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An improved equation of state under solar interior conditions

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Abstract. This paper presents a simple and efficient equation of state which can be used for quick and accurate computing of the thermodynamic functions of partly ionized and weakly coupled plasmas. Based on the free energy minimization method, the improvement of the equation of state includes a detailed account of the physical processes of non-ideal effects consisting of electron degeneracy, Coulomb coupling and pressure ionization. The treatment of Coulomb coupling combines the results of the quantum exchange effect of degenerate electrons at finite temperature, N-body semi-analytic theory and the extended Debye-Hückel theory with hard-sphere correction. For the complicated physical processes of pressure ionization an approximate model is adopted. The nonideal corrections to equation of state are calculated under solar interior conditions.

Key words: equation of state – Sun: interior – stars: interiors

1. Introduction

The modeling of high-quality helioseismic data requires great accuracy in an equation of state (EOS), thus providing a basis for checking input physics about stellar envelopes and interiors. Although nonideal effects are fairly weak in the Sun, they influence the structure of solar interior significantly. The complexity of physical effects mainly includes two processes, i.e., Coulomb coupling and pressure ionization, both of which should be incorporated into the equation of state of stellar evolutionary codes covering a wide range of density and temperature variables.

Several equations of state have been developed in order to include nonideal effects for fully ionized or partially ionized plasmas. A theoretical description of improved equations of state beyond the ideal gas law can be based either on the physical or the chemical picture of the plasma. In the chemical picture, the simplest improved equation of state is the so called CEFF equation of state (Christensen-Dalsgaard et al. 1988; Christensen-Dalsgaard & Däppen 1992) by adding Debye-Hückel free energy term to the EFF model (Eggleton et al. 1973). Mihalas et al. (Hummer & Mihalas 1988; Mihalas et al. 1988; Däppen et al. 1988) have presented the so called MHD equation of state which takes into account the effect of excited levels of atoms and ions on the properties of the plasma. The MHD equation of state considers only the lowest-order Coulomb coupling term through the Debye-Hückel approximation. In contrast to the chemical picture, there exists a more complicated physical picture, in which nuclei and electrons (free or bound) are the only fundamental constituents of the thermodynamic ensemble, as employed in the OPAL equation of state (Rogers 1986; Rogers et al. 1996).

The MHD equation of state and the OPAL equation of state are given with their results in tabular form and can not be called directly. This is because the complex formalism and time-consuming calculation of the EOS stem from many physical processes. Although a number of shortcomings in the EFF equation of state have been known for a long time, the EFF equation of state possesses many advantages over tabulated EOSs due to its being analytical. Its obvious merit is flexibility in varying compositions, which have been routinely dealt with, and the possibility of introducing and investigating new physics. In order to model high accurate EOS, we attempt to present an algorithm for explicit and simplified expressions of the improved EFF equation of state under the solar interior conditions on the basis of free-energy minimization method in the chemical picture (Harris et al. 1960; Graboske et al. 1969). The EOS presented in this paper is formulated for a hydrogen-helium mixture and takes into account the physical processes of electron degeneracy, Coulomb coupling and pressure ionization.

The paper is organized as follows. A thermodynamic model of the hydrogen-helium mixture is presented in Sect. 2. In Sect. 3, we propose simple and accurate analytic approximations for the non-ideal free energies of the plasma arising from Coulomb coupling and pressure ionization. The algorithm for calculating thermal equilibrium is given in Sect. 4. In Sect. 5 the calculated results of the EOS are compared with those of other EOSs.

2. Free energy model for a H-He mixture

Since the main matter constituting the Sun is a mixture of hydrogen and helium, we need an expression for the free energy including the contribution of at least six chemical species with free and bound state, i.e., electrons, ions H^+, He^{++}, He^+, and

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neutral particles H, He. The total free energy F can be written as the sum of four terms (Saumon et al. 1995; Potekhin et al. 1999):

$$F\left(T, V, \{N_{\mathrm{k}}\}, N_{\mathrm{e}}\right) = F_{\mathrm{id}}^{(k)} + F_{\mathrm{id}}^{(e)} + F_{\mathrm{rad}} + F_{\mathrm{ex}}, \tag{1}$$

where $F_{\mathrm{id}}^{(k)}$ is the ideal-gas contribution of the particles; $F_{\mathrm{id}}^{(e)}$, the contribution from the uniform electron gas; F_{rad}, the radiation term of free energy; F_{ex}, the excess free energy arising from nonideal effects.

The pressure P, enthalpy H and the electron chemical potential μ_{e} can be given by differentiating the free energy with respect to either V and T, at fixed N_{e} and N_{k}, or N_{k}, at fixed V and T, respectively:

$$P = -\left(\frac{\partial F}{\partial V}\right)_{\mathrm{T},\{\mathrm{N_e},\mathrm{N_k}\}} \, , \tag{2}$$

$$H = -T^2\left(\frac{\partial}{\partial T}\frac{F}{T}\right)_{\mathrm{V},\{\mathrm{N_e},\mathrm{N_k}\}} - V\left(\frac{\partial F}{\partial V}\right)_{\mathrm{T},\{\mathrm{N_e},\mathrm{N_k}\}} \, , \tag{3}$$

and

$$\mu_{\mathrm{e}} = \frac{1}{k_{\mathrm{B}}T}\left(\frac{\partial F}{\partial N_{\mathrm{e}}}\right)_{\mathrm{T},\mathrm{V},\{\mathrm{N_k}\}} \, . \tag{4}$$

2.1. *Plasma parameters*

The behaviour of a H-He mixture manifests nonideal effects of interacting charged particles. Degeneracy of electron, Coulomb coupling and pressure ionization are important features of the plasma. To describe nonideal effects of the plasma, it is convenient to introduce dimensionless parameters to characterize the plasma. We consider the plasma consisting of N_{i} ions of species $i = \{\mathrm{H}^+, \mathrm{He}^{++}, \mathrm{He}^+\}$, with charges $Z_{\mathrm{i}}e$, N_{j} neutral particles of species $j = \{\mathrm{H}, \mathrm{He}\}$, and N_{e} electrons in a volume V at a temperature T. The mean ionic charge is defined as

$$\langle Z^\nu \rangle = \frac{\sum_{\mathrm{i}} Z_{\mathrm{i}}^\nu N_{\mathrm{i}}}{\sum_{\mathrm{i}} N_{\mathrm{i}}} \, . \tag{5}$$

In the multicomponent plasma, the averaged Coulomb coupling parameters for ions and for electrons are given by (Ichimaru et al. 1987; Stolzmann & Böcher 1996):

$$\Gamma_{\mathrm{ion}} = \langle Z \rangle^{1/3} \left\langle Z^{5/3} \right\rangle \frac{e^2}{k_{\mathrm{B}}Ta} \, , \tag{6}$$

and

$$\Gamma_{\mathrm{e}} = \frac{e^2}{k_{\mathrm{B}}T}\left(\frac{4\pi}{3V}N_{\mathrm{e}}\right)^{1/3} = \Gamma_{\mathrm{ion}} / \left\langle Z^{5/3} \right\rangle \, , \tag{7}$$

where

$$a = \left(\frac{4\pi N_{\mathrm{ion}}}{3V}\right)^{-1/3} \, , \tag{8}$$

is the mean ion-sphere radius, and k_{B} is the Boltzmann constant. The total number of ions is $N_{\mathrm{ion}} = \sum_{\mathrm{i}} N_{\mathrm{i}}$. The charge neutrality condition requires $N_{\mathrm{e}} = \langle Z \rangle N_{\mathrm{ion}}$.

The dimensionless density parameter of electrons r_{s} and the degree of Fermi degeneracy θ are described as, respectively

$$r_{\mathrm{s}} = \left(\frac{3V}{4\pi N_{\mathrm{e}}}\right)^{1/3} \frac{m_{\mathrm{e}}e^2}{\hbar^2} \, , \tag{9}$$

and

$$\theta = 2\left(\frac{4}{9\pi}\right)^{2/3} r_{\mathrm{s}}/\Gamma_{\mathrm{e}} \, , \tag{10}$$

where m_{e} is the mass of an electron.

2.2. *Ideal part of the free energy*

The main purpose of this work is the investigation of the thermodynamic functions of the plasma. We stress that charged and neutral particles behave classically. In this paper, we limit ourselves to the consideration of one-component plasma (OCP) where the particles are regarded as point particles while the electrons are assumed to form a uniform background of neutralizing space charges. Thus $F_{\mathrm{id}}^{(k)}$ and $F_{\mathrm{id}}^{(e)}$ can be given by Maxwell-Boltzmann statistic and Fermi-Dirac integrals. The ideal free energy of classical particles can be written as

$$F_{\mathrm{id}}^{(k)} = k_{\mathrm{B}}T \sum_{\mathrm{k}} N_{\mathrm{k}} \left[\ln\left(\frac{N_{\mathrm{k}}}{V w_{\mathrm{k}}}\lambda_{\mathrm{k}}^3\right) + \frac{\chi_{\mathrm{k}}}{k_{\mathrm{B}}T}\right] \tag{11}$$

with the thermal de-Broglie wavelength of particles

$$\lambda_{\mathrm{k}} = \left(\frac{2\pi\hbar^2}{k_{\mathrm{B}}Tm_{\mathrm{k}}}\right)^{1/2} \, , \tag{12}$$

where k runs over five species $\{\mathrm{H}^+, \mathrm{H}, \mathrm{He}^{++}, \mathrm{He}^+, \mathrm{He}\}$; w_{k} is the statistical weights both in bound and free states; the corresponding energies χ_{k} of ionization for five species have values $0, -13.60, 0, -54.40$ and -78.98 in electron volts.

For partially degenerate electrons, the ideal part of the free energy for electrons is

$$F_{\mathrm{id}}^{(e)} = N_{\mathrm{e}}\mu_{\mathrm{e}} - P_{\mathrm{e}}V \, , \tag{13}$$

where P_{e} is the pressure of the ideal Fermi gas. The pressure P_{e} and electron density n_{e}, in turn, are functions of chemical potential μ_{e} and temperature T, which can be given by

$$P_{\mathrm{e}} = \frac{8}{3\sqrt{\pi}}\frac{k_{\mathrm{B}}T}{\lambda_{\mathrm{e}}^3} I_{3/2}\left(\psi\right) \, , \tag{14}$$

and

$$n_{\mathrm{e}} = \frac{4}{\sqrt{\pi}\lambda_{\mathrm{e}}^3} I_{1/2}\left(\psi\right) \, , \tag{15}$$

where the degeneracy parameter is defined as $\psi \equiv \mu_{\mathrm{e}}\left(k_{\mathrm{B}}T\right)^{-1}$, and

$$I_{\mathrm{n}}\left(\psi\right) = \int_0^\infty \frac{x^n \mathrm{d}x}{e^{x-\psi} + 1} \tag{16}$$

is the usual nonrelativistic Fermi-Dirac integral. The chemical potential is obtained from the relationship

$$I_{1/2}\left(\psi\right) = \frac{2}{3}\theta^{-3/2} \, . \tag{17}$$

Furthermore, ψ can be expressed in useful analytic formula (Ichimaru & Kitamura 1996):

$$\psi = -\frac{3}{2}\ln\theta + \ln\frac{4}{3\sqrt{\pi}} + \frac{A\theta^{-(b+1)} + B\theta^{-(b+1)/2}}{1 + A\theta^{-b}} \tag{18}$$

with $A = 0.025954$, $B = 0.072$, and $b = 0.858$, as a function of the degeneracy parameter θ.

The third term on the right of Eq. (1), i.e., radiative term $F_{\rm rad}$, is

$$F_{\rm rad} = \frac{4\sigma}{3c}VT^4 \ , \tag{19}$$

where σ and c are the Stefan-Boltzmann constant and speed of light, respectively.

The excess free energy, $F_{\rm ex}$, from the contribution of non-ideal effects, will be discussed in Sect. 3.

3. Non-ideal effects

The excess free energy arising from nonideal effects is written as

$$F_{\rm ex} = F_{\rm C} + F_{\rm neu} \ . \tag{20}$$

where $F_{\rm C}$ denotes Coulomb coupling, and $F_{\rm neu}$ takes account of the contributions from interactions of neutral species with electrons, ions and other neutral species.

Two physical processes, i.e., Coulomb correction of charged particles and pressure ionization of neutral species, have been taken into account in this paper. Owing to the complexity of such physical processes, we only consider simplified and approximate models.

3.1. Improvement of Coulomb coupling

The interaction contributions of Coulomb coupling, as presented in the work of Bi et al. (2000), allow fast access to different thermodynamic properties in wide ranges of density and temperature. The Debye-Hückel approximation overestimates Coulomb effects when the coupling becomes significant at moderately coupling value. Therefore, the present improvements are made on the basis of the available analytical formulae for the quantum exchange effect of electrons at finite temperature, N-body semi-analytic theory for ions, and the extended Debye-Hückel theory with hard-core correction for ion-electron interaction under the weakly coupled and weakly degenerate conditions. These modifications not only can be applied to the weak coupling region, but can also yield the Debye-Hückel limiting law in the classical limit.

The Coulomb term of free energy can be expressed as the sum of the separate contributions, electron-electron, ion-ion and ion-electron interaction, that is,

$$F_{\rm C} = N_{\rm e}k_{\rm B}Tf_{\rm ee} + N_{\rm ion}k_{\rm B}T\left(f_{\rm ii} + f_{\rm ie}\right) \ , \tag{21}$$

where the dimensionless form of excess free energy in Eq. (21) can be written by the linear-mixing rule (Ichimaru & Kitamura 1996):

$$\begin{aligned} f_{\rm ee}\left(N_{\rm e}\right) &= f_{\rm ee}\left(\Gamma_{\rm e},\theta\right) \ , \\ f_{\rm ii}\left(\{N_{\rm i}\}\right) &= \sum_{\rm i=1}^{3}\zeta_{\rm i}f_{\rm ii}\left(N_{\rm i}\right) \ , \\ f_{\rm ie}\left(\{N_{\rm i}\},N_{\rm e}\right) &= \sum_{\rm i=1}^{3}\zeta_{\rm i}f_{\rm ie}\left(N_{\rm i},N_{\rm e}\right) \ . \end{aligned} \tag{22}$$

where $\zeta_{\rm i} \equiv N_{\rm i}/N_{\rm ion}$ represents the number fraction of ions of species i in the total ionic configurations $\{{\rm H}^+, {\rm He}^{++}, {\rm He}^+\}$. Since $m_{\rm e} \ll m_{\rm i}$, we may approximately regard the electron-electron and ion-ion interaction terms as being the functions of only $N_{\rm e}$ and $N_{\rm ion}$, respectively. In general, the excess free energy due to Coulomb coupling is calculated through the coupling constant integration of the internal energy (Ichimaru et al. 1987), namely

$$f_{\rm C} = \int_0^{\Gamma} u_{\rm C}\left(\Gamma'\right)\frac{{\rm d}\Gamma'}{\Gamma'} \ , \tag{23}$$

where $u_{\rm C}$ is the dimensionless form of the Coulomb internal energy.

3.1.1. Electron-electron interaction

For the electron-electron contribution, we adopt the expression of interaction energy proposed by Bi et al. (2000), which is based on the results of quantum-statistic calculations of electrons at the finite temperature:

$$u_{\rm ee}\left(\Gamma_{\rm e},\theta\right) = a_0\left(\theta\right)\Gamma_{\rm e} + a_1\left(\theta\right)\Gamma_{\rm e}^{3/2} + a_2\left(\theta\right)\Gamma_{\rm e}^2 \ , \tag{24}$$

where

$$\begin{aligned} a_0\left(\theta\right) &= 0.44973\exp\left(-0.54712/\theta\right) - 0.44335 \ , \\ a_1\left(\theta\right) &= -0.38618\exp\left(-0.47357/\theta\right) - 0.34389 \ , \\ a_2\left(\theta\right) &= 0.28162\exp\left(-0.16000/\theta\right) + 0.21628 \ . \end{aligned} \tag{25}$$

The excess free energy arising from electron-electron interaction is then obtained by performing $\Gamma_{\rm e}$ integration:

$$f_{\rm ee}\left(\Gamma_{\rm e},\theta\right) = a_0\left(\theta\right)\Gamma_{\rm e} + \frac{2}{3}a_1\left(\theta\right)\Gamma_{\rm e}^{3/2} + \frac{1}{2}a_2\left(\theta\right)\Gamma_{\rm e}^2 \ . \tag{26}$$

In the weak coupling limit ($\Gamma_{\rm e} \ll 1$), the values of $f_{\rm ee}$ asymptically approach the lowest-order exchange energy, i.e., Hartree-Fock energy. In the classical and weak coupling limits, the Debye-Hückel value $f_{\rm ee} = -1/\sqrt{3}\Gamma_{\rm e}^{3/2}$ then becomes the leading contribution to the electron-electron interaction. Considering those boundary conditions mentioned above, Eq. (26) reproduces the RPA values (Fetter & Walecka 1971; Tanaka et al. 1985) and the STLS values (Singwi et al. 1968) within 1% for $\Gamma_{\rm e} < 1$.

3.1.2. Ion-ion interaction

For the ion-ion interaction, we adopt a simplified internal energy formula for ions of species i proposed by Chabrier & Potekhin

(1998), which accurately reproduces the Debye-Hückel value $u_{\rm ii} = -\sqrt{3}/2\Gamma_{\rm i}^{3/2}$ for $\Gamma_{\rm i} \ll 1$ and provides a smoother transition from $\Gamma_{\rm i} > 1$ to $\Gamma_{\rm i} < 1$:

$$u_{\rm ii}\left(\Gamma_{\rm i}\right) = \Gamma_{\rm i}^{3/2}\left[\frac{c_1}{\sqrt{c_2+\Gamma_{\rm i}}} + \frac{c_3}{1+\Gamma_{\rm i}}\right] , \tag{27}$$

where $\Gamma_{\rm i} = \Gamma_{\rm e} Z_{\rm i}^{5/3}$ denotes coupling parameter of ions of species i. The fitting parameters in Eq. (27) are $c_1 = -0.9052$, $c_2 = 0.6322$, and $c_3 = 0.2724$. It should be noted that $u_{\rm ii}$ is expressed as functions of the only parameter $\Gamma_{\rm i}$ in a uniform electron background for the classical ions. The excess free energy of ions of species i is calculated according to Eq. (23), that is

$$\begin{aligned} f_{\rm ii}\left(\Gamma_{\rm i}\right) \;=\; & c_1[\sqrt{\Gamma_{\rm i}\left(c_2+\Gamma_{\rm i}\right)} - c_2 \ln(\sqrt{\Gamma_{\rm i}/c_2} \\ & + \sqrt{1+\Gamma_{\rm i}/c_2})] + 2c_3\left[\sqrt{\Gamma_{\rm i}} - \arctan\left(\sqrt{\Gamma_{\rm i}}\right)\right] . \end{aligned} \tag{28}$$

Neglecting the interactions between the charged hydrogen and helium species, the total internal energy and the excess free energy arising from the contribution of ion-ion interaction can be given by the linear-mixing rule at good accuracy,

$$u_{\rm ii}\left(\{N_{\rm i}\}\right) = \sum_{\rm i=1}^{3} \zeta_{\rm i} u_{\rm ii}\left(\Gamma_{\rm i}, \zeta_{\rm i}=1\right) , \tag{29}$$

and

$$f_{\rm ii} = \sum_{\rm i=1}^{3} \zeta_{\rm i} f_{\rm ii}\left(\Gamma_{\rm i}, \zeta_{\rm i}=1\right) . \tag{30}$$

3.1.3. Ion-electron interaction

If we assume that ion-electron interaction is weak, in which the Poisson-Boltzmann equation for the electrostatic potential can be linearized, the screened OCP model for the description of the thermodynamic properties of the two-component ion-electron plasma can be adopted. When the Fermi degeneracy of the electrons is also weak, we can farther assume that electrons and ions obey Maxwell -Boltzmann statistics. For ion-electron screening effect, we adopt the internal energy formula given by Bi et al. (2000) on the basis of the extended Debye-Hückel theory with hard-core correction, namely

$$u_{\rm ie}\left(N_{\rm i}\right) = -\frac{1}{2}\frac{Z_{\rm i}^2 e^2 \Theta\left(k_{\rm D} a\right)}{r_{\rm D} k_{\rm B} T} , \tag{31}$$

where the function $\Theta\left(k_{\rm D} a\right)$ is defined as

$$\Theta\left(k_{\rm D} a\right) = \frac{e^{k_{\rm D} a}}{1+k_{\rm D} a} , \tag{32}$$

and the reciprocal of the Debye shielding length $r_{\rm D}$ is given by

$$\begin{aligned} k_{\rm D} = r_{\rm D}^{-1} \;&=\; \left[\frac{4\pi e^2\left(\sum_{\rm i} Z_{\rm i}^2 N_{\rm i} + \theta_{\rm e} N_{\rm e}\right)}{V k_{\rm B} T}\right]^{1/2} \\ &=\; \left[\frac{4\pi e^2 N_{\rm e}\left(\theta_{\rm e} + \left\langle Z^2\right\rangle / \left\langle Z\right\rangle\right)}{V k_{\rm B} T}\right]^{1/2} . \end{aligned} \tag{33}$$

Here

$$\theta_{\rm e} = \frac{1}{2}\frac{I_{-1/2}\left(\psi\right)}{I_{1/2}\left(\psi\right)} \tag{34}$$

is a correction for degenerate electrons. In the non-degenerate limit, $\theta_{\rm e} = 1$.

By using Eqs. (6), (8) and (33), after some operations, we have a relation

$$k_{\rm D} a = \sqrt{3}\frac{\left(\theta_{\rm e}\left\langle Z\right\rangle + \left\langle Z^2\right\rangle\right)^{1/2}}{\left\langle Z\right\rangle^{1/6}\left\langle Z^{5/3}\right\rangle^{1/2}}\Gamma_{\rm ion}^{1/2} . \tag{35}$$

With the aid of Eqs. (5) and (35), the total internal energy from the contribution of ion-electron interaction is given by the liner-mixing rule, so that

$$\begin{aligned} u_{\rm ie}\left(\{N_{\rm i}\}\right) \;&=\; -\frac{1}{2}\sum_{\rm i}^{3} \zeta_{\rm i}\frac{Z_{\rm i}^2 e^2 \Theta\left(k_{\rm D}\, a\right)}{r_{\rm D} k_{\rm B} T} \\ &=\; -\frac{1}{2}\sum_{\rm i=1}^{3} \zeta_{\rm i}\frac{Z_{\rm i}^2}{\left\langle Z\right\rangle^{1/3}\left\langle Z^{5/3}\right\rangle}\Theta\left(k_{\rm D} a\right) k_{\rm D} a \Gamma_{\rm ion} \\ &=\; -\frac{\sqrt{3}}{2}\frac{\left\langle Z^2\right\rangle\left(\theta_{\rm e}\left\langle Z\right\rangle + \left\langle Z^2\right\rangle\right)^{1/2}}{\left\langle Z\right\rangle^{1/2}\left\langle Z^{5/3}\right\rangle^{3/2}}\Theta\left(k_{\rm D} a\right)\Gamma_{\rm ion}^{3/2}, \end{aligned} \tag{36}$$

Thus, the excess free energy due to ion-electron interaction is obtained by performing $\Gamma_{\rm ion}$ integration in Eq. (23) under weakly coupled limit, as

$$f_{\rm ie} = -\frac{\left\langle Z^2\right\rangle\left(\theta_{\rm e}\left\langle Z\right\rangle + \left\langle Z^2\right\rangle\right)^{1/2}}{\sqrt{3}\left\langle Z\right\rangle^{1/2}\left\langle Z^{5/3}\right\rangle^{3/2}}\Theta\left(k_{\rm D}\, a\right)\Gamma_{\rm ion}^{3/2} . \tag{37}$$

As a result, corresponding Coulomb corrections to the thermodynamic functions, i.e., the pressure $P_{\rm C}$, the electron chemical potential $\Delta\mu_{\rm C}$ and the enthalpy $H_{\rm C}$, can be calculated from

$$\begin{aligned} P_{\rm C} \;&=\; -\left(\frac{\partial F_{\rm C}}{\partial V}\right)_{\rm T,\{N_e,N_i\}} \\ &=\; \frac{k_{\rm B} T}{3}\left[n_{\rm e} u_{\rm ee} + n_{\rm ion}\left(u_{\rm ii} + u_{\rm ie}\right)\right] \\ &\quad + \frac{n_{\rm e} k_{\rm B} T}{\theta}\left[b_0\left(\theta\right)\Gamma_{\rm e} + b_1\left(\theta\right)\Gamma_{\rm e}^{3/2} + b_2\left(\theta\right)\Gamma_{\rm e}^2\right] \end{aligned} \tag{38}$$

with

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

$$\begin{aligned} \Delta\mu_{\rm C} \;&=\; -\frac{1}{k_{\rm B} T}\left(\frac{\partial F_{\rm C}}{\partial N_e}\right)_{\rm V,T} \\ &=\; -f_{\rm ee} - \frac{1}{3}\left(u_{\rm ee} + \frac{u_{\rm ie}}{\left\langle Z\right\rangle}\right) , \end{aligned} \tag{40}$$

and

$$\begin{aligned} H_{\rm C} \;&=\; -T^2\left(\frac{\partial}{\partial T}\frac{F_{\rm C}}{T}\right)_{\rm V,\{N_e,N_i\}} - V\left(\frac{\partial F_{\rm C}}{\partial V}\right)_{\rm T,\{N_e,N_i\}} \\ &=\; U_{\rm C} + P_{\rm C} V , \end{aligned} \tag{41}$$

where the Coulomb correction of the internal energy is given by

$$U_{\rm C} = N_{\rm e}k_{\rm B}Tu_{\rm ee} + N_{\rm ion}k_{\rm B}T\left(u_{\rm ii}+u_{\rm ie}\right) \ . \tag{42}$$

3.2. Approximate treatment of pressure ionization

The nonideal part of the atomic free energy $F_{\rm neu}$, which takes account of the contributions from interactions of an atom with surrounding particles, can be given by

$$F_{\rm neu} = F_{\rm HS} + F_{\rm e} \ . \tag{43}$$

Here the first term $F_{\rm HS}$ denotes the neutral-neutral interactions based on the hard-sphere excluded-volume treatment. This excluded volume contribution is the lowest-order approximation to the total configuration of the free energy. The second term $F_{\rm e}$ represents the neutral-charged interaction.

In the plasma with high temperatures ($T \geq 10^5 K$), pressure ionization of atoms is predominantly based on Stark-ionization theory. For the cooler surface of the Sun, however, neutral atoms dominate the interaction between interparticles. Rather sophisticated physical models for the interactions based on advanced physics theory are discussed in Saumon & Chabrier (1991; 1992). For astrophysical application and research, we only adopt an approximate model for the complicated physical processes of pressure ionization to produce the essential thermodynamic features.

The free energy of the hard-sphere mixture is represented by the occupation probabilities according to the definition given by Potekhin et al. (1999):

$$k_{\rm B}T\ln w_{\rm j} = -\frac{\partial F_{\rm HS}}{\partial N_{\rm j}} \tag{44}$$

with the occupation probability formalism given approximately by Luo (1997)

$$\ln w_{\rm j} = -\frac{4\pi}{3}r_{\rm j}^3\left(\frac{N_{\rm H}+N_{\rm He}}{V}\right), \tag{45}$$

where $N_{\rm H}+N_{\rm He}$ is the total number of atomic nuclei. j includes three configurations, i.e., $\{{\rm H}, {\rm He}, {\rm He}^+\}$; $r_{\rm j}$ is an effective radius of species j. The radii of atomic ${\rm H}$, ${\rm He}$ and singly ionized helium ${\rm He}^+$ are taken to be $r_{\rm H^0} = a_{\rm B}$, $r_{\rm He^0} = 0.5a_{\rm B}$ and $r_{\rm He^+} = 0.8a_{\rm B}$, respectively, with Bohr radius $a_{\rm B} = \hbar^2/m_{\rm e}e^2$.

A detailed treatment of the neutral-charged interaction requires complicated and time-consuming calculation. Pressure ionization is predominantly a volume effect. Owing to the destruction of relatively loosely bound states by interactions of both charged and neutral particles in the plasma, the particles are jammed closely together, bound electron orbitals filling too large a volume fail to survive, and the electrons migrate from atom to atom. The electrons in a bound state are so called "acting" electrons. We consider that "acting" electron in a bound state can move freely with respect to a particle in bound, thus making the gross simplification that the "acting" electrons depend only on the density of free electrons. For simplicity, we adopt the expression for $F_{\rm e}$ by EFF (1973) and Christensen-Dalsgaard (1977), namely

$$F_{\rm e} = \frac{C_1}{V\langle Z\rangle^3}\left(k_{\rm B}T + C_2\langle Z\rangle^2\right)\left(N_{\rm e0}^2 - N_{\rm e}^2\right) \ , \tag{46}$$

where C_1 and C_2 are constants, and $N_{\rm e0}$ is the total number of electrons per unit mass, in bound or free

$$N_{\rm e0} = N_{\rm A}\left(\frac{X}{A_{\rm H}} + \frac{Y}{A_{\rm He}} + \frac{Z}{2}\right) \ . \tag{47}$$

Here X, Y and Z are the mass abundance of H, ${\rm He}$ and elements beyond hydrogen and helium, respectively. $N_{\rm A}$ is Avogadro's number. $A_{\rm H} = 1.0079$ and $A_{\rm He} = 4.0026$ are the atomic weights. Eq. (46) ensures that the effect of pressure ionization on the thermodynamic functions becomes zero as $N_{\rm e} \rightarrow N_{\rm e0}$.

As a result, the contribution from pressure ionization to the pressure $P_{\rm PI}$, the electron chemical potential $\Delta\mu_{\rm PI}$ and the enthalpy $H_{\rm PI}$ can be formulated in terms of

$$\begin{aligned} P_{\rm PI} &= -\left(\frac{\partial F_{\rm neu}}{\partial V}\right)_{\rm T,\{N_e,N_j\}} \\ &= \frac{1}{2}\sum_{\rm j}k_{\rm B}T\frac{N_{\rm j}}{V}\left(\frac{\partial\ln w_{\rm j}}{\partial\ln V}\right)_{\rm T,N_j} \\ &\quad + \frac{C_1}{\langle Z\rangle^3}\left(k_{\rm B}T + C_2\langle Z\rangle^2\right)\left(n_{\rm e0}^2 - n_{\rm e}^2\right) \ , \end{aligned} \tag{48}$$

$$\begin{aligned} \Delta\mu_{\rm PI} &= -\frac{1}{k_{\rm B}T}\left(\frac{\partial F_{\rm neu}}{\partial N_{\rm e}}\right)_{\rm T,V} \\ &= \frac{2C_1}{\langle Z\rangle^3}\left(k_{\rm B}T + C_2\langle Z\rangle^2\right)\frac{n_{\rm e}}{k_{\rm B}T}, \end{aligned} \tag{49}$$

and

$$\begin{aligned} H_{\rm PI} &= -T^2\left(\frac{\partial}{\partial T}\frac{F_{\rm neu}}{T}\right)_{\rm V,\{N_e,N_j\}} - V\left(\frac{\partial F_{\rm neu}}{\partial V}\right)_{\rm T,\{N_e,N_j\}} \\ &= \frac{C_1}{\langle Z\rangle^3}\left(k_{\rm B}T + 2C_2\langle Z\rangle^2\right)\left(n_{\rm e0}^2 - n_{\rm e}^2\right)V \\ &\quad + \frac{1}{2}\sum_{\rm j}k_{\rm B}TN_{\rm j}\left(\frac{\partial\ln w_{\rm j}}{\partial\ln V}\right)_{\rm T,N_j} \ , \end{aligned} \tag{50}$$

where $n_{\rm e}$ is the number of electrons per unit volume. The hard-sphere term of Eqs. (48) and (50) is explicit functions of T, $N_{\rm H^0}$, $N_{\rm He^0}$ and $N_{\rm He^+}$. Here $N_{\rm H^0}$ and $N_{\rm He^0}$ denote the number of hydrogen atoms and helium atoms, respectively. The factor $\frac{1}{2}$ is introduced to take account of the fact that the interactions of particles have actually been counted twice for each atom in the sum.

4. Thermal equilibrium quantities

For simplicity, we only employ the partition functions in the ground state for the dominant elements H and ${\rm He}$. Considering

Table 1. Reference solar models

Model	EOS	Z/X	$T_c(10^6K)$	$\rho_c(g/cm^3)$
1	EFF	0.0248	15.74	157.4
2	Present	0.0248	15.74	157.4
3	MHD	0.0245	15.67	154.5
4	OPAL	0.0245	15.67	154.2

the correction of nonideality and electron degeneracy to thermodynamic quantities, the modified Saha equation can be written as (Christensen-Dalsgaard 1977; Pols et al. 1995):

$$\frac{N_{\rm H^+}}{N_{\rm H^0}} = \frac{1}{2}\exp\left(-\psi + \Delta\mu - E_{\rm H^0}/k_{\rm B}T\right) \ , \quad (51)$$

$$\frac{N_{\rm He^+}}{N_{\rm He^0}} = 2\exp\left(-\psi + \Delta\mu - E_{\rm He^0}/k_{\rm B}T\right) \ , \quad (52)$$

and

$$\frac{N_{\rm He^{++}}}{N_{\rm He^+}} = \frac{1}{2}\exp\left(-\psi + \Delta\mu - E_{\rm He^+}/k_{\rm B}T\right) , \quad (53)$$

where the total correction to the electron chemical potential is

$$\Delta\mu = \Delta\mu_{\rm C} + \Delta\mu_{\rm PI}; \quad (54)$$

$E_{\rm ij}$ is the configuration energies in unit of electron volts, i.e.,

$$\begin{aligned} E_{\rm H^0} &= -\chi_{\rm H^0}, \qquad E_{\rm H^+} = 0 \ , \\ E_{\rm He^0} &= -\chi_{\rm He^0} - \chi_{\rm He^+} \ , \quad (55) \\ E_{\rm He^+} &= -\chi_{\rm He^+}, \qquad E_{\rm He^{++}} = 0 \ . \end{aligned}$$

For the number $N_{\rm H^0}$, $N_{\rm H^+}$, $N_{\rm He^0}$, $N_{\rm He^+}$ and $N_{\rm He^{++}}$ of neutral and ionized hydrogen and helium particles, we introduce a set of dependent variables, i.e., $x_{\rm H^0}$, $x_{\rm H^+}$, $x_{\rm He^0}$, $x_{\rm He^+}$ and $x_{\rm He^{++}}$, being the occupation numbers of particles divided by the number of nuclei of the respective H or He species. With these definitions, we have the occupation number for hydrogen species

$$x_{\rm H^+} = Z_{\rm H^0}/Z_{\rm H} \ , \quad (56)$$

where the partition functions are given according to

$$\begin{aligned} Z_{\rm H^0} &= \frac{1}{2}\exp\left(-\psi + \Delta\mu - E_{\rm H^0}/k_{\rm B}T\right) \ , \\ Z_{\rm H^+} &= 1 \ , \quad (57) \\ Z_{\rm H} &= 1 + Z_{\rm H^0} \ , \end{aligned}$$

with the normalization condition

$$x_{\rm H^0} + x_{\rm H^+} = 1. \quad (58)$$

For helium species

$$\begin{aligned} x_{\rm He^+} &= Z_{\rm He^0}/Z_{\rm He} \ , \\ x_{\rm He^{++}} &= Z_{\rm He^+}/Z_{\rm He}, \quad (59) \end{aligned}$$

where the partition functions are

$$\begin{aligned} Z_{\rm He^0} &= 2\exp\left(-\psi + \Delta\mu - E_{\rm He^0}/k_{\rm B}T\right) \ , \\ Z_{\rm He^+} &= \frac{1}{2}\exp\left(-\psi + \Delta\mu - E_{\rm He^+}/k_{\rm B}T\right) \ , \quad (60) \\ Z_{\rm He^{++}} &= 1 \ , \\ Z_{\rm He} &= 1 + Z_{\rm He^0} + Z_{\rm He^+} \ , \end{aligned}$$

Table 2. Non-ideal effects in the equation of state

Effects	EFF	MHD	OPAL	Present
Coulomb coupling	No	Yes	Yes	Yes
Pressure ionization	Yes	Yes	Yes	Yes
Electron exchange relativistic-	No	No	Yes	Yes
Electron degeneracy	Yes	No	No	No
Excited states	No	Yes	Yes	No
Classical ions	Yes	Yes	Yes	Yes

with the normalization condition

$$x_{\rm He^0} + x_{\rm He^+} + x_{\rm He^{++}} = 1 \ . \quad (61)$$

Under conservation constraints, the number of free electrons per unit mass is given by

$$N_{\rm e} = N_{\rm H}x_{\rm H^+} + N_{\rm He}\left(x_{\rm He^+} + 2x_{\rm He^{++}}\right) + Z/2 \ . \quad (62)$$

Since the present model considers six species $\{e, {\rm H}, {\rm H}^+, {\rm He}, {\rm He}^+, {\rm He}^{++}\}$, Eqs. (56) and (58)-(62) are six simultaneous equations for the six unknown $\{N_{\rm e}, x_{\rm H^0}, x_{\rm H^+}, x_{\rm He^0}, x_{\rm He^+}, x_{\rm He^{++}}\}$ with a unique unknown variable, i.e., the electron degeneracy ψ. Here $\Delta\mu$ defined in Eq. (54) is also an explicit function of the electron degeneracy ψ by means of the free electron number $N_{\rm e}$.

5. Results and comparison

Coulomb coupling and pressure ionization lead to influence of nonideality on the equation of state. In order to examine the importance of nonideal effects on the EOS and compare the results with those of other EOS, we have employed four solar models for this paper. All models have been constructed with OPAL opacities (Iglesias et al. 1992) at $T > 10^4K$ and Kurucz tables (Kurucz 1991) at lower temperatures. Table 1 summarizes the main properties of the models and displays the values of the ratio Z/X of metallicity to initial hydrogen abundance, the central temperature and density. The nonideal effects in the different equation of state are listed in Table 2.

The simplicity of our improved EOS formalism allows us to obtain the solution easily and investigate the properties of thermodynamic functions. Contributions of Coulomb coupling, pressure ionization and electron degeneracy to the total pressure can be seen in Fig. 1. The ratio of non-ideal part to ideal pressure, e.g., $\delta P/P_{\rm id}$, is plotted in Fig. 1 with respect to $\log T$ of temperature from surface to the center throughout the solar model. Here $P_{\rm id}$ is the total pressure of Model 1 employed EFF EOS without including any nonideal effects, and δP is any of the fractional contributions to the pressure calculated according to Eqs. (38) and (48). In Fig. 1 the dashed line indicates the Coulomb pressure for fully ionized H-He mixture, the dotted line is the Coulomb pressure under Debye-Hückle approximation, and the solid line is the pressure correction due to Coulomb coupling and pressure ionization for the partially ionized plasma.

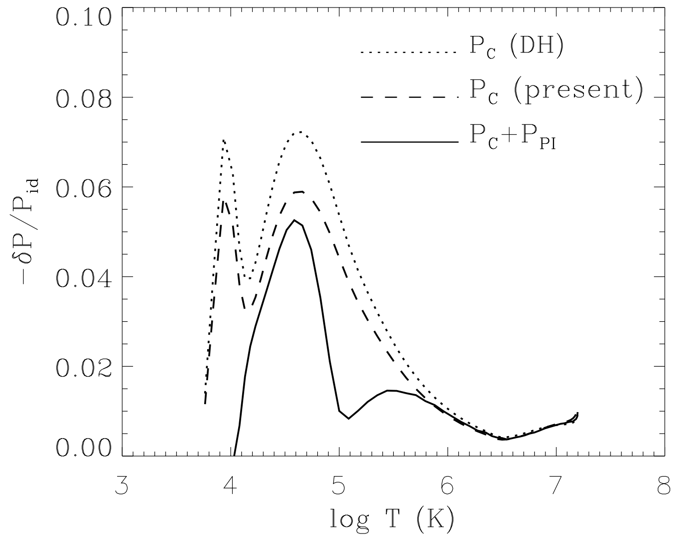

Fig. 1. The fractional contribution arising from nonideal effects to the ideal pressure of the reference solar model 1 which employed the EFF EOS. The solid line refers to the calculation of pressure correction including Coulomb coupling and pressure ionization for the partially ionized plasma, in the sense $\delta P = P_{\rm C} + P_{\rm PI}$; the dashed and dotted lines denote pure Coulomb pressure correction, $\delta P = P_{\rm C}$, for the fully ionized plasms by means of the present formula and Debye-Hückel approximation, respectively.

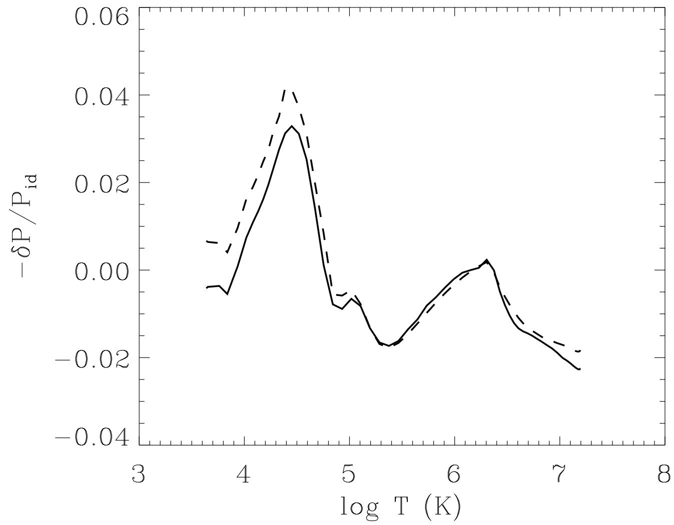

Fig. 2. The relative pressure difference with respect to Model 1 with the EFF EOS. The solid and dashed lines correspond to the pressure change $\delta P = P_{\rm present} - P_{\rm id}$ and $\delta P = P_{\rm MHD} - P_{\rm id}$, respectively.

Comparison of the Coulomb pressure corrections in Fig. 1 shows the following points: (1) At the solar surface, either the present formula or the Debye-Hückle approximation overestimates Coulomb effects. Contribution of the Coulomb potential to the total pressure is maximum ($\log T = 4.6$ and 4.7), at which point the most abundant species (hydrogen and helium) are completely and singly ionized, respectively. This means that the Debye radius is sufficiently small. (2) In the intermediate regions, the Debye-Hückle approximation also overestimates the Coulomb effects. (3) As the temperature and the density increase, the Coulomb contribution becomes smaller, until partial degeneracy of the electrons sets in near the center of the Sun. At the centre, the values of Debye-Hückle term without electron exchange contribution (dotted line) are smaller than our calculated values. As a result, we may conclude that the terms of higher order in the Coulomb correction play an important role even under the weakly-coupled limit.

Pressure ionization is caused by interparticle interactions and contributes to the pressure $P_{\rm id}$. The fully ionized ions, e.g., H^+ and He^{++}, have no contribution to the pressure, because they have no bound systems interacting with surroundings. The comparison of solid line and dash line in Fig. 1. shows the difference of the pressure corrections mainly at low temperature. The contribution from pressure ionization starts to play a role and increases the pressure before pressure ionization takes place. In contrast, Coulomb correction becomes important only after pressure ionization takes place. As the degree of ionization increases, a great number of charged particles are produced, therefore fractional change, i.e., $\delta P/P_{\rm id}$, increases a few percent. The increase of the pressure due to pressure ionization compensates the decrease of the pressure due to Coulomb coupling in the region of pressure ionization. Consequently, the pressure correction which corresponds to a partially ionized plasma is smaller than that of a fully ionized gas. The Coulomb coupling makes a negative pressure correction with respect to the ideal-gas value, while pressure ionization makes a positive contribution to it.

Our improved EOS has simple and explicit expression for its practical use, however, its reliability requires comparison with the EOS data calculated by other EOS. Fig. 2 shows the profile of $\delta P/P_{\rm id}$ for the two different formalism of the EOS with Model 1 as the reference model, where the relative pressure difference is $\delta P = P_{\rm s} - P_{\rm id}$ with the pressure labeled "s" corresponding to our EOS or the MHD EOS. In Fig. 2, we can see that the MHD and our improved EOS are similar throughout the Sun except near the surface. This discovery reveal that the Coulomb interaction term is the dominant nonideal correction in solar interior. Comparision of the pressure corrections in Fig. 2 shows that the central pressure is smaller in our EOS than in the MHD EOS. Although the MHD EOS takes into account the Coulomb correction to the pressure in the Debye-Hückel approximation, it fails to account for the contributions of the electron-electron interaction and screened potential in the weak coupling central regime. At the surface, the MHD EOS includes several factors ignored by us, e.g., the formation of H_2 and H^-, and excited states in bound systems. Therefore, it seems much more realistic than our simple EOS.

The adiabatic sound speed $c = (\Gamma_1 P/\rho)^{1/2}$ is very sensitive to changes in the equation of state. The relative difference in the sound speed with respect to the depth inside both models are shown in Fig. 3. Comparision of the sound speeds corresponding to the EFF EOS and our EOS shows that the computation of solar model has been truly improved through improved equation of state in physics. From Fig. 3, we also can see that the overall agreement between our analytical formalism and the results ob-

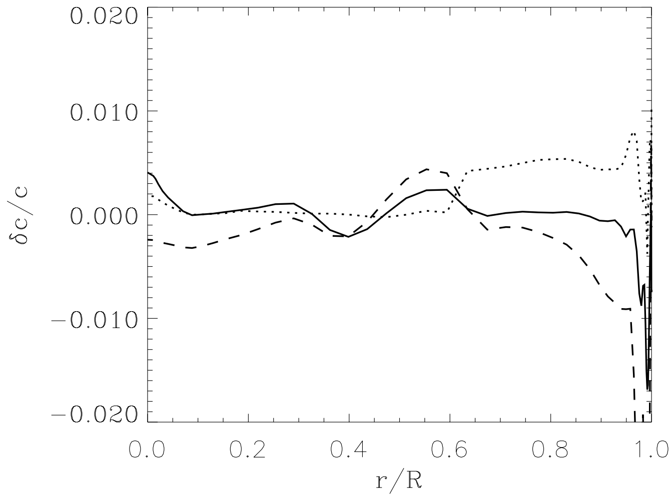

Fig. 3. The relative difference in the sound speed against fractional redius between Model 4 and 2 (solid line), between Model 4 and Model 3 (dotted line) and between Model 4 and 1 (dashed line).

tained by MHD is rather good. The divergence is found mainly at the surface because of the occurrence of many complicated physics processes. Under conditions of weak coupling and weak degeneracy, however, our EOS yields quite reasonable results and time-saving calculations.

6. Conclusions

Starting from the free-energy minimization method in the chemical picture, we have derived analytical and simplified expressions for the physical processes of Coulomb coupling, pressure ionization and electron degeneracy. Thus, we are able to establish a single algorithm of equation of state involving a sum of terms, each including a different physical contribution. This makes it possible to incorporate nonideal effects into the stellar evolution codes with direct call of EOS. Therefore, the thermodynamic quantities of the plasma may be calculated explicitly and very quickly over a wide range of temperature and density.

The purpose of this paper is to examine the nonideal effects on the EOS for solar interior matter. We have found that the corrections have a significant effect on the solar equation of state. In addition, our simple and comprehensive algorithm also allows us to incorporate more physical processes or add more elements into the EOS. Although our improved formulation of the equation of state can be of benefit to the study of the complexity of physical processes concerned in the EOS, the influence of the nonideality on the EOS as shown in this paper remains approximate. More studies would be needed to fully understand finer infulence of nonideality on the equation of state.

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