}{\exp[(\varepsilon - \mu_e)/k_B T] + 1},$$

with  $x = k_B/k_F$  and  $\varepsilon = \hbar^2(k_F x)^2/2m_e$ . Eq. (30), based on the random-phase approximation (RPA), gives good results in calculating the Coulomb coupling for a weakly coupled plasma because the kinetic energy is dominant.

In order to derive the equation of state, we must find an analytic formula for interaction energy which is sufficiently accurate to enable the necessary integration and differentiation. The formula should include limiting conditions for  $u_{ee}(\Gamma_e, \theta)$

1.  $\theta \ll 1$ . When  $\Gamma_e$  is kept at a finite value, the electrons thus form an unpolarizable negatively charged background to the

ions. The contribution  $u_{ee}$  of the electrons to the interaction energy is given by the Hartree-Fock value

$$-\frac{1}{\Gamma_e} u_{ee} = \frac{3}{4\pi} \left( \frac{9\pi}{4} \right)^{1/3} \simeq 0.45817. \quad (32)$$

2. In the weak-coupling limit  $\Gamma_e \ll 1$ , the lowest-order Hartree-Fock exchange energy of the electrons is the dominant contribution to  $u_{ee}$ , so that

$$-\frac{1}{\Gamma_e} u_{ee} = a(\theta) + O\left(\Gamma_e^{1/2}\right), \quad (33)$$

where an accurate fitting formula for  $a(\theta)$  has been obtained by Perrot & Dharma-wardana (1984) as

$$\begin{aligned} a(\theta) &= \left( \frac{9}{4\pi^2} \right)^{1/3} \tanh\left(\frac{1}{\theta}\right) \times \\ &\frac{0.75 + 3.04363\theta^2 - 0.092270\theta^3 + 1.70350\theta^4}{1 + 8.31051\theta^2 + 5.1105\theta^4}. \end{aligned} \quad (34)$$

In the classical limit  $\theta \gg 1$ ,  $a(\theta) \rightarrow 0$ , and the second term in Eq. (33) proportional to  $\Gamma_e^{1/2}$  becomes the leading contribution in the weak coupling regime; this term can be approximately evaluated in the Debye-Hückel theory as  $O(\Gamma_e^{1/2}) = (\sqrt{3}/2)\Gamma_e^{1/2}$ .

Considering these limiting cases, we adopt an approximate expression for the contribution arising from the electron-electron interaction. Tanaka et al. (1985a); Tanaka et al. (1985b) and Tanaka & Ichimaru (1989) computed the interaction energy of the finite-temperature electron liquids in the RPA and the Singwi-Tosi-Land-Sjölander approximation (STLS) (Singwi et al. 1968). The values of  $u_{ee}$  obtained in the RPA and the STLS approximations may provide accurate estimates of the exact free energy  $f_{ee}$  at finite temperatures as an interpolation between the classical and degenerate limits. A fitting formula may be constructed which parametrizes the computed values, valid when  $\Gamma_e < 1$ ;  $\theta > 0.1$ ; not only can this be applied to the weak coupling region ( $\Gamma_e < 1$ ), but it also yields the Debye-Hückel limiting law in the classical limit ( $\Gamma_e \ll 1$ ):

$$u_{ee} = a_0(\theta) \Gamma_e + a_1(\theta) \Gamma_e^{3/2} + a_2(\theta) \Gamma_e^2, \quad (35)$$

where

$$\begin{aligned} a_0(\theta) &= 0.44973 \exp(-0.54712/\theta) - 0.44335, \\ a_1(\theta) &= -0.48618 \exp(-0.47357/\theta) - 0.34389, \\ a_2(\theta) &= 0.28162 \exp(-0.16000/\theta) + 0.21628. \end{aligned} \quad (36)$$

Eq. (35) reproduces the RPA values and the STLS values within 1% for  $\Gamma_e < 1$ . The excess free energy  $f_{ee}$  can be derived from the above expression with the aid of Eq. (26):

$$f_{ee}(\Gamma_e, \theta) = a_0(\theta) \Gamma_e + \frac{2}{3} a_1(\theta) \Gamma_e^{3/2} + \frac{1}{2} a_2(\theta) \Gamma_e^2. \quad (37)$$

The Coulomb pressure  $P_{ee}$  can be obtained from Eqs (35) and (37) as

$$\frac{P_{ee} V}{N_e k_B T} = -V \left( \frac{\partial f_{ee}(\Gamma_e, \theta)}{\partial V} \right)_{T, N}$$

$$\begin{aligned}
&= \frac{\Gamma_e}{3} \left( \frac{\partial f_{ee}}{\partial \Gamma_e} \right)_\theta - \frac{2\theta}{3} \left( \frac{\partial f_{ee}}{\partial \theta} \right)_{\Gamma_e} \quad (38) \\
&= \frac{1}{3} u_{ee} + \frac{1}{\theta} \left[ b_0(\theta) \Gamma_e + b_1(\theta) \Gamma_e^{3/2} + b_2(\theta) \Gamma_e^2 \right],
\end{aligned}$$

where

$$\begin{aligned}
b_0(\theta) &= -0.16404 \exp(-0.54712/\theta), \\
b_1(\theta) &= 0.08128 \exp(-0.47357/\theta), \\
b_2(\theta) &= -0.01502 \exp(-0.16000/\theta).
\end{aligned} \quad (39)$$

### 3.2. Ion-ion interaction

All the thermodynamic functions of classical ions in a uniform (rigid) electron background can be expressed as functions of the single parameter  $\Gamma_j$ , where  $\Gamma_j = \Gamma_e Z_j^{5/3}$  denotes the coupling parameter of ions of species  $j$ . An accurate analytic fit of the internal energy of ions must recover the Debye-Hückel limit  $u_{ii} = -(\sqrt{3}/2)\Gamma_j^{3/2}$ . For the ion-ion interaction, we adopt a simplified internal energy formula proposed by Chabrier & Potekhin (1998) in the framework of the  $N$ -body HNC theory, which accurately reproduces the Debye-Hückel value for  $\Gamma_j \ll 1$  and provides a smooth transition from  $\Gamma_j > 1$  to  $\Gamma_j < 1$ :

$$u_{ii}(\Gamma_j) = \Gamma_j^{3/2} \left[ \frac{c_1}{\sqrt{c_2 + \Gamma_j}} + \frac{c_3}{1 + \Gamma_j} \right], \quad (40)$$

where the fitting parameters are  $c_1 = -0.9052$ ,  $c_2 = 0.6322$  and  $c_3 = 0.2724$ .

The excess free energy  $f_{ii}$  for ions of species  $j$  arising from the contribution of ion-ion interaction can be derived from the above expression with the aid of Eq. (26):

$$\begin{aligned}
f_{ii}(\Gamma_j) &= c_1 \left[ \sqrt{\Gamma_j (c_2 + \Gamma_j)} - c_2 \ln(\sqrt{\Gamma_j/c_2} \right. \\
&\quad \left. + \sqrt{1 + \Gamma_j/c_2}) \right] + 2c_3 \left[ \sqrt{\Gamma_j} - \arctan(\sqrt{\Gamma_j}) \right].
\end{aligned} \quad (41)$$

For a H-He mixture, the total ion-ion contribution to the free energy is given by the linear-mixing formula Eq. (29) to good accuracy

$$f_{ii}(N_1, N_2, N_e) = \sum_{j=1}^2 \zeta_j f_{ii}(\Gamma_j, \zeta_j = 1). \quad (42)$$

The corresponding changes in pressure due to ion-ion interaction is obtained by using Eq. (14):

$$\begin{aligned}
\frac{P_{ii}V}{N_{\text{ion}}k_B T} &= -V \left( \frac{\partial f_{ii}}{\partial V} \right)_{T,N} \\
&= \frac{1}{3} \sum_{j=1}^2 \zeta_j u_{ii}(\Gamma_j, \zeta_j = 1).
\end{aligned} \quad (43)$$

### 3.3. Ion-electron interaction

When the Fermi degeneracy of the electrons is weak, we can assume classical statistics both for the electrons and for the ions.

We consider here a modified Coulomb interaction rather than the bare Coulomb potential through which purely classical particles would interact. Suppose that a point charge  $Z_j e$  is introduced into the thermal uniform plasma. We allow the plasma to settle down to a steady state after the charge is introduced. Now the electron and ion densities will be determined by the Maxwell-Boltzmann distribution, so that the changes in density are given by the Boltzmann factors:

$$n_e(r) = n_e \exp\left(\frac{e\phi}{k_B T}\right), \quad (44)$$

$$n_j(r) = n_j \exp\left(-\frac{Z_j e \phi}{k_B T}\right). \quad (45)$$

Since the unperturbed state has zero charge density, so that  $n_e = \sum_j Z_j n_j$ , the electrostatic potential  $\phi(\mathbf{r})$  is related to the charge density through the Poisson-Boltzmann equation, which can be written as (Sturrock 1994; Brügggen & Gough 1997):

$$\begin{aligned}
\nabla^2 \phi &= 4\pi n_e e \left[ \exp\left(\frac{e\phi}{k_B T}\right) - \exp\left(-\frac{\langle Z^2 \rangle e \phi}{\langle Z \rangle k_B T}\right) \right] \\
&\quad - 4\pi \sum_j Z_j e \delta(\mathbf{r} - \mathbf{r}_j),
\end{aligned} \quad (46)$$

where  $\mathbf{r}_j$  is the position of the ion  $j$ , and  $\delta$  is the Dirac delta function. Furthermore, linearization yields

$$\phi = \sum_j \phi_j. \quad (47)$$

If  $\phi_j$  is a weak potential then expansion of the exponentials in Eq. (46) leads to

$$(\nabla^2 - k_D^2) \phi_j = 4\pi Z_j e \delta(\mathbf{r} - \mathbf{r}_j), \quad (48)$$

In solving Eq. (48) one must require that both  $\phi_j(r)$  and the electric field  $-\nabla \phi_j(r)$  be continuous across the exclusion sphere  $|\mathbf{r}| = a$  and that  $\phi_j(r)$  vanish as  $\mathbf{r} \rightarrow \infty$ . In the exterior region,  $r > a$ , the screened potential of a given ion  $j$  is given by the extend Debye-Hückel theory with hard-core correction (Lee & Fisher 1996; Levin & Fisher 1996):

$$\phi_j = \frac{Z_j e}{r_j} \Theta(k_D a) e^{-k_D r_j}, \quad (49)$$

with

$$\Theta(k_D a) = \frac{e^{k_D a}}{1 + k_D a}. \quad (50)$$

Since Eq. (49) is the solution of Eq. (48), the net electron density in the cloud around ion  $j$  is given by

$$\rho_e = - \left[ \frac{1}{4\pi} \nabla^2 \phi_j \right]_{\mathbf{r}=\mathbf{r}_j>0} = - \frac{e^2 n \phi_j}{k_B T}, \quad (51)$$

or alternatively

$$\rho_e = - \frac{Z_j e k_D^2 \Theta(k_D a)}{4\pi r} \exp(-k_D r), \quad (52)$$

and the ion density  $\rho_j$  is

$$\rho_j = Z_j e \delta(\mathbf{r}) . \quad (53)$$

The ion-electron interaction energy for ions of species  $j$  is obtained by (Shaviv & Shaviv 1996):

$$U_{ie}(N_j, N_e) = \frac{1}{2} \sum_j \int \frac{\rho_j(\mathbf{r}) \rho_e(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' . \quad (54)$$

On the basis of the spherically symmetric approximation, substituting Eqs (52) and (53) into Eq. (54), the dimensionless form of Eq. (54) is given by

$$\begin{aligned} u_{ie}(N_j, N_e) &= -\frac{\Theta(k_D a)}{2k_B T} \\ &\times \int \frac{Z_j^2 e^2 k_D^2 \exp(-k_D |\mathbf{r}'|) \delta(\mathbf{r})}{4\pi |\mathbf{r} - \mathbf{r}'| |\mathbf{r}'|} d^3r d^3r' \\ &= -\frac{\Theta(k_D a)}{2k_B T} \int \frac{Z_j^2 e^2 k_D^2}{r^2} 4\pi r^2 dr \\ &= -\frac{(Z_j e)^2 \Theta(k_D a)}{2r_D k_B T} . \end{aligned} \quad (55)$$

By using Eq. (4), Eq. (55) becomes

$$u_{ie}(N_j, N_e) = -\frac{1}{2} \left( \frac{Z_j}{\langle Z \rangle} \right)^2 \Theta(k_D a) k_D a \Gamma_{ion} . \quad (56)$$

In order to consider screening effects of the degenerate electrons, Eq. (9) can be rewritten as

$$k_D = \left[ \frac{4\pi N_e e^2 (\theta_e + \langle Z^2 \rangle / \langle Z \rangle)}{V k_B T} \right]^{1/2} , \quad (57)$$

where

$$\theta_e = \frac{1}{2} \frac{I_{-1/2}(\eta_e)}{I_{1/2}(\eta_e)} \quad (58)$$

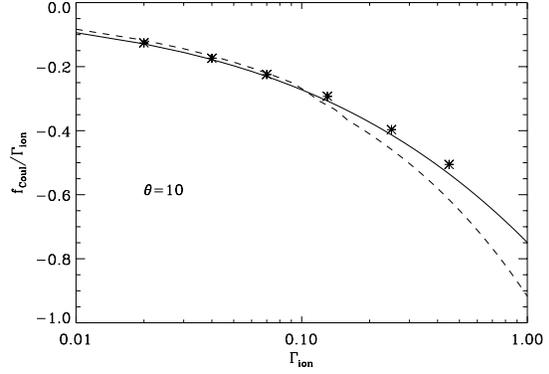
is a correction for degenerate electrons. In the non-degenerate limit,  $\theta_e = 1$ .

By using Eqs (3), (4) and (57), we obtain the relation

$$k_D a = \sqrt{3} \frac{(\theta_e \langle Z \rangle + \langle Z^2 \rangle)^{1/2}}{\langle Z \rangle} \Gamma_{ion}^{1/2} . \quad (59)$$

With the aid of Eqs (26), (29) and (59), the excess free energy  $f_{ie}$  due to the ion-electron interaction for the weak coupling limit is approximately given by the linear-mixing rule

$$\begin{aligned} f_{ie}(N_1, N_2, N_e) &= -\sum_{j=1}^2 \zeta_j \frac{Z_j^2 e^2 \Theta(k_D a)}{3r_D k_B T} \\ &= -\frac{1}{3} \sum_{j=1}^2 \zeta_j \left( \frac{Z_j}{\langle Z \rangle} \right)^2 \Theta(k_D a) k_D a \Gamma_{ion} \\ &= -\frac{1}{3} \frac{\langle Z^2 \rangle}{\langle Z \rangle^2} \Theta(k_D a) k_D a \Gamma_{ion} . \end{aligned} \quad (60)$$



**Fig. 1.** Total excess free energy due to Coulomb coupling for a H-He mixture divided by the coupling parameter  $\Gamma_{ion}$  at weak degeneracy  $\theta = 10$ . The solid and dashed lines refer to the calculations of the present formula and Debye-Hückel approximation, respectively; the stars illustrate the Padé formula of Stolzmann & Blöcker (1996).

The corresponding change in pressure due to screening effects of degenerate electrons is obtained by using Eq. (14)

$$\begin{aligned} \frac{P_{ie} V}{N_{ion} k_B T} &= -V \left( \frac{\partial f_{ie}}{\partial V} \right)_{T, N} \\ &= -\frac{1}{6} \frac{\langle Z^2 \rangle}{\langle Z \rangle^2} \Theta(k_D a) k_D a \Gamma_{ion} . \end{aligned} \quad (61)$$

Finally, the Coulomb pressure  $P_{Coul}$  is given by

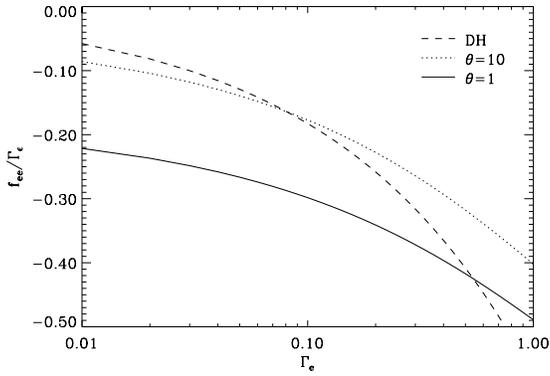
$$P_{Coul} = P_{ee} + P_{ii} + P_{ie} . \quad (62)$$

## 4. Results and discussion

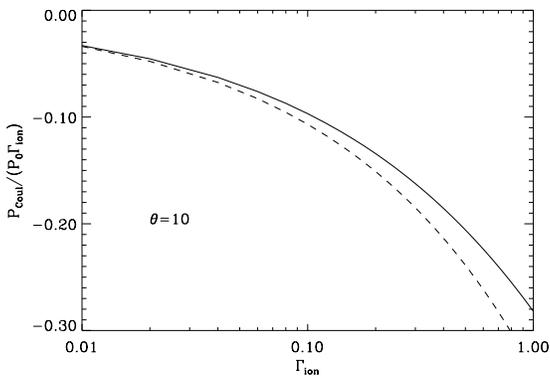
The Coulomb coupling leads to non-ideal effects in the EOS and modifies the thermodynamic functions. In the present work, we examine the contribution of the Coulomb coupling to the thermodynamic quantities of a fully ionized and weakly coupled H-He mixture, with abundances by mass of hydrogen and helium of  $X = 0.70$  and  $Y = 0.30$ , respectively.

Fig. 1 shows the total excess free energy  $f_{Coul}$  divided by  $\Gamma_{ion}$  at  $\theta = 10$  calculated according to Eqs (37), (42) and (60). In Fig. 1 we compare the value of  $f_{Coul}$  with values obtained from other theoretical expressions. As one would expect, our result is closed available representation of Stolzmann & Blöcker (1996) from a Padé approximation. For  $\Gamma_{ion} < 0.05$ , the electron-electron exchange contribution is dominant; the Debye-Hückel approximation fails to account appropriately for the electron-electron exchange effects in the weak coupling regime, and hence it predicts a value of  $f_{Coul}$  even lower than the RPA values over a significant domain of  $\Gamma_{ion}$ . It can also be seen from Fig. 1 that the simple Debye-Hückel approximation overestimates the Coulomb effects when the coupling becomes significant at moderately small  $\Gamma_{ion}$ . However, it is easy to add the fitted formula to the Debye-Hückel approximation to obtain improved results.

Fig. 2 shows the contributions of the electron-electron interaction  $f_{ee}$  divided by  $\Gamma_e$  at  $\theta = 1$  and 10. In Fig. 2 we note that



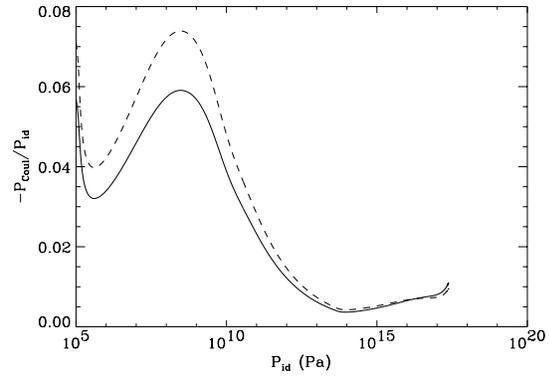
**Fig. 2.** Excess free energy arising from the electron-electron interaction  $f_{ee}$  divided by  $\Gamma_e$  at  $\theta = 1$  and 10, respectively.



**Fig. 3.** Calculated Coulomb pressure  $P_{Coul} = P_{ee} + P_{ii} + P_{ie}$  in units of  $P_0\Gamma_{ion}$ , where  $P_0 = nk_B T$ , at weak degeneracy ( $\theta = 10$ ). Solid line: the present formula; dashed line: the Debye-Hückel approximation.

the magnitude of the electron-electron exchange contribution decreases as  $\theta$  increases owing to reduction in the exchange energy. Since no electron exchange contribution (at fixed  $\Gamma_e$  regardless of  $\theta$ ) to the free energy is included in the Debye-Hückel approximation, the value of the Debye-Hückel term deviates widely from the present calculations. The result indicates that the electron-electron exchange effect and electron finite-temperature effect substantially modify the plasma properties.

The total excess pressure  $P_{Coul}$  due to Coulomb coupling is plotted in Fig. 3 at weak degeneracy,  $\theta = 10$ . The Debye-Hückel pressure is calculated on the basis of a two-component plasma (TCP) for electron-ion interaction, and a one-component (OCP) for the electron and ion. The computed data are compared with the Debye-Hückel values. It can be seen that non-ideal contributions to the pressure increase systematically with increasing  $\Gamma_{ion}$ , and the Debye-Hückel approximation overestimates the Coulomb effects. Fig. 3 also reveals that the Coulomb coupling makes a negative contribution to the pressure term, and hence reduces the total pressure  $P$ .



**Fig. 4.** Ratio of Coulomb pressure to the ideal-gas pressure of the reference solar model with the EFF equation of state. The present formula (solid line:); the Debye-Hückel approximation (dashed line).

Fig. 4 shows the relative pressure, i.e., the ratio of the Coulomb pressure  $P_{Coul}$  to the pressure  $P_{id}$  corresponding to an ideal gas for the plasma parameters of the solar interior. The reference solar model was constructed with OPAL and Kurucz opacities (Iglesias et al. 1992; Kurucz 1991) and employed the EFF equation of state without any Coulomb term. In Fig. 4 we see, at the centre ( $P \sim 10^{17}$  Pa), the values of Debye-Hückel term without electron exchange contribution are smaller than our calculated values. On the other hand, in the intermediate regions, the results indicate a smaller Coulomb correction than that obtained with the Debye-Hückel theory. It seems that the terms of higher order in the Coulomb correction play an important role. Moreover, we find that the contribution to the pressure from the Coulomb correction is up to 1%, and thus it indeed reflects the fact that the Coulomb term has a significant effect on the thermodynamic properties of the plasma, at the centre and intermediate regions (Däppen 1998).

However, at the solar surface, either the present formula or the Debye-Hückel approximation overestimates Coulomb effects. It indicates that the influence of Coulomb term is not adequate by helioseismic constraint. At the solar surface, especially in the second helium ionization zone, complex physical effects, such as pressure ionization and the formation of bound states, should be taken into account.

## 5. Summary

We have developed a completely semi-analytic model for the free energy of a fully ionized, weakly coupled plasma consisting of a H-He mixture, which is valid in the whole temperature-density regime and applicable to arbitrary mixtures. For the excess free energy of the electron fluid at finite temperature, we provide an analytic approximation based on quantum-statistics calculations. For the excess free energy of the classical ionic OCP, we adopt the present formula in the framework of the  $N$ -body HNC theory. Finally, we have taken into account the electron-ion interaction by using the extended Debye-Hückel theory with hard-sphere correction under the weakly coupled

and weakly degenerate limits. Our formulae are compared with other available approximations, and provide quick and accurate computation of the thermodynamic functions of fully ionized and weakly coupled plasmas.

A more elaborate equation of state aimed at describing the thermodynamic properties of partially ionized plasmas and ionization equilibrium will be discussed in a later paper.

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