

Theoretical Description of the Coulomb Interaction by Padé-Jacobi Approximants

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Abstract

Coulomb interactions for the Free Helmholtz energy and the pressure are studied in a partial new formulation which described more exactly the numerical evaluation of many body theories.

41.1 Introduction

With regard to the EOS many activities have been developed to yield results which consider different phenomena, for instance pressure dissoziation and ionisation, degeneracy, relativity, Coulomb- and non-Coulombic interactions, pair production and charge mixing in different chemical compositions.

Various theoretical approaches are used in order to include exchange and correlation effects for fully ionized or partially ionized matter (see e.g. Salpeter and Zapolski 1967, Graboske et al. 1969, Hansen 1973, Pokrant 1977, Fontaine et al. 1977, March and Tosi 1984, Perrot and Dharmawardana 1984, Hubbard and Dewitt 1985, Dandrea et al. 1986, van Horn 1987, Kraeft et al. 1986, Ichimaru et al. 1987, Rogers and DeWitt 1987, Däppen et al. 1988, Ichimaru 1990, Eliezer and Ricci 1991, Saumon and Chabrier 1992).

For many applications (e.g. stellar evolution calculations or astroseis-mology) it is necessary either to have algebraic formulae for the EOS or extensive tables which supply the input informations at any density and temperature. As a first step we present an analytical EOS for fully ionized

multicomponent plasmas covering a large density-temperature range. The EOS includes non-ideal effects due to exchange-correlation interactions of charged particles at any degeneracy and is applicable to any chemical mixture. Relativistic effects as well as ionic quantum corrections are taken into account. The aim of this contribution is to derive explicit exchange and correlation corrections for the Coulombic part of the EOS in an algebraic form.

Recently, we presented results for the pressure (Stolzmann and Blöcker 1993a,b) and a first application to the mass-radius relationship of white dwarfs (Stolzmann et al. 1993). This paper will be devoted to a brief overview of the theoretical background of our EOS concept.

41.2 Theoretical Background

We start with the Helmholtz free energy F of a fully ionized plasma consisting of a species which is given by

$$F(T, V, N_a) = \sum_a F_a^{\text{id}} + F^{\text{coul}} \quad (1)$$

with F_a^{id} being the ideal free energy and F^{coul} representing the Coulomb interaction contributions of the free energy. We splitted the Coulomb contributions in the following parts:

$$F^{\text{coul}} = F_{\text{ee}}^{\text{x}} + F_{\text{ee}}^{\text{c}} + F_{\text{ii}}^{\text{x}} + F_{\text{ii}}^{\text{c}} + F_{\text{ii}}^{\text{cq}} + F_{\text{ie}}^{\text{c}} \quad (2)$$

where x and c denote the exchange and the correlation term, resp. F_{ee} , F_{ii} and F_{ie} correspond to the electron-electron, ion-ion and ion-electron interaction. In this notation $F_{\text{ii}}^{\text{cq}}$ and F_{ii}^{x} describe ionic quantum corrections.

The pressure is given by the thermodynamic relation

$$P(V, T, N_a) = - \left(\frac{\partial F}{\partial V} \right)_{T, N} \quad (3)$$

or equivalent by the grand potential Ω

$$- \Omega = P \cdot V = G - F \quad (4)$$

with the definition of the Gibbs free energy

$$G = \sum_a \mu_a N_a \quad \text{and} \quad \mu_a = \left(\frac{\partial F}{\partial N_a} \right)_{T, V, N \neq N_a} \quad (5)$$

The equivalence between (3) and (4) is achieved by the elimination of the chemical potential from the pressure (4) by means of an inversion procedure

described in detail by Kohn and Luttinger (1960), Stolzmann and Kraeft (1979), Perrot and Dharma-wardana (1984), Rösler and Stolzmann (1987).

In equivalence to (2) the Coulombic pressure contribution is given by

$$P^{\text{coul}} = P_{ee}^{\text{x}} + P_{ee}^{\text{c}} + P_{ii}^{\text{x}} + P_{ii}^{\text{c}} + P_{ii}^{\text{cq}} + P_{ie}^{\text{c}} \quad (6)$$

Consequently, we apply in (2)

$$F_e^{\text{id}} = \frac{2kTV}{\Lambda_e^3} \left\{ \psi \left(J_{1/2}(\psi, \lambda) + \frac{3}{2} \lambda J_{3/2}(\psi, \lambda) \right) - \left(J_{3/2}(\psi, \lambda) + \frac{5}{2} \lambda J_{5/2}(\psi, \lambda) \right) \right\} \quad (7)$$

with the De Broglie wavelength Λ_e and the relativity parameter λ

$$\Lambda_e = \frac{2\pi\hbar}{\sqrt{2m_e\pi kT}} \quad \lambda = \frac{kT}{mc^2} \quad (8)$$

The electron degeneracy parameter ψ is defined implicitly by the density

$$n_e = \frac{2}{\Lambda_e^3} \left(J_{1/2}(\psi, \lambda) + \lambda \frac{3}{2} J_{3/2}(\psi, \lambda) \right) \quad (9)$$

$$F_i^{\text{id}} = kTV \sum_j n_j \left\{ \ln \left(\frac{n_j \Lambda_j^3}{2} \right) - 1 \right\} \quad (10)$$

According to Kovetz et al. 1972 we used for the lowest order exchange interaction

$$\frac{F_{ee}^{\text{x}}}{N_e kT} = f_{ee}^{\text{x}} = \frac{e^2}{\pi \Lambda_e^4} \frac{1}{n_e kT} J_{\text{rel}}^{\text{x}}(\psi, \lambda). \quad (11)$$

with the relativistic Hartree-Fock integral $J_{\text{rel}}^{\text{x}}(\psi, \lambda)$. The non-relativistic conditions can be described by the fit formula of Perrot and Dharma-wardana (1984). We determine for the electron-electron correlation term the new Jacobi-Padé approximation

$$\frac{F_{ee}^{\text{c}}}{N_e kT} = f_{ee}^{\text{c}} = - \frac{a_0 \Gamma_e^{3/2} - a_2 \Gamma_e^6 \varepsilon_c(r_s, 0)/kT}{1 + a_1 \Gamma_e^{3/2} + a_2 \Gamma_e^6} \quad (12)$$

The ground state energy ε_c can be taken from Salpeter and Zalpolsky (1967), Vosko et al. (1980) or Ebeling and Richert (1985). The Coulomb coupling parameter Γ describes the ratio of the Coulomb potential to the kinetic

energy. The Jacobi-Padé approximants of the ion-electron and ion-ion interaction are proposed by Ebeling (1990):

$$\frac{F_{ie}^c}{N_i kT} = f_{ie}^c = \frac{-c_0 \Gamma_i^{3/2} - c_2 \Gamma_e^{9/2} \epsilon_{ie}}{1 + \Gamma_i^{3/2} (c_1 + 2c_4 \ln[1 + (c_5/\Gamma_i^3)^{1/2}]) + c_2 \Gamma_e^{9/2}} \quad (13)$$

$$\frac{F_{ii}^c}{N_i kT} = f_{ii}^c = -\frac{b_0 \Gamma_i^{3/2} + b_2 \Gamma_i^{9/2} \epsilon_{ii}}{1 + b_1 \Gamma_i^{3/2} + b_2 \Gamma_i^{9/2}} \quad (14)$$

The energy ϵ_{ie} is adopted from Ebeling (1990), Hubbard and DeWitt (1985), DeWitt and Hubbard (1976) and Galam and Hansen (1974) whereas ϵ_{ii} consists of Madelung-like and thermal energy and is taken from Stringfellow et al. (1990). Ionic quantum corrections (for the near-classical limit) can be considered according to Chabrier et al. (1992) (see also Nagara et al. 1987):

$$\begin{aligned} \frac{F_{ii}^{cq}}{N_i kT} = f_{ii}^{cq} = & \frac{3}{2} z_1 \Theta_i + 2 \ln(1 - e^{-\alpha \Theta_i}) + \ln(1 - e^{-\gamma \Theta_i}) \\ & - 3 \ln \Theta_i + 2.71848 - \mathfrak{S}_{\text{Deb}}(\Theta_i) \end{aligned} \quad (15)$$

with the approximation for the Debye integral $\mathfrak{S}_{\text{Deb}}(\Theta_i)$:

$$\mathfrak{S}_{\text{Deb}}(\Theta_i) = \frac{2}{3} \frac{1}{1 + 0.43\alpha\Theta_i + \frac{5}{\pi^4} (\alpha\Theta_i)^3} \quad (16)$$

Leaving the classical region symmetry effects become important. We try to determine the exchange free energy in the lowest order approximation (Hartree-Fock exchange) by

$$\frac{F_{ii}^x}{N_i kT} = f_{ii}^x = -t_0 \Gamma_i \frac{t_1 + t_2 \xi_i^2 - t_3 \xi_i^3 + t_4 \xi_i^4}{1 + t_5 \xi_i^2 + t_6 \xi_i^4} \tanh \frac{1}{\xi_i} \quad (17)$$

analogous to the treatment of the electrons by Perrot and Dharma-wardana (1984).

$$\xi_i = 6 \cdot \left(\frac{4}{9\pi}\right)^{2/3} \cdot \frac{\Gamma_i}{\Theta_i^2} \quad \Theta_i = \frac{\hbar\omega_p}{kT} \quad (18)$$

Straightforward we obtain with (3) - (5) for the pressure

$$P_e^{\text{id}} = \frac{2kT}{\Lambda_e^3} \left(J_{3/2}(\psi, \lambda) + \frac{5}{4} \lambda J_{5/2}(\psi, \lambda) \right) \quad (19)$$

$$P_i^{\text{id}} = kT \sum_j n_j \quad (20)$$

$$\frac{P_{ee}^c}{n_e kT} = -\frac{s_0 \Gamma_e^{3/2} - s_2 \Gamma_e^6 \mu_c(r_s, 0)/kT}{1 + s_1 \Gamma_e^{3/2} + s_2 \Gamma_e^6} - f_{ee}^c \quad (21)$$

$$\mu_c(r_s, 0) = \varepsilon_c(r_s, 0) - \frac{r_s}{3} \frac{\partial \varepsilon_c(r_s, 0)}{\partial r_s} \quad (22)$$

The pressure of the ion-electron and the ion-ion interaction is given by

$$\begin{aligned} \frac{P_{ie}^c}{n_i kT} = & -D_{ie} \cdot \left\{ \frac{c_0}{2} \Gamma_i^{3/2} + \left(\frac{3}{2} \varepsilon_{ie} + \frac{1}{3} (h_{ie} - d_{ie}) \right) c_2 \Gamma_e^{9/2} \right. \\ & \left. + \left(\frac{c_1}{2} \Gamma_i^{3/2} + c_4 \left(\ln c_6 - 1 + \frac{1}{c_6} \right) \Gamma_i^{3/2} + \frac{3}{2} c_2 \Gamma_e^{9/2} \right) \cdot f_{ie}^c \right\} \quad (23) \end{aligned}$$

$$\frac{P_{ii}^c}{n_i kT} = -D_{ii} \Gamma_i^{3/2} \cdot \left\{ \frac{b_0}{2} + \left(\frac{3}{2} \varepsilon_{ii} + \frac{h_{ii}}{3} \right) b_2 \Gamma_i^3 + \left(\frac{b_1}{2} + \frac{3}{2} b_2 \Gamma_i^3 \right) f_{ii}^c \right\} \quad (24)$$

D_{ie} and D_{ii} are the denominators of (13) and (14), resp., whereas h_{lm} and d_{lm} are defined by

$$h_{lm} = \Gamma_i \frac{\partial \varepsilon_{lm}}{\partial \Gamma_i} \quad d_{lm} = r_s \frac{\partial \varepsilon_{lm}}{\partial r_s} \quad r_s = \left(\frac{3}{4\pi n_e} \right)^{1/3} \quad (25)$$

Finally, the ionic quantum corrections can be determined by

$$\frac{P_{ii}^{cq}}{n_i kT} = \frac{3}{4} z_1 \Theta_i + \frac{1}{2} \gamma \frac{\Theta_i}{e^{\gamma \Theta_i} - 1} + \frac{3}{2} \mathfrak{S}_{\text{Deb}}(\Theta_i) \quad (26)$$

$$\frac{P_{ii}^x}{n_i kT} = -\Gamma_i q_0 \frac{1 + q_1 \xi_i^2 - q_2 \xi_i^3 + q_3 \xi_i^4}{1 + q_4 \xi_i^2 + q_5 \xi_i^4} - f_{ii}^x \quad (27)$$

A detailed description of our investigations is given by Stolzmann and Blöcker (1993c).

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