

Thermodynamical properties of stellar matter

II. Internal energy, temperature and density exponents, and specific heats for stellar interiors

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Abstract. Starting from the Helmholtz free energy we calculate analytically first- and second-order derivatives, as internal energy and specific heats, for the ideal system and the exchange and correlation interactions covering a broad range of degeneracy and relativity. The complex physics of Coulomb interactions is expressed by Padé Approximants, which reflect the actual state of our knowledge with high accuracy. We assume complete ionization and provide a base system of thermodynamical functions from which any other thermodynamical quantities can be calculated. We chose for the base system the free energy, the pressure, the internal energy, the isothermal compressibility (or density exponent), the coefficient of strain (or temperature exponent), and the isochoric specific heat. By means of the latter potentials entropy, isobaric specific heat and adiabatic temperature gradient can be determined. We give comparisons with quantities which are composed by numerical second-order derivatives of the free energy and show that numerical derivatives of the free energy as calculated, for instance, from EOS tables, may produce discontinuities for astrophysically relevant quantities as, e.g., the adiabatic temperature gradient. Adiabatic temperature gradients are shown for different chemical compositions (hydrogen, helium, carbon). Finally the used formalism of Padé Approximants allows immediate incorporation of recent results from many particle statistics.

Key words: equation of state – plasmas – stars: interiors – stars: evolution – stars: low-mass, brown dwarfs – stars: white dwarfs

1. Introduction

For an accurate modelling of stellar objects we have to compute a complete set of thermodynamical quantities which meets the physical conditions of various evolutionary stages. Based on the framework presented in Stolzmann & Blöcker (1996a, hereafter paper I) we derive further thermodynamical potentials in order to provide a base system from which *any* other thermodynamical quantity can be calculated. Such a system requires

six quantities consisting of the Helmholtz free energy, two of its single derivatives, one of its second mixed derivatives, and two of its second pure derivatives with respect to temperature and density (see e.g. Däppen et al. 1988). We complement the Helmholtz free energy with the pressure and the internal energy, with the isochoric specific heat, and with the temperature and density exponents in the equation of state (EOS), χ_T and χ_ρ . This paper will be devoted to the ideal, exchange and correlation contributions according to the expansions given in paper I, viz. for *case a*: weak relativity and arbitrary degeneracy, and *case b*: strong degeneracy and arbitrary relativity. These cases cover a large area in the density-temperature plane. The correlations between the charged particles are formulated by the technique of Padé Approximants as in paper I. Here we give improved versions of our earlier applied Padé Approximants. In particular we have rearranged terms of the quantum virial function.

Explicit expressions for the Helmholtz free energy and the pressure have already been derived in paper I for ideality as well as for exchange and correlation interaction. This paper aims at providing analytical formulae with high accuracy which supply quick computing with reliable accuracy in practical applications. Furthermore the expressions of the thermodynamical functions given here can be easily included as a part of the thermodynamical description of arbitrary degree of ionization.

This paper is organized as follows. In Sect. 2 we list the set of thermodynamical potentials to be considered. Sect. 3 gives a brief overview of the concept for the calculation of the EOS terms. Sect. 4 deals with the detailed determination of the ideal, exchange and correlation parts for the EOS. Numerical results and comparisons are presented in Sect. 5, and a summary is given in Sect. 6.

2. Thermodynamical relations and identities

We summarize briefly some well-known standard relations, which are frequently used to provide the thermodynamics for astrophysical applications.

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We have to determine the first and second-order quantities which are related by the ratio C_P/C_V of isochoric to isobaric specific heat:

$$\gamma = \frac{C_P}{C_V} = 1 + \frac{V}{K_T} \frac{\lambda_P^2}{C_V T}, \quad (1)$$

The (isobaric) thermal expansion coefficient λ_P can be expressed by

$$\lambda_P = \frac{K_T}{V} C_V T \gamma_G = K_T \Phi_S, \quad (2)$$

with γ_G being the Grüneisen coefficient

$$\gamma_G = \frac{PV}{C_V T} \chi_T. \quad (3)$$

Φ_S is the coefficient of strain

$$\Phi_S = P \chi_T, \quad (4)$$

and K_T is the isothermal compressibility

$$\frac{1}{K_T} = P \chi_\rho. \quad (5)$$

The so-called temperature and density exponents in the equation of state (Cox & Giuli 1968) are defined by

$$\chi_T = \left(\frac{\partial \ln P}{\partial \ln T} \right)_\rho = \frac{T}{P} \left(\frac{\partial P}{\partial T} \right)_V \quad (6)$$

$$\chi_\rho = \left(\frac{\partial \ln P}{\partial \ln \rho} \right)_T = -\frac{V}{P} \left(\frac{\partial P}{\partial V} \right)_T. \quad (7)$$

The adiabatic temperature gradient defined by $\nabla_{\text{ad}} = (\partial \ln T / \partial \ln P)_S$ (S denotes the entropy) can be expressed by

$$\nabla_{\text{ad}} = \frac{PV}{C_P T} \lambda_P = \frac{PV}{C_P T} \chi_T. \quad (8)$$

Another possibility to calculate the adiabatic gradient is given by the three adiabatic exponents Γ_1 , Γ_2 , and Γ_3 (Cox & Giuli 1968, Rogers et al. 1996)

$$\nabla_{\text{ad}} = \frac{\Gamma_2 - 1}{\Gamma_2} = \frac{\Gamma_3 - 1}{\Gamma_1}, \quad (9)$$

which can be obtained by

$$\Gamma_1 = \frac{\gamma}{PK_T}, \quad \Gamma_2 = \frac{\gamma}{\gamma - PK_T \gamma_G}, \quad \Gamma_3 = 1 + \gamma_G. \quad (10)$$

In order to calculate the quantities given by Eqs. (1)-(10) we start with the Helmholtz free energy $F(V, T, N)$ and determine by means of standard thermodynamic relations the Gibbs energy,

$$G = N \left(\frac{\partial F}{\partial N} \right)_{T, V}, \quad (11)$$

the pressure,

$$PV = G - F, \quad (12)$$

and the internal energy,

$$U = F - T \left(\frac{\partial F}{\partial T} \right)_{V, N}, \quad (13)$$

leading to the entropy S according to

$$TS = U - F \quad (14)$$

and to the isochoric specific heat via

$$C_V = \left(\frac{\partial U}{\partial T} \right)_{V, N} = -T \left(\frac{\partial^2 F}{\partial T^2} \right)_{V, N}. \quad (15)$$

Moreover, we have to calculate the coefficient of strain and the inverse compressibility (bulk modulus) by means of Eqs. (4)-(7).

3. Theoretical model

As in paper I we start with the Helmholtz free energy F of a fully ionized plasma consisting of ideal and Coulomb interaction parts

$$F(T, V, N_a) = \sum_a F_a^{\text{id}} + F^{\text{coul}}, \quad (16)$$

where the Coulomb term contains the following parts:

$$F^{\text{coul}} = F_{\text{ee}}^{\text{x}} + F_{\text{ee}}^{\text{c}} + F_{\text{ii}}^{\text{c}} + F_{\text{ii}}^{\text{cq}} + F_{\text{ie}}^{\text{c}}, \quad (17)$$

with x and c marking the exchange and correlation contributions and cq the quantum correction term. The pairs ab denote the interaction between particles of species a and b (electrons, ions), respectively.

For convenience we introduce dimensionless thermodynamical potentials defined by

$$f = \frac{F}{NkT}, \quad g = \frac{G}{NkT}, \quad p = \frac{P}{nkT}, \quad (18)$$

$$u = \frac{U}{NkT}$$

$$s = \frac{S}{Nk}, \quad \frac{1}{k_T} = \frac{1}{K_T nkT}, \quad \phi_S = \frac{\Phi_S}{nkT},$$

$$c_V = \frac{C_V}{Nk} \quad (19)$$

where $n = N/V$ refers to the total particle number density of the ions *or* the electrons, and k denotes the Boltzmann constant. Eq. (16), or correspondingly the potentials summarized by Eq. (18) and Eq. (19), can be written by

$$\Sigma = N_e kT [\sigma_e^{\text{id}} + \sigma_{\text{ee}}^{\text{x}} + \sigma_{\text{ee}}^{\text{c}}] + N_i kT [\sigma_i^{\text{id}} + \sigma_{\text{ii}}^{\text{c}} + \sigma_{\text{ii}}^{\text{cq}} + \sigma_{\text{ie}}^{\text{c}}] \quad (20)$$

where $\Sigma = \{F, G, P \cdot V, U, S \cdot T, V/K_T, \Phi_S \cdot V, C_V \cdot T\}$ and $\sigma = \{f, g, p, u, s, 1/k_T, \phi_S, c_V\}$ symbolize the various thermodynamic functions defined in the previous section.

4. Thermodynamical potentials

This section deals in detail with the calculation of the potentials listed in Eq. (20). By introducing definitions and for the sake of the integrity we repeat here few expressions concerning Helmholtz free energy and pressure, which are already given in paper I.

4.1. Ideality

The ideality of the nonrelativistic and nondegenerate ions is described by the well-known classical expressions for the Helmholtz free energy

$$f_i^{\text{id}} = [\ln(n_i \Lambda_i^3) - 1] . \quad (21)$$

The thermal de Broglie wavelength for particles of species a is $\Lambda_a = 2\pi\hbar/\sqrt{2m_a\pi kT}$. In the classical description we get for the pressure, the compressibility, and the coefficient of strain

$$p_i^{\text{id}} = \frac{1}{k_{T,i}^{\text{id}}} = \phi_{S,i}^{\text{id}} = 1 , \quad (22)$$

and for the internal energy and the isochoric specific heat

$$u_i^{\text{id}} = c_{V,i}^{\text{id}} = \frac{3}{2} . \quad (23)$$

The ideal pressure of the electrons at any relativity and degeneracy (Chandrasekhar 1939, Cox & Giuli 1968) can be calculated by

$$p_e^{\text{id}} = \frac{2}{n_e \Lambda_e^3} \left[J_{3/2}(\psi, \lambda) + \frac{5}{4} \lambda J_{5/2}(\psi, \lambda) \right] , \quad (24)$$

with the corresponding particle number density

$$n_e = \frac{2}{\Lambda_e^3} \left[J_{1/2}(\psi, \lambda) + \frac{3}{2} \lambda J_{3/2}(\psi, \lambda) \right] . \quad (25)$$

The thermodynamical potentials of the electrons are characterized by the relativistic Fermi-Dirac integrals $J_\nu(\psi, \lambda)$, which depend on the degeneracy (ψ) and the relativity (λ) parameters

$$\psi = \frac{\mu}{kT} , \quad \lambda = \frac{kT}{mc^2} . \quad (26)$$

Generally, the degeneracy parameter ψ in (26) is a function of the density and temperature defined by Eq. (25). In order to evaluate the free energy

$$f_e^{\text{id}} = \psi - p_e^{\text{id}} \quad (27)$$

we have to determine ψ explicitly from Eq. (25) by an inversion procedure which has to be performed numerically. Note, that ψ in (26) is identical with the ideal contribution of g in (18), i.e. $\psi = g_e^{\text{id}}$. Lamb (1974) and Lamb & Van Horn (1975) evaluated the thermodynamical potentials applying the parametrizations of Eggleton et al. (1973) for the relativistic Fermi-Dirac integrals. Johns et al. (1996) improved the accuracy of the polynomials given by Eggleton et al. (1973). Straniero (1988) calculated the complete set of thermodynamical functions based on the expressions given in Eqs. (24)-(27) by numerical integrations to

determine the adiabatic temperature gradient. Recently, Blinnikov et al. (1996) and Miralles & Van Riper (1996) presented parametrizations and used various approximations to evaluate the fully relativistic ideality for the set of thermodynamical potentials, which are listed in Sect. 3. However, all calculational schemes are characterized by an immense effort in order to determine temperature- and density derivations even for asymptotic regions. For details, see e.g. Miralles & Van Riper (1996).

We pursue to include relativistic effects over a broad region of astrophysically relevant densities and temperatures for ideality and exchange. Furthermore we evaluate the set of thermodynamical potentials analytically avoiding the well-known noise problems of second-order quantities apparent in purely numerical approaches.

This can be realized by introducing two approximations:

- a) arbitrary degeneracy, but weak relativity (*case a*) and
- b) arbitrary relativity, but strong degeneracy (*case b*)

A numerical study on the density-temperature validity region of these approximations was carried out in paper I. Note, that *case a*, based on λ -expansions $\sim O(\lambda^4)$, is limited to $T \lesssim 2 \cdot 10^9 \text{K}$ and $\rho \lesssim 10^6 \text{g/cm}^3$, whereas *case b*, based on $1/\psi$ -Sommerfeld-Chandrasekhar expansions $\sim O(\psi^{-6})$ holds for $\psi \gtrsim 5$ (see Fig. 1 in paper I).

Carrying out the expansions ($\sim O(\lambda^4)$) in *case a* we get for Eqs. (24) and (25)

$$p_e^{\text{id}} = \frac{I_{3/2}(\psi)}{I_{1/2}(\psi)} \frac{U^a(\psi, \lambda)}{V^a(\psi, \lambda)} \quad (28)$$

$$n_e = \frac{2}{\Lambda_e^3} I_{1/2}(\psi) V^a(\psi, \lambda) , \quad (29)$$

with the abbreviations U^a and V^a (not to be confused with the internal energy or the volume)

$$U^a = 1 + \frac{15}{8} \lambda \frac{I_{5/2}}{I_{3/2}} \left[1 + \frac{7}{16} \lambda \frac{I_{7/2}}{I_{5/2}} \left(1 - \frac{3}{8} \lambda \frac{I_{9/2}}{I_{7/2}} \right) \right] \quad (30)$$

and

$$V^a = 1 + \frac{15}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \left[1 + \frac{7}{16} \lambda \frac{I_{5/2}}{I_{3/2}} \left(1 - \frac{3}{8} \lambda \frac{I_{7/2}}{I_{5/2}} \right) \right] \quad (31)$$

taking into account relativistic corrections. $I_\nu = I_\nu(\psi) = \int_0^\infty dz z^\nu (e^{z-\psi} + 1)^{-1} / \Gamma(\nu + 1)$ are the nonrelativistic Fermi-Dirac integrals considered by parametrizations and expansions (see e.g. paper I).

For the Helmholtz free energy in Eq. (27) we have performed the inversion $\psi = \psi(n_e, T)$ analytically (see paper I). Using the Maxwell relation Eq. (13) and Eqs. (4)-(7) we obtain for the internal energy, compressibility, and coefficient of strain

$$u_e^{\text{id}} = \frac{3}{2} p_e^{\text{id}} + \frac{15}{8} \lambda \frac{I_{5/2}}{I_{1/2}} \frac{U_\lambda^a}{V^a} \quad (32)$$

$$\frac{1}{k_{T,e}^{\text{id}}} = \frac{I_{1/2}}{I_{-1/2}} \frac{V^a}{V_\psi^a} \quad (33)$$

$$\phi_{S,e}^{\text{id}} = u_e^{\text{id}} + p_e^{\text{id}} - \frac{3}{2} \frac{I_{1/2}}{I_{-1/2}} \left[\frac{V^a}{V_\psi^a} + \frac{5}{4} \lambda \frac{I_{3/2}}{I_{1/2}} \frac{V_\lambda^a}{V_\psi^a} \right] . \quad (34)$$

Obviously, Eq. (32) results for $\lambda \rightarrow 0$ in the well-known nonrelativistic relation $u^{\text{id}} = \frac{3}{2}p^{\text{id}}$. Calculating the derivatives of the free energy with respect to the temperature in order to get the isochoric specific heat (Eq. 15) we have to execute explicitly

$$C_V = -T \left[\frac{\partial^2 F}{\partial T^2} + 2 \frac{d\psi}{dT} \frac{\partial^2 F}{\partial \psi \partial T} + \left(\frac{d\psi}{dT} \right)^2 \frac{\partial^2 F}{\partial \psi^2} + \frac{d^2 \psi}{dT^2} \frac{\partial F}{\partial \psi} \right]_{V, N_a}. \quad (35)$$

The temperature derivatives of ψ at constant V and N_e must be calculated from Eq. (29) giving

$$T \frac{d\psi}{dT} = -\frac{3}{2} \frac{I_{1/2}}{I_{-1/2}} \left[\frac{V^a}{V_\psi^a} + \frac{5}{4} \lambda \frac{I_{3/2}}{I_{1/2}} \frac{V_\lambda^a}{V_\psi^a} \right], \quad (36)$$

$$T^2 \frac{d^2 \psi}{dT^2} = \frac{15}{4} \frac{I_{1/2}}{I_{-1/2}} \frac{V^a}{V_\psi^a} - \left[\frac{3}{5} \frac{I_{1/2}}{I_{-1/2}} \frac{V^a}{V_\psi^a} \frac{I_{-3/2}}{I_{-1/2}} \frac{V_{\psi\psi}^a}{V_\psi^a} + \frac{3}{4} \lambda \left(\frac{I_{1/2}}{I_{-1/2}} \frac{V_{\lambda\psi}^a}{V_\psi^a} - \frac{I_{3/2}}{I_{-1/2}} \frac{V_\lambda^a}{V_\psi^a} \frac{I_{-3/2}}{I_{-1/2}} \frac{V_{\psi\psi}^a}{V_\psi^a} \right) + \frac{15}{8} \lambda^2 \frac{I_{3/2}}{I_{-1/2}} \frac{V_\lambda^a}{V^a} \left(\frac{I_{1/2}}{I_{-1/2}} \frac{V_{\lambda\psi}^a}{V_\psi^a} - \frac{1}{2} \frac{I_{3/2}}{I_{1/2}} \frac{V_\lambda^a}{V_\psi^a} \frac{I_{-3/2}}{I_{-1/2}} \frac{V_{\psi\psi}^a}{V_\psi^a} - \frac{7}{30} \frac{I_{5/2}}{I_{3/2}} \frac{V_{\lambda\lambda}^a}{V_\lambda^a} \right) \right]. \quad (37)$$

Finally, Eq. (35) divided by $N_e k$ yields the ideal part of the electronic specific heat

$$c_{V,e}^{\text{id}} = \frac{15}{4} \left[\frac{I_{3/2}}{I_{1/2}} \frac{U^a}{V^a} - \frac{3}{5} \frac{I_{1/2}}{I_{-1/2}} \frac{V^a}{V_\psi^a} \right] + \frac{75}{8} \lambda \left[\frac{I_{5/2}}{I_{1/2}} \frac{U_\lambda^a}{V^a} - \frac{3}{5} \frac{I_{3/2}}{I_{-1/2}} \frac{V_\lambda^a}{V_\psi^a} \right] + \frac{105}{64} \lambda^2 \left[\frac{I_{7/2}}{I_{1/2}} \frac{U_{\lambda\lambda}^a}{V^a} - \frac{15}{7} \frac{I_{3/2}}{I_{-1/2}} \frac{V_\lambda^a}{V_\psi^a} \frac{I_{3/2}}{I_{1/2}} \frac{V_\lambda^a}{V^a} \right], \quad (38)$$

where the abbreviations are given by

$$U_\lambda^a = 1 + \frac{7}{8} \lambda \frac{I_{7/2}}{I_{5/2}} \left(1 - \frac{9}{16} \lambda \frac{I_{9/2}}{I_{7/2}} \right) \quad (39)$$

$$U_{\lambda\lambda}^a = 1 - \frac{9}{8} \lambda \frac{I_{9/2}}{I_{7/2}} \quad (40)$$

$$V_\lambda^a = 1 + \frac{7}{8} \lambda \frac{I_{5/2}}{I_{3/2}} \left(1 - \frac{9}{16} \lambda \frac{I_{7/2}}{I_{5/2}} \right) \quad (41)$$

$$V_{\lambda\lambda}^a = 1 - \frac{9}{16} \lambda \frac{I_{7/2}}{I_{5/2}} \quad (42)$$

$$V_\psi^a = 1 + \frac{15}{8} \lambda \frac{I_{1/2}}{I_{-1/2}} \left[1 + \frac{7}{16} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 - \frac{3}{8} \lambda \frac{I_{5/2}}{I_{3/2}} \right) \right] \quad (43)$$

$$V_{\psi\psi}^a = 1 + \frac{15}{8} \lambda \frac{I_{-1/2}}{I_{-3/2}} \left[1 + \frac{7}{16} \lambda \frac{I_{1/2}}{I_{1/2}} \left(1 - \frac{3}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \right) \right] \quad (44)$$

$$V_{\psi\lambda}^a = 1 + \frac{7}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 - \frac{9}{16} \lambda \frac{I_{5/2}}{I_{3/2}} \right). \quad (45)$$

From these relations we can read off immediately various asymptotics. The nonrelativistic ($\lambda \ll 1$) and nondegenerate limit ($\psi \ll -1$) of Eq. (38) results to the well-known classical value

$$c_{V,e}^{\text{id}} = \frac{3}{2}. \quad (46)$$

Furthermore in the nonrelativistic limit and at arbitrary degeneracy the comparison of Eqs. (34) and (38) yields

$$\phi_{S,e}^{\text{id}} = \frac{2}{3} c_{V,e}^{\text{id}}. \quad (47)$$

Case *b* describes the regime where the Sommerfeld-Chandrasekhar expansion (Chandrasekhar 1939, Cox & Giuli 1968) becomes valid. The degeneracy parameter ψ is related for the strong-degenerate limit by

$$\psi\lambda = \sqrt{1 + \alpha^2} - 1, \quad (48)$$

where $\alpha = p_F/mc$ is the fraction of the Fermi- to the relativistic momentum. The Sommerfeld-Chandrasekhar expansion with $\sim O(\psi^{-6})$ provides (Cox & Giuli 1968)

$$p_e^{\text{id}} = \frac{1}{4\lambda} \frac{U^b(\psi, \lambda)}{V^b(\psi, \lambda)}, \quad (49)$$

$$n_e = \frac{2}{\Lambda_e^3} \sqrt{\frac{2}{\pi}} \frac{\alpha^3}{3\lambda^{3/2}} V^b(\psi, \lambda) = \left(\frac{mc}{\hbar} \right)^3 \frac{\alpha^3}{3\pi^2} V^b(\psi, \lambda), \quad (50)$$

with the abbreviations

$$U^b = \sqrt{1 + \alpha^2} \left[1 - \frac{3}{2\alpha^2} + \frac{3}{2\alpha^3 \sqrt{1 + \alpha^2}} \times \ln \left(\alpha + \sqrt{1 + \alpha^2} \right) + \frac{2\pi^2 \lambda^2}{\alpha^2} \left(1 - \frac{7}{60} \frac{\pi^2 \lambda^2}{\alpha^4} (1 - 2\alpha^2) \right) \right] \quad (51)$$

and

$$V^b = 1 + \frac{\pi^2 \lambda^2}{2\alpha^4} \left(1 + 2\alpha^2 + \frac{7}{20} \frac{\pi^2 \lambda^2}{\alpha^4} \right). \quad (52)$$

For the Helmholtz free energy represented by Eq. (27) the inversion $\psi = \psi(n_e, T)$ for case *b* is already given by Eq. (48). In order to correct Eq. (48) to the order $\sim O(\psi^{-6})$ analytical inversions have been performed by Yakovlev & Shalybkov (1989) and paper I.

For the internal energy, compressibility, and coefficient of strain we get

$$u_e^{\text{id}} = \frac{1}{\lambda} \left[\sqrt{1 + \alpha^2} - 1 + \frac{1}{4} \left(\frac{U^b}{V^b} + \frac{U_\lambda^b}{V_\lambda^b} \right) \right] \quad (53)$$

$$\frac{1}{k_e^{\text{id}}} = \frac{1}{\lambda} \left[\frac{\alpha^2}{\sqrt{1+\alpha^2}} \left(\frac{V^{\text{b}}}{3V^{\text{b}} + V_{\alpha}^{\text{b}}} \right) \right] \quad (54)$$

$$\phi_e^{\text{id}} = \frac{1}{\lambda} \left[\frac{1}{4} \frac{U_{\lambda}^{\text{b}}}{V^{\text{b}}} - \frac{\alpha^2}{\sqrt{1+\alpha^2}} \left(\frac{V_{\lambda}^{\text{b}}}{3V^{\text{b}} + V_{\alpha}^{\text{b}}} \right) \right]. \quad (55)$$

Neglecting the order ψ^{-6} in Eq. (53) we get the Chandrasekhar approximation for the internal energy (Chandrasekhar 1939, Cox & Giuli 1968, Lamb 1974, Eliezer et al. 1986, Yakovlev & Shalybkov 1989)

$$u_e^{\text{id}} = \frac{1}{N_e k T} \frac{m c^2}{8 \pi^2} \left(\frac{m c}{\hbar} \right)^3 \times \left[\alpha \sqrt{1+\alpha^2} (1+2\alpha^2) - \frac{8}{3\alpha^3} - \ln \left(\alpha + \sqrt{1+\alpha^2} \right) + \frac{4}{3} \frac{\pi^2 \lambda^2}{\alpha} \left(\sqrt{1+\alpha^2} (1+3\alpha^2) - (1+2\alpha^2) \right) \right]. \quad (56)$$

The specific heat Eq. (15) can be calculated for *case b* via

$$C_V = -T \left[\frac{\partial^2 F}{\partial T^2} + 2 \frac{d\alpha}{dT} \frac{\partial^2 F}{\partial \alpha \partial T} + \left(\frac{d\alpha}{dT} \right)^2 \frac{\partial^2 F}{\partial \alpha^2} + \frac{d^2 \alpha}{dT^2} \frac{\partial F}{\partial \alpha} \right]_{V, N_e} \quad (57)$$

The temperature derivatives of α at constant V and N_e must be calculated from Eq. (50)

$$\frac{T}{\alpha} \frac{d\alpha}{dT} = - \frac{V_{\lambda}^{\text{b}}}{3V^{\text{b}} + V_{\alpha}^{\text{b}}}, \quad (58)$$

$$\frac{T^2}{\alpha} \frac{d^2 \alpha}{dT^2} = \frac{T}{\alpha} \frac{d\alpha}{dT} \left[\frac{V_{\lambda\lambda}^{\text{b}}}{V_{\lambda}^{\text{b}}} + 2 \frac{T}{\alpha} \frac{d\alpha}{dT} \frac{V_{\alpha\lambda}^{\text{b}}}{V_{\lambda}^{\text{b}}} - \left(\frac{T}{\alpha} \frac{d\alpha}{dT} \right)^2 \left(\frac{12V^{\text{b}}}{V_{\lambda}^{\text{b}}} - \frac{V_{\alpha\alpha}^{\text{b}}}{V_{\lambda}^{\text{b}}} \right) \right]. \quad (59)$$

Finally, Eq. (57) divided by $N_e k$ yields

$$c_{V,e}^{\text{id}} = - \frac{1}{\lambda} \left\{ \left(\sqrt{1+\alpha^2} - 1 \right) \frac{V_{\lambda\lambda}^{\text{b}}}{V^{\text{b}}} - \frac{1}{4} \frac{U_{\lambda\lambda}^{\text{b}}}{V^{\text{b}}} + 2 \frac{T}{\alpha} \frac{d\alpha}{dT} \left[\left(\sqrt{1+\alpha^2} - 1 \right) \left(\frac{3V_{\lambda}^{\text{b}}}{V^{\text{b}}} + \frac{V_{\alpha\lambda}^{\text{b}}}{V^{\text{b}}} \right) - \left(\frac{T}{\alpha} \frac{d\alpha}{dT} \right)^2 \left[6 \left(\sqrt{1+\alpha^2} - 1 \right) \left(1 + \frac{V_{\alpha}^{\text{b}}}{V^{\text{b}}} + \frac{1}{6} \frac{V_{\alpha\alpha}^{\text{b}}}{V^{\text{b}}} \right) - \frac{3U^{\text{b}}}{V^{\text{b}}} + \frac{1}{4} \frac{U_{\alpha\alpha}^{\text{b}}}{V^{\text{b}}} - \frac{\alpha^2}{(1+\alpha^2)^{3/2}} \left(1 + 2(1+\alpha^2) \frac{V_{\alpha}^{\text{b}}}{V^{\text{b}}} \right) \right] + \frac{T^2}{\alpha} \frac{d^2 \alpha}{dT^2} \left[\left(\sqrt{1+\alpha^2} - 1 \right) \left(3 + \frac{V_{\alpha}^{\text{b}}}{V^{\text{b}}} \right) \right] \right\}. \quad (60)$$

Here the abbreviations labeled by the superscript *b* are given by the simple derivatives with $X = \{U^{\text{b}}, V^{\text{b}}\}$

$$X_{\lambda} = \lambda \frac{\partial}{\partial \lambda} X, \quad X_{\lambda\lambda} = \lambda^2 \frac{\partial^2}{\partial \lambda^2} X, \quad (61)$$

$$X_{\alpha} = \alpha \frac{\partial}{\partial \alpha} X, \quad X_{\alpha\alpha} = \alpha^2 \frac{\partial^2}{\partial \alpha^2} X, \quad (62)$$

$$X_{\alpha\lambda} = \alpha \lambda \frac{\partial^2}{\partial \alpha \partial \lambda} X. \quad (63)$$

Eq. (60) yields by neglecting the order ψ^{-6} (Chandrasekhar 1939, Eliezer et al. 1986, Yakovlev & Shalybkov 1989)

$$c_{V,e}^{\text{id}} = \frac{\pi^2 \lambda}{\alpha^2} \sqrt{1+\alpha^2}, \quad (64)$$

which delivers the strong-relativistic ($\alpha \gg 1$)

$$c_{V,e}^{\text{id}} = \frac{\pi^2}{\psi} \quad (65)$$

and the nonrelativistic ($\alpha \ll 1$)

$$c_{V,e}^{\text{id}} = \frac{\pi^2}{2\psi} \quad (66)$$

limiting laws. Let us remark that both Eqs. (38) and (60) have in the degenerate, weak-relativistic limit a wide overlap, which we use to combine *case a* and *b* in order to realize numerical continuity (see paper I).

4.2. Exchange

The lowest order exchange (Hartree-Fock) free energy for relativistic electrons is given by

$$f_{ee}^{\text{x}} = \frac{e^2}{\pi \Lambda_e^4} \frac{1}{n_e k T} J_{\text{rel}}^{\text{x}}(\psi, \lambda), \quad (67)$$

where $J_{\text{rel}}^{\text{x}}(\psi, \lambda)$ is the relativistic Hartree-Fock integral (Kovetz et al. 1972, paper I).

The λ -expansion in *case a* results in

$$f_{ee}^{\text{x}} = - \frac{e^2}{k T \Lambda_e} \frac{I^{\text{x}}(\psi)}{I_{1/2}(\psi)} \frac{W^{\text{a}}(\psi, \lambda)}{V^{\text{a}}(\psi, \lambda)}, \quad (68)$$

where

$$W^{\text{a}} = 1 - \frac{3}{8} \lambda \frac{I_{1/2}^2}{I^{\text{x}}} \left[1 + \frac{9}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 + \frac{11}{72} \lambda \frac{I_{3/2}}{I_{1/2}} \times \left(1 - \frac{25}{11} \lambda \frac{I_{5/2}}{I_{3/2}} \frac{I_{1/2}}{I_{3/2}} \right) \right) \right]. \quad (69)$$

Parametrizations for the nonrelativistic Hartree-Fock integral

$$I^{\text{x}}(\psi) = \int_{-\infty}^{\psi} d\psi' I_{-1/2}^2(\psi') \quad (70)$$

are given by Perrot & Dharma-wardana (1984) and Kalitkin & Ritus (1986) (see Stolzmann & Blöcker 1996b). Note, that for $\lambda = 0$ the following relation holds

$$J_{\text{rel}}^{\text{x}}(\psi, \lambda = 0) = -2\pi I^{\text{x}}(\psi). \quad (71)$$

The exchange pressure $p_{ee}^{\text{x}} = g_{ee}^{\text{x}} - f_{ee}^{\text{x}}$ is determined via the exchange Gibbs energy (cf. paper I)

$$g_{ee}^{\text{x}} = - \frac{e^2}{k T \Lambda_e} I_{-1/2} \frac{W_{\psi}^{\text{a}}}{V_{\psi}^{\text{a}}}, \quad (72)$$

where

$$W_{\psi}^a = 1 - \frac{3}{4} \lambda \frac{I_{1/2}}{I_{-1/2}} \left[1 + \frac{9}{16} \lambda \frac{I_{1/2}}{I_{-1/2}} \left(1 + \frac{I_{3/2}}{I_{1/2}} \frac{I_{-1/2}}{I_{1/2}} - \frac{1}{24} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 + \frac{25}{3} \frac{I_{5/2}}{I_{3/2}} \frac{I_{-1/2}}{I_{1/2}} \right) \right) \right] \quad (73)$$

For the exchange contribution of the internal energy, compressibility, and coefficient of strain we get

$$u_{ee}^x = \frac{3}{2} p_{ee}^x - \frac{1}{2} \frac{e^2}{kT\Lambda_e} \frac{I^x}{I_{1/2}} \frac{W_{\lambda}^a}{V^a} + \frac{15}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \frac{V_{\lambda}^a}{V^a} g_{ee}^x \quad (74)$$

$$\frac{1}{k_{T,ee}^x} = -\frac{e^2}{kT\Lambda_e} \frac{I_{1/2} I_{-3/2}}{I_{-1/2}} \frac{V^a}{V_{\psi}^a} \left[2 \frac{W_{\psi\psi}^a}{V_{\psi}^a} - \frac{V_{\psi\psi}^a}{V_{\psi}^a} \frac{W_{\psi}^a}{V_{\psi}^a} \right] \quad (75)$$

$$\phi_{S,ee}^x = p_{ee}^x + u_{ee}^x + \frac{1}{2} \frac{e^2}{kT\Lambda_e} I_{-1/2} \left[3 \frac{I_{1/2}}{I_{-1/2}} \frac{I_{-3/2}}{I_{-1/2}} \times \left(2 \frac{W_{\psi\psi}^a}{V_{\psi}^a} - \frac{V_{\psi\psi}^a}{V_{\psi}^a} \frac{W_{\psi}^a}{V_{\psi}^a} \right) \left(\frac{V^a}{V_{\psi}^a} + \frac{5}{4} \lambda \frac{I_{3/2}}{I_{1/2}} \frac{V_{\lambda}^a}{V_{\psi}^a} \right) + \frac{W_{\psi\lambda}^a}{V_{\psi}^a} + \frac{15}{4} \lambda \frac{I_{1/2}}{I_{-1/2}} \frac{V_{\psi\lambda}^a}{V_{\psi}^a} \frac{W_{\psi}^a}{V_{\psi}^a} \right] \quad (76)$$

Using (35) we obtain for the exchange part of the isochoric specific heat

$$\begin{aligned} c_{V,e}^x &= \frac{e^2}{kT\Lambda_e} \left[\frac{15}{4} \left[\frac{I^x}{I_{1/2}} \left(\frac{W^a}{V^a} - \frac{2}{3} \frac{W_{\lambda}^a}{V^a} + \frac{1}{5} \frac{W_{\lambda\lambda}^a}{V^a} \right) + \frac{3}{5} \frac{I_{1/2} I_{-3/2}}{I_{-1/2}} \frac{V^a}{V_{\psi}^a} \left(2 \frac{W_{\psi\psi}^a}{V_{\psi}^a} - \frac{V_{\psi\psi}^a}{V_{\psi}^a} \frac{W_{\psi}^a}{V_{\psi}^a} \right) - I_{-1/2} \left(\frac{W_{\psi}^a}{V_{\psi}^a} - \frac{2}{5} \frac{W_{\psi\lambda}^a}{V_{\psi}^a} \right) \right] \right. \\ &+ \frac{75}{8} \lambda \left[-\frac{I_{3/2} I_{-1/2}}{I_{1/2}} \frac{V_{\lambda}^a}{V^a} \left(\frac{W_{\psi}^a}{V_{\psi}^a} - \frac{1}{5} \frac{W_{\psi\lambda}^a}{V_{\psi}^a} \right) + \frac{3}{5} \frac{I_{3/2} I_{-3/2}}{I_{1/2}} \frac{V_{\lambda}^a}{V_{\psi}^a} \left(2 \frac{W_{\psi\psi}^a}{V_{\psi}^a} - \frac{V_{\psi\psi}^a}{V_{\psi}^a} \frac{W_{\psi}^a}{V_{\psi}^a} \right) + \frac{3}{5} I_{1/2} \frac{V_{\psi\lambda}^a}{V_{\psi}^a} \frac{W_{\psi}^a}{V_{\psi}^a} \right] \\ &+ \frac{225}{64} \lambda^2 \left[\frac{I_{3/2}^2 I_{-3/2}}{I_{1/2} I_{-1/2}} \frac{V_{\lambda}^a}{V^a \psi} \left(2 \frac{W_{\psi\psi}^a}{V^a} - \frac{V_{\psi\psi}^a}{V^a} \frac{W_{\psi}^a}{V^a} \right) + 4 \frac{I_{3/2} I_{-3/2}}{I_{1/2}} \left(\frac{I_{1/2}}{I_{-1/2}} \frac{V_{\lambda}^a}{V_{\psi}^a} \frac{V_{\psi\lambda}^a}{V_{\psi}^a} - \frac{7}{30} \frac{I_{5/2}}{I_{3/2}} \frac{V_{\lambda\lambda}^a}{V_{\psi}^a} \right) \right] \quad (77) \end{aligned}$$

with the relativistic corrections

$$W_{\lambda}^a = 1 + \frac{3}{8} \lambda \frac{I_{1/2}^2}{I^x} \left[1 + \frac{27}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 + \frac{55}{216} \lambda \frac{I_{3/2}}{I_{1/2}} \times \left(1 - \frac{25}{11} \frac{I_{5/2}}{I_{3/2}} \frac{I_{1/2}}{I_{3/2}} \right) \right) \right] \quad (78)$$

$$W_{\lambda\lambda}^a = 1 + \frac{1}{8} \lambda \frac{I_{1/2}^2}{I^x} \left[1 - \frac{27}{8} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 + \frac{55}{72} \lambda \frac{I_{3/2}}{I_{1/2}} \times \left(1 - \frac{25}{11} \frac{I_{5/2}}{I_{3/2}} \frac{I_{1/2}}{I_{3/2}} \right) \right) \right] \quad (79)$$

$$W_{\psi\psi}^a = 1 - \frac{3}{8} \lambda \frac{I_{1/2}}{I_{-1/2}} \left[1 + \frac{I_{-1/2}}{I_{-3/2}} \frac{I_{-1/2}}{I_{1/2}} + \frac{9}{16} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 + 3 \frac{I_{-1/2}}{I_{-3/2}} \frac{I_{1/2}}{I_{3/2}} - \frac{7}{9} \lambda \frac{I_{-1/2}}{I_{-3/2}} \times \left(1 + \frac{3}{28} \frac{I_{1/2}}{I_{-1/2}} \frac{I_{1/2}}{I_{3/2}} + \frac{25}{28} \frac{I_{5/2}}{I_{3/2}} \frac{I_{-3/2}}{I_{-1/2}} \right) \right) \right] \quad (80)$$

$$W_{\psi\lambda}^a = 1 + \frac{3}{4} \lambda \frac{I_{1/2}}{I_{-1/2}} \left[1 + \frac{27}{16} \lambda \frac{I_{3/2}}{I_{1/2}} \left(1 + \frac{I_{1/2}}{I_{-1/2}} \frac{I_{1/2}}{I_{3/2}} - \frac{125}{216} \lambda \frac{I_{5/2}}{I_{3/2}} \left(1 + \frac{3}{25} \frac{I_{3/2}}{I_{5/2}} \right) \right) \right] \quad (81)$$

The Sommerfeld-Chandrasekhar expansion for the exchange free energy in *case b* (Salpeter & Zapolsky 1967, Kovetz et al. 1972, Lamb 1974) delivers for $\sim O(\psi^{-6})$ (see paper I)

$$f_{ee}^x = -\frac{e^2}{kT\Lambda_e} \frac{3}{2\alpha^3} \frac{1}{\sqrt{2\pi\lambda}} \frac{W^b(\alpha, \lambda)}{V^b(\alpha, \lambda)}, \quad (82)$$

where

$$\begin{aligned} W^b &= \frac{3B^2}{2(1+\alpha^2)} - 3\alpha B + \frac{3}{2}\alpha^2 + \frac{1}{2}\alpha^4 \\ &+ \frac{\pi^2\lambda^2}{3} \left[-0.7046 + 2 \ln \frac{2\alpha^2}{\lambda} + \alpha^2 - \frac{3B}{\alpha} \right] \\ &+ \frac{\pi^4\lambda^4}{18} \left[1 - \frac{11}{10\alpha^2} \left(1 + \frac{37}{11\alpha^2} + \frac{63B}{11\alpha^3} \right) \right] \quad (83) \end{aligned}$$

with $B = \sqrt{1+\alpha^2} \ln(\alpha + \sqrt{1+\alpha^2})$.

With the Gibbs energy (see paper I)

$$g_{ee}^x = -\frac{e^2}{kT\Lambda_e} \frac{3}{2\alpha^3} \frac{1}{\sqrt{2\pi\lambda}} \frac{W_{\alpha}^b}{3V^b + V_{\alpha}^b} \quad (84)$$

it is possible to provide the exchange pressure $p_{ee}^x = g_{ee}^x - f_{ee}^x$ again.

In a straightforward manner, the exchange contribution for internal energy, compressibility, and coefficient of strain are represented by

$$u_{ee}^x = \frac{e^2}{kT\Lambda_e} \frac{3}{2\alpha^3} \frac{1}{\sqrt{2\pi\lambda}} \left[\frac{W_{\lambda}^b}{V^b} - \frac{W_{\lambda}^b}{V^b} + \frac{W_{\alpha}^b}{V^b} \left(\frac{V_{\lambda}^b}{3V^b + V_{\alpha}^b} \right) \right] \quad (85)$$

$$\begin{aligned} \frac{1}{k_{T,ee}^x} &= \frac{e^2}{kT\Lambda_e} \frac{3}{2\alpha^3} \frac{1}{\sqrt{2\pi\lambda}} \left(\frac{V^b}{3V^b + V_{\alpha}^b} \right)^2 \times \\ &\left[\frac{W_{\alpha\alpha}^b}{V^b} - \frac{6W_{\alpha}^b}{3V^b + V_{\alpha}^b} \left(1 + \frac{V_{\alpha}^b}{V^b} + \frac{1}{6} \frac{V_{\alpha\alpha}^b}{V^b} \right) \right] \quad (86) \end{aligned}$$

$$\phi_{S,ee}^x = p_{ee}^x + u_{ee}^x - g_{ee}^x \left[1 + \frac{3V_\lambda^b + V_{\alpha\lambda}^b}{3V^b + V_\alpha^b} - \frac{W_{\alpha\lambda}^b}{W_\alpha^b} - \frac{V_\lambda^b}{3V^b + V_\alpha^b} \left(2 + \frac{4V_\lambda^b + V_{\alpha\alpha}^b}{3V^b + V_\alpha^b} - \frac{W_{\alpha\lambda}^b}{W_\alpha^b} \right) \right]. \quad (87)$$

The exchange specific heat can be formulated by

$$c_{V,e}^x = -\frac{e^2}{kT\Lambda_e} \frac{3}{2\alpha^3} \frac{1}{\sqrt{2\pi\lambda}} \left[\frac{W_{\lambda\lambda}^b}{V^b} + 2\frac{T}{\alpha} \frac{d\alpha}{dT} \frac{W_{\alpha\lambda}^b}{V^b} + \left(\frac{T}{\alpha} \frac{d\alpha}{dT} \right)^2 \frac{W_{\alpha\alpha}^b}{V^b} + \frac{T^2}{\alpha} \frac{d^2\alpha}{dT^2} \frac{W_{\alpha\lambda}^b}{V^b} \right] \quad (88)$$

The temperature derivatives of α in Eq. (88) are given by (58) and (59). The derivatives of W with respect to λ and α for the exchange contributions are determined by

$$W_\lambda^b = \lambda \frac{\partial}{\partial \lambda} W^b, \quad W_{\lambda\lambda}^b = \lambda^2 \frac{\partial^2}{\partial \lambda^2} W^b, \quad (89)$$

$$W_\alpha^b = \alpha \frac{\partial}{\partial \alpha} W^b, \quad W_{\alpha\alpha}^b = \alpha^2 \frac{\partial^2}{\partial \alpha^2} W^b, \quad (90)$$

$$W_{\alpha\lambda}^b = \alpha\lambda \frac{\partial^2}{\partial \alpha \partial \lambda} W^b. \quad (91)$$

The adiabatic temperature gradient (8) expressed by our dimensionless potentials (18) and (19) is given by

$$\nabla_{ad} = pk_T \frac{\phi_S}{c_P} = \frac{p}{\phi_S} \left(1 - \frac{c_V}{c_P} \right) \quad (92)$$

with the isobaric specific heat

$$c_P = c_V + k_T \phi_S^2 \quad (93)$$

The Figs. 1 and 2 illustrate the adiabatic temperature gradient (92) of the ideal gas in comparison with a gas where additionally the exchange term is taken into account. Note, that the representation in Figs. 1 and 2 for extremely high densities serves only to illustrate the asymptotics of the theoretical expressions. Processes relevant to such high densities as, e.g., pycnonuclear reactions or electron captures, are not taken into account. Fig. 1 illustrates the course of ∇_{ad} for the elements hydrogen, helium and oxygen along a nonrelativistic and a weak-relativistic temperature. A comparison with the corresponding data for carbon from Lamb (1974) is given in Fig. 2. Note a disagreement for $T = 10^5$ K. This deviation could be caused by an erroneous constant for the exchange contribution used by Kovetz et al. (1972) and Lamb (1974) and is discussed in detail in paper I. A numerical procedure to guarantee a smooth transition between the approximations given by *case a* and *case b* is developed in paper I. The curves as seen in Figs. 1 and 2 show how exchange effects vanish with increasing temperature. Considering the isotherms in the high density region exchange effects are negligible. Nevertheless Eqs. (82)-(88) guarantee the accurate asymptotics, which is a fundamental problem for the calculation of EOS derivatives for quantities with vanishingly small temperature dependence (Miralles & Van Riper 1996).

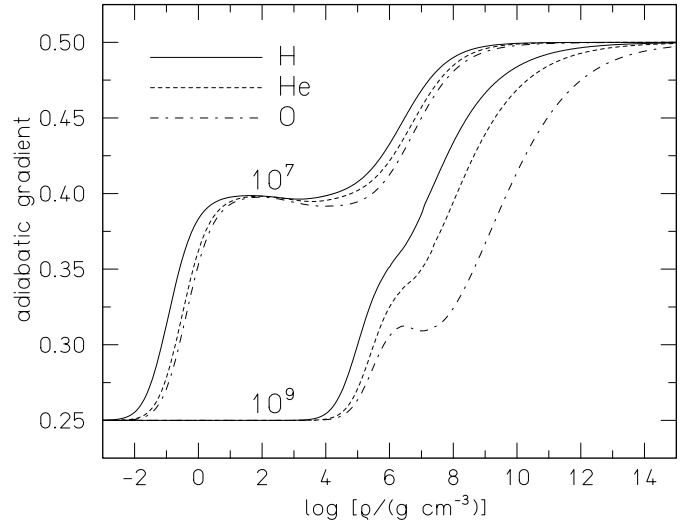


Fig. 1. Adiabatic temperature gradient ∇_{ad} vs. density at $T = 10^7$ K and $T = 10^9$ K for various elements. The curves refer to the sum of ideality, exchange and radiation. The presentation towards extremely high densities serves only to illustrate the asymptotic behaviour of the adiabatic gradient in our model (processes relevant to very high densities as, e.g., pycnonuclear reactions or electron captures, are not considered).

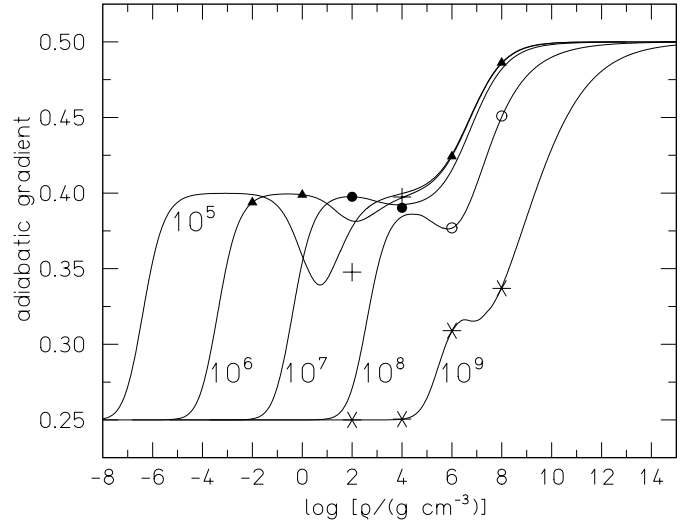


Fig. 2. Adiabatic temperature gradient ∇_{ad} vs. density for carbon along various isotherms compared with Lamb (1974) (+ : 10^5 K, Δ : 10^6 K, \bullet : 10^7 K, \circ : 10^8 K, * : 10^9 K). The curves refer to the sum of ideality, exchange and radiation. The presentation towards extremely high densities serves only to illustrate the asymptotic behaviour of the adiabatic gradient in our model (processes relevant to very high densities as, e.g., pycnonuclear reactions or electron captures, are not considered).

4.3. Correlations

According to Eq. (20) we have to determine the terms labeled by the superscript c, which are based on correlation effects. As in paper I we aim to present closed-form parametrizations formed by Padé Approximants to get explicit expressions for

the correlation contributions of the thermodynamical potentials. The thermodynamical potentials resulting from the correlation contributions are characterized by the electronic and ionic Coulomb-coupling parameters $\Gamma_e = (4\pi n_e/3)^{1/3} e^2/kT$ and $\Gamma_i = \Gamma_e \langle Z^{5/3} \rangle$ giving the strength of the Coulomb interaction, and by the degeneracy parameter $\Theta = T/T_F = 2(4/9\pi)^{2/3} r_s/\Gamma_e$ describing the quantum state of the system. The parameter $r_s = m_e e^2/\hbar^2 (3/4\pi n_e)^{1/3}$ is the ratio of the mean interelectronic distance to the (electronic) Bohr-radius.

4.3.1. Electron-electron interaction

The Padé Approximants for free Helmholtz- and Gibbs energies of the nonrelativistic electronic subsystem at arbitrary degeneration and Coulomb coupling have the general structure

$$f_{ee}^c = -\frac{a_0 \Gamma_e^{3/2} - a_2 \Gamma_e^6 [\varepsilon_c(r_s, 0) + \Delta\varepsilon_c(r_s, \tau)]/\tau}{1 + a_1 \Gamma_e^{3/2} + a_2 \Gamma_e^6}, \quad (94)$$

$$g_{ee}^c = -\frac{s_0 \Gamma_e^{3/2} - s_2 \Gamma_e^6 [\mu_c(r_s, 0) + \Delta\mu_c(r_s, \tau)]/\tau}{1 + s_1 \Gamma_e^{3/2} + s_2 \Gamma_e^6}, \quad (95)$$

with ground-state energies $\varepsilon_c(r_s, 0)$ and $\mu_c(r_s, 0)$ derived by Vosko et al. (1980) and low-temperature corrections $\Delta\varepsilon_c(r_s, \tau)$ and $\Delta\mu_c(r_s, \tau)$, which are given in paper I. The coefficients read

$$a_0 = \frac{1}{\sqrt{3}} f_0(\Gamma_e), \quad s_0 = \frac{3}{2} a_0 + \frac{1}{3} \Gamma_e \frac{da_0}{d\Gamma_e} \quad (96)$$

$$f_0(\Gamma) = \frac{1}{2} \left(\frac{1}{(1 + 0.1088\Gamma_e)^{1/2}} + \frac{1}{(1 + 0.3566\Gamma_e)^{3/2}} \right) \quad (97)$$

$$a_1 = \frac{3\sqrt{3}}{32} \sqrt{2\pi\tau} \left[1 + K_e^* \left(\sqrt{2/\tau} \right) \right], \quad s_1 = \frac{8}{9} a_1 \quad (98)$$

$$a_2 = 6 \frac{\tau}{r_s^2}, \quad s_2 = a_2. \quad (99)$$

Note that we have modified the coefficients a_1 and s_1 as compared to paper I by a rearrangement of the quantum virial function (Ebeling et al. 1976)

$$K_e^*(x) = E_2^*(-x) - \frac{8x}{\sqrt{\pi}} \left[Q_3^*(-x) - \frac{1}{6} \ln|x| - C_0 \right] \quad (100)$$

In paper I we incorporated for $K_e^*(x)$ in Eq. (98) only the first part of Eq. (100) as proposed by Ebeling (1993). The second term was considered by the coefficient c_1 of the ion-electron contribution (see Eq. (85) in paper I). The justification to rearrange these summations over the electrons is the omission of the coefficient a_3 in Eq. (53) in paper I, which has only been introduced to optimize the interpolation. For E_2^* and Q_3^* we derived Padé approximations as given in paper I with improvements to achieve higher accuracy.

$$E_2^*(-x) = \frac{\ln 2 + 0.0113x^2 + 0.1x^5 \left(\frac{2}{\sqrt{\pi x}} - \frac{1}{x^2} \right)}{1 + \pi^{3/2} x / (18 \ln 2) + 0.1x^5} \quad (101)$$

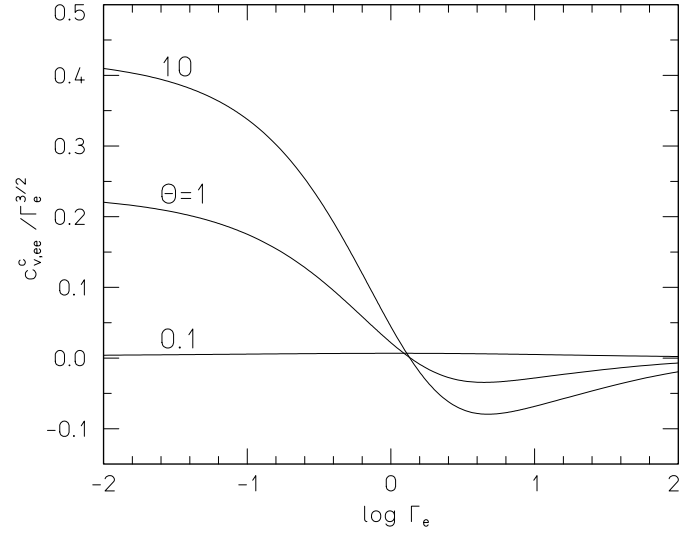


Fig. 3. The isochoric specific heat for the electronic subsystem at different degeneracy ($\Theta = 10$ (classical), 1 (intermediate), 0.1 (strong)) vs. Coulomb-coupling parameter.

$$Q_3^*(-x) = \frac{C_1 + x^5 \left(\frac{1}{6} \ln|x| + C_0 + \frac{\sqrt{\pi}}{8x} - \frac{1}{9x^2} \right)}{1 - \frac{9}{10C_1} \left(\frac{\pi^{5/2} x}{192} - \frac{x^2}{75} \right) + x^5} \quad (102)$$

with $C_0 = \frac{1}{6} (\ln 3 + 2C_E - \frac{11}{6})$ and $C_1 = \frac{1}{6} (\ln 3 + \frac{C_E}{2} - \frac{1}{2})$.

A detailed comparison of the Padé formula (94) with most advanced many body calculations is given in paper I and recently in Stolzmann & Rösler (1998b). The electronic correlation contribution for the pressure is obtained by

$$p_{ee}^c = g_{ee}^c - f_{ee}^c, \quad (103)$$

The internal energy can be described by the Padé approximant

$$u_{ee}^c = -\frac{u_0 \Gamma_e^{3/2} - u_2 \Gamma_e^6 [\varepsilon_c(r_s, 0) + \Delta\varepsilon_c(r_s, \tau)]/\tau}{1 + u_1 \Gamma_e^{3/2} + u_2 \Gamma_e^6}, \quad (104)$$

with the coefficients

$$u_0 = \frac{3}{2} a_0 + \Gamma_e \frac{da_0}{d\Gamma_e}, \quad u_2 = a_2 \quad (105)$$

$$u_1 = 2 \left(a_1 - \frac{\tau}{3} \frac{da_1}{d\tau} \right) = \frac{5}{3} a_1 - \frac{\sqrt{3}}{16} \sqrt{2\pi\tau} \left(\tau \frac{d}{d\tau} K_e^*(x) \right) \quad (106)$$

The temperature derivative of the quantum virial function (100) is given by

$$\tau \frac{d}{d\tau} K_e^*(x) = \tau \frac{d}{d\tau} E_2^*(-\tau) - \frac{1}{2} K_e^*(-\tau) + \frac{1}{2} E_2^*(-\tau) - \frac{16}{\sqrt{2\pi\tau}} \left[\tau \frac{d}{d\tau} Q_3^*(-\tau) + \frac{1}{12} \right]. \quad (107)$$

For the temperature derivatives of E_2^* and Q_3^* we derive the Padé Approximants

$$\tau \frac{d}{d\tau} E_2^*(-\tau) = \frac{\frac{\pi^{3/2}}{36} x + \frac{x^5}{12} \left(\frac{1}{\sqrt{\pi x}} - \frac{1}{x^2} \right)}{1 + 0.113 \frac{36}{\pi^{3/2}} x (1 - 0.473x) + \frac{x^5}{12}} \quad (108)$$

$$\tau \frac{d}{d\tau} Q_3^*(-\tau) = \frac{-\frac{\pi^{5/2}}{384}x + 0.1x^{4.5} \left(-\frac{1}{12} + \frac{\pi^{1/2}}{16x} - \frac{1}{6x^2}\right)}{1 + \frac{384}{25\pi^{5/2}}x + 0.1x^{4.5}}. \quad (109)$$

The correlation contribution $1/k_{T,ee}^c$ for the bulk modulus is given by

$$\frac{1}{k_{T,ee}^c} = \frac{k_0\Gamma_e^{3/2} + k_2\Gamma_e^6 [p_c(r_s, 0) (1 - 1/k_c(r_s, 0))] / \tau}{1 + k_1\Gamma_e^{3/2} + k_2\Gamma_e^6} \quad (110)$$

with the coefficients

$$k_0 = -\frac{3}{4}a_0 - \frac{\Gamma_e}{4} \frac{da_0}{d\Gamma_e}, \quad k_2 = 10a_2, \quad k_1 = 30a_1. \quad (111)$$

The ground-state bulk modulus is given by

$$\frac{1}{k_c(r_s, 0)} = \frac{3}{0.062181} \frac{r_s}{3} \frac{d}{dr_s} p_c(r_s, 0). \quad (112)$$

Using the Monte-Carlo data-fit from Vosko et al. (1980) for $p_c(r_s, 0)$ (see paper I) we apply

$$\frac{1}{k_c(r_s, 0)} = \left[\frac{\frac{1}{2}m_1\sqrt{r_s}}{1 + m_1\sqrt{r_s}} - \frac{\frac{1}{2}m_1\sqrt{r_s} + m_2r_s + \frac{3}{2}m_3r_s^{3/2}}{1 + m_1\sqrt{r_s} + m_2r_s + m_3r_s^{3/2}} \right] \quad (113)$$

The coefficient of strain $\phi_{S,ee}^c$ can be expressed by

$$\phi_{S,ee}^c = p_{ee}^c + u_{ee}^c + \frac{\phi_0\Gamma_e^{3/2} - \phi_2\Gamma_e^6 [\mu_c(r_s, 0) - \frac{3}{2}\Delta\varepsilon_c(r_s, \tau)] / \tau}{1 + \phi_1\Gamma_e^{3/2} + \phi_2\Gamma_e^6} \quad (114)$$

with the coefficients

$$\phi_0 = \frac{9}{4}a_0 + \frac{3}{4}\Gamma_e \frac{da_0}{d\Gamma_e}, \quad \phi_2 = \frac{1}{2}a_2, \quad (115)$$

$$\phi_1 = \frac{16}{9}a_1 - \frac{2}{3}\tau \frac{da_1}{d\tau} \quad (116)$$

and for the isochoric specific heat $c_{V,ee}^c$ the Padé Approximant can be obtained by

$$c_{V,ee}^c = \frac{v_0\Gamma_e^{3/2} - v_2\Gamma_e^6 [2f(r_s)\Theta^2 (1 + \frac{2}{9}\ln\Theta)] / \tau}{1 + v_1\Gamma_e^{3/2} + v_2\Gamma_e^6} \quad (117)$$

with the coefficients

$$v_0 = \frac{3}{4} \left[a_0 + \frac{1}{4}\Gamma_e \frac{da_0}{d\Gamma_e} \right], \quad v_2 = a_2, \quad (118)$$

$$v_1 = \frac{3\sqrt{3}}{32} \sqrt{2\pi\tau} \left[1 + \frac{7}{12} \left(1 - \frac{\sqrt{2\pi\tau}}{16} K_e^*(-\tau) \right) + \frac{1}{24} (1 + E_2^*(-\tau)) - \frac{1}{2} \left(\tau \frac{d}{d\tau} E_2^*(-\tau) \right) - \frac{5}{6} \frac{16}{\sqrt{2\pi\tau}} \left(\tau \frac{d}{d\tau} Q_3^*(-\tau) + \frac{1}{12} \right) \right]. \quad (119)$$

Fig. 3 shows that the electronic correlation part of the isochoric specific heat can be neglected in the case of strongly degenerate electrons.

4.3.2. Ion-ion interaction

The classical one-component plasma (OCP) is a thoroughly studied plasma system and the results are unified in closed-form parametrizations (Hansen 1973, Graboske et al. 1975, Bami et al. 1979, Ebeling & Richert 1985, Ichimaru 1993, Kahlbaum 1996, Chabrier & Potekhin 1998). For the ion-ion correlation we modify the Padé Approximants used in paper I by the new formula (Stolzmann & Blöcker 1998, 1999) for the free energy

$$f_{ii}^c = -\frac{b_0\Gamma_i^{3/2} \left[1 + b_3\Gamma_i^{3/2} F(\Gamma_i) \right] + b_2\Gamma_i^6 \varepsilon_{ii}(\Gamma_i)}{1 - b_1\Gamma_i^3 G(\Gamma_i) + b_2\Gamma_i^6}, \quad (120)$$

with $F(\Gamma_i) = \ln \Gamma_i + B_0$ and $G(\Gamma_i) = \ln \Gamma_i + B_1$

$$B_0 = \frac{2}{3} \left(2C_E + \frac{3}{2} \ln 3 - \frac{11}{6} \right), \quad (121)$$

$$B_1 = \frac{2}{3} \left(2C_E + \frac{1}{2} \ln 3 + 2 \ln 2 - \frac{17}{6} \right) - 0.4765 \quad (122)$$

and the coefficients

$$b_0 = \frac{1}{\sqrt{3}} \frac{\langle Z^2 \rangle^{3/2}}{\langle Z \rangle^{1/2} \langle Z^{5/3} \rangle^{3/2}}, \quad b_1 = \frac{3\sqrt{3}}{8b_0}, \quad (123)$$

$$b_2 = 100, \quad b_3 = \frac{b_1}{\sqrt{3}}, \quad (124)$$

Eq. (120) is based on the classical $\Gamma_i < 1$ result from Cohen & Murphy (1969) and for $\Gamma_i \gtrsim 1$ we take into account the most recent Monte-Carlo fit for the free energy $\varepsilon_{ii}(\Gamma_i)$ of the liquid OCP from DeWitt & Slattery (1999)

$$\varepsilon_{ii}(\Gamma_i) = 0.899172\Gamma_i + 0.274823 \ln \Gamma_i - 1.864179\Gamma_i^{0.323064} + 1.4018. \quad (125)$$

We remark, that in our notation of Eq. (20) for $\varepsilon_{ii}(\Gamma_i)$ we have to take for $\Gamma_i \gtrsim 178$

$$\varepsilon_{ii}(\Gamma_i) = 0.895929\Gamma_i - 1.5 \ln \Gamma_i + 3.9437\Gamma_i^{-1} + 1245\Gamma_i^{-2} + 1.1703 \quad (126)$$

which, with Eq. (21) rewritten by

$$f_i^{\text{id}} = \frac{3}{2} \ln \frac{kT}{\text{Ryd}_i} + 3 \ln \Gamma_i - 0.7155, \quad (127)$$

delivers the thermal (solid phase) energy of the OCP given by Hansen (1972), Pollock & Hansen (1973), Slattery et al. (1980), and Stringfellow et al. (1990). The quantity $\text{Ryd}_i = AZ^4 m_p / m_e \text{Ryd}$ denotes the ionic Rydberg energy with the (electronic) Rydberg unit $\text{Ryd} = m_e e^4 / 2\hbar^2$.

The free Gibbs energy g_{ii}^c and the isochoric specific heat $c_{V,ii}^c$ are expressed by the Padé Approximants

$$g_{ii}^c = -\frac{\frac{3}{2}b_0\Gamma_i^{3/2} \left[1 + \frac{4}{3}b_3\Gamma_i^{3/2} (F(\Gamma_i) + \frac{1}{6}) \right] + b_2\Gamma_i^6 \mu_{ii}(\Gamma_i)}{1 - \frac{5}{3}b_1\Gamma_i^3 (G(\Gamma_i) + \frac{2}{15}) \left[1 + \frac{3}{4}\Gamma_i^{3/2} \right] + b_2\Gamma_i^6} \quad (128)$$

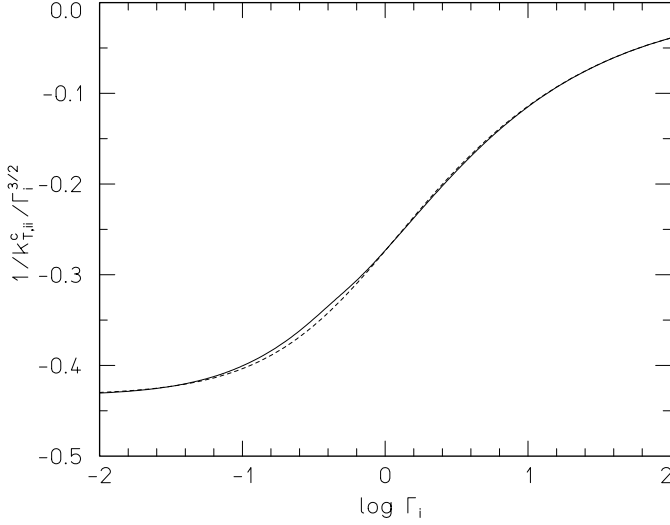


Fig. 4. The compressibility for the ionic subsystem vs. coupling parameter Γ_i . The solid line represents the correlation contribution (133) and the dashed line refers to the parametrization from Hansen (1973).

$$c_{V,ii}^c = \frac{\frac{3}{4}b_0\Gamma_i^{3/2} \left[1 + 8b_3\Gamma_i^{3/2} \left(F(\Gamma_i) + \frac{5}{6} \right) \right] + 6b_2\Gamma_i^6 \varrho_{ii}(\Gamma_i)}{1 - 7b_1\Gamma_i^3 \left(G(\Gamma_i) + \frac{32}{63} \right) + 6b_2\Gamma_i^6} \quad (129)$$

with

$$\begin{aligned} \mu_{ii}(\Gamma_i) &= \varepsilon_{ii}(\Gamma_i) + \frac{1}{3}\Gamma_i \frac{d\varepsilon_{ii}(\Gamma_i)}{d\Gamma_i}, \\ \varrho_{ii}(\Gamma_i) &= \Gamma_i^2 \frac{d^2\varepsilon_{ii}(\Gamma_i)}{d\Gamma_i^2}. \end{aligned} \quad (130)$$

The pressure, internal energy, isothermal compressibility, and coefficient of strain (Hansen 1973, Stolzmann & Blöcker 1999) are calculated by

$$p_{ii}^c = g_{ii}^c - f_{ii}^c, \quad (131)$$

$$u_{ii}^c = 3 p_{ii}^c, \quad (132)$$

$$\frac{1}{k_{T,ii}^c} = -\frac{1}{9} c_{V,ii}^c + \frac{4}{9} u_{ii}^c, \quad (133)$$

$$\phi_{S,ii}^c = \frac{1}{3} c_{V,ii}^c. \quad (134)$$

Fig. 4 compares our Padé Approximants of the isothermal compressibility with the fit formulae from Hansen (1973). Further comparisons between different interpolation formulae for the classically ionic subsystem, e.g. from Hansen (1973), Ichimaru (1994), Kahlbaum (1996), Chabrier & Potekhin (1998) can be found in Stolzmann & Blöcker (1999).

Ionic quantum effects, which were included approximately in our earlier Padé Approximants for the ionic subsystem (see paper I) will be considered separately in the following section.

4.3.3. Ionic quantum effects

The classical description for the subsystem of ionic OCP becomes inaccurate in the region of high densities at moderate temperatures. A measure for the quantum effects of the ions is the parameter (weight fraction X_i , molecular weight A_i , proton mass m_p , atomic mass unit $m_u = 1.66053 \cdot 10^{-24}$ g)

$$\Theta_i = \frac{\hbar\omega_p}{kT} = \frac{4\sqrt{\pi}}{kT} \left(\frac{\rho}{m_u} \frac{m_e}{m_p} \left(\frac{\hbar^2}{m_e e^2} \right)^3 \sum_i \frac{Z_i^2 X_i}{A_i^2} \right)^{1/2} \quad (135)$$

which is related by

$$\Theta_i = \sqrt{\frac{3}{R_S}} \Gamma_i, \quad (136)$$

and whereas ω_p denotes the (ionic) plasma frequency and $R_S = m_i Z^2 e^2 / \hbar^2 (3/4\pi n_i)^{1/3}$ is the ratio of the (ionic) Wigner-Seitz-radius to the (ionic) Bohr-radius. Quantum corrections for a solid OCP over a broad region of Θ_i were calculated first by Pollock & Hansen (1973). Chabrier et al. (1992) (see also Chabrier 1993) and Iyetomi et al. (1993) derived a free energy for a solid OCP model with quantum corrections. Nagara et al. (1987) calculated quantum corrections for the free energy of the OCP valid for fluid and solid phases by a new expansion method. In our model ionic quantum effects according to Nagara et al. (1987) as well as Chabrier et al. (1992) will be included.

Following paper I, the free energy calculated within the so-called “sixth reduced moment approximation” of Nagara et al. (1987) is given by

$$f_{ii}^{cq} = 3 \left[q_0(t) + z_4 q_4(t) - \frac{3}{4} \frac{t}{\Gamma_i} z_5 q_5(t) + z_6 q_6(t) \right] \quad (137)$$

with $t = \Theta_i/2\sqrt{3}$. Generally, the reduced moments z_i are dependent of Γ_i . For simplicity we choose for the solid phase the values for the rigid bcc lattice (Nagara et al. 1987):

$$z_4 = 0.827702, \quad z_5 = 1.131, \quad z_6 = 0.55045. \quad (138)$$

The functions $q_i(t)$ are given by

$$q_0(t) = \ln \left(\frac{\sinh t}{t} \right) \quad (139)$$

$$q_4(t) = \frac{1}{4} - \frac{t}{8} \coth t - \frac{t^2}{8} \frac{1}{\sinh^2 t} \quad (140)$$

$$q_5(t) = \frac{t}{3} \coth^2 t - \frac{3}{2} \coth t - \frac{5}{6} t \frac{1}{\sinh^2 t} + \frac{2}{t} \quad (141)$$

$$q_6(t) = -\frac{1}{6} + \frac{t}{16} \coth t + \frac{t^2}{16} \frac{1}{\sinh^2 t} \left(1 + \frac{2t}{3} \coth t \right). \quad (142)$$

The free energy expansion (137) reproduces the Wigner-Kirkwood expansion (Wigner 1932, Kirkwood 1933) up to the order Θ_i^6 . Furthermore the expansion of Nagara et al. (1987) delivers the high- Θ_i asymptotics of the Coulomb lattice by

$$f_{ii}^{cq} = \frac{3}{2} \mu_1 \Theta_i \quad (143)$$

with $\mu_1 = 0.564$. For the harmonic lattice approximation one obtains $\mu_1 = 0.511$ (Hansen & Vieflefosse 1975).

The ionic quantum effects for our set of potentials are given by the resulting formulae

$$p_{ii}^{\text{cq}} = \frac{3}{2}t \left[q_0'(t) + z_4 q_4'(t) + z_6 q_6'(t) - \frac{3}{4} \frac{t}{\Gamma_i} z_5 q_5'(t) \right] - \frac{3}{8} \frac{t}{\Gamma_i} z_5 q_5(t) \quad (144)$$

$$g_{ii}^{\text{cq}} = p_{ii}^{\text{cq}} + f_{ii}^{\text{cq}} \quad (145)$$

$$u_{ii}^{\text{cq}} = 2p_{ii}^{\text{cq}} + \frac{3}{4} \frac{t}{\Gamma_i} z_5 q_5(t) \quad (146)$$

$$c_{V,ii}^{\text{cq}} = -3t^2 \left[q_0''(t) + z_4 q_4''(t) - \frac{3}{4} \frac{t}{\Gamma_i} z_5 q_5''(t) + z_6 q_6''(t) \right] \quad (147)$$

$$\frac{1}{k_{T,ii}^{\text{cq}}} = \frac{1}{4} \left[3u_{ii}^{\text{cq}} - c_{V,ii}^{\text{cq}} - \frac{3}{4} \frac{t}{\Gamma_i} z_5 \left(\frac{7}{3} q_5(t) + 2tq_5'(t) \right) \right] \quad (148)$$

$$\phi_{S,ii}^{\text{cq}} = \frac{1}{2} \left[c_{V,ii}^{\text{cq}} - \frac{3}{4} \frac{t}{\Gamma_i} z_5 \left(q_5(t) - tq_5'(t) \right) \right] \quad (149)$$

The functions $q_i'(t)$ and $q_i''(t)$ are first and second derivatives of the functions $q_i(t)$ with respect to t .

Although the expansion of Nagara et al. (1987) can be applied to estimate quantum effects for fluid ionic phases as well as for solid phases this expansion is restricted to $\Theta_i \lesssim 17$, which is equivalent to $\Gamma_i \lesssim 4 \cdot 10^3 (AZ^4/(T/K))^{1/3}$ or to $\rho \lesssim 5 \cdot 10^{-6} (T/K)^2 (A/Z)^2$ for the density-temperature regime. For $\Gamma_i \approx \Gamma_m \gtrsim 180$ it is convenient to use the quantum crystal models from Iyetomi et al. (1993) or from Chabrier et al. (1992), which are applicable for a wide region of Θ_i .

If we extract the ionic quantum corrections for the free energy of a crystal from Chabrier et al. (1992) one obtains (Stolzmann & Blöcker 1994)

$$f_{ii}^{\text{cq}} = -\frac{2}{3} D_3(\alpha\Theta_i) + 2 \ln [1 - e^{-\alpha\Theta_i}] + \ln [1 - e^{-\gamma\Theta_i}] + \beta\Theta_i - 3 \ln(\delta\Theta_i) \quad (150)$$

with (Chabrier 1993)

$$\alpha = 0.399, \quad \gamma = 0.899, \quad \beta = 0.767. \quad (151)$$

The last term in (150) with $\delta = 0.4355$ guarantees the pure ionic quantum correction in our formalism. $D_3(\eta)$ is the Debye integral, which can be approximated by (see e.g. Iben & Tutukov 1984)

$$D_3(\eta) = \frac{3}{\eta^3} \int_0^\eta dt \frac{t^3}{e^t - 1} \approx \left(1 + 0.43\eta + \frac{5}{\pi^4} \eta^3 \right)^{-1}. \quad (152)$$

With (150) our set of potentials is given by

$$p_{ii}^{\text{cq}} = D_3(\alpha\Theta_i) + \frac{1}{2} \frac{\gamma\Theta_i \exp(-\gamma\Theta_i)}{1 - \exp(-\gamma\Theta_i)} - \frac{3}{2} + \frac{1}{2} \beta\Theta_i \quad (153)$$

$$g_{ii}^{\text{cq}} = p_{ii}^{\text{cq}} + f_{ii}^{\text{cq}} \quad (154)$$

$$u_{ii}^{\text{cq}} = 2p_{ii}^{\text{cq}} \quad (155)$$

$$\frac{1}{k_{T,ii}^{\text{cq}}} = p_{ii}^{\text{cq}} - \frac{3}{2} D_3(\alpha\Theta_i) + \frac{3}{2} \frac{\alpha\Theta_i \exp(-\alpha\Theta_i)}{1 - \exp(-\alpha\Theta_i)} + \frac{1}{4} \beta\Theta_i + \frac{1}{4} \frac{\gamma\Theta_i \exp(-\gamma\Theta_i)}{1 - \exp(-\gamma\Theta_i)} \left[1 - \frac{\gamma\Theta_i}{1 - \exp(-\gamma\Theta_i)} \right] + \frac{3}{2} \frac{\alpha\Theta_i \exp(-\alpha\Theta_i)}{1 - \exp(-\alpha\Theta_i)} \quad (156)$$

$$\phi_{S,ii}^{\text{cq}} = 3p_{ii}^{\text{cq}} - 2 \frac{1}{k_{T,ii}^{\text{cq}}} \quad (157)$$

$$c_{V,ii}^{\text{cq}} = 2\phi_{S,ii}^{\text{cq}} \quad (158)$$

An explicite expression for (158) is given by Chabrier (1993). Figs. 5-8 compare the ionic quantum corrections for the free energy as well as the isochoric specific heat calculated by different approaches. Note, the end of the solid lines in the Figs. 5-8 reflects the validity of the moment expansion as pointed out by Nagara et al. (1987). Fig. 5 shows ionic quantum corrections for $Z = 6$ calculated with different theories. Ionic quantum corrections in the vicinity of phase transition at $\Gamma_i \approx 180$ are shown in Fig. 6. Fig. 6 illustrates that the quantum corrections calculated by Iyetomi et al. (1993) decrease with increasing Θ_i . This behaviour is caused by the inclusion of the anharmonic contribution of the zero-temperature oscillations (see e.g. Nagara et al. 1987, Iyetomi et al. 1993), which is neglected by Chabrier et al. (1992). Fig. 7 shows the ionic quantum corrections for the isochoric specific heat derived from the corresponding free energies. Fig. 8 illustrates the course of the electronic and ionic contributions of the isochoric specific heat vs. temperature and shows how different prescriptions for the quantum corrections affect the results. The discontinuities in the curves for the ionic contribution in Fig. 8 refer to the fluid-solid phase transition at $\Gamma_i \approx 180$.

4.3.4. Ion-electron interaction

Next we have to include the screening effect between electrons and ions. We adopt the new Padé Approximant based on the Unsöld-Berlin-Montroll asymptotics of Stolzmann & Ebeling (1998) and Ebeling et al. (1999)

$$f_{ie}^c = -\frac{c_0 \Gamma_i^{3/2} + c_2 \Gamma_e^{5/2} \varepsilon_{ie}(r_s, \Gamma_i) + c_3 c_4 \Gamma_e^{5/2}}{1 + c_1 \Gamma_i^{3/2} + c_2 \Gamma_e^{5/2} + c_3 \Gamma_e^{5/2}} \quad (159)$$

The weak coupling limit ($\Gamma_i \ll 1$) is given here by the Debye-Hückel two component plasma (DHTCP) law. The coefficients c_k are defined by

$$c_0 = \frac{1}{\sqrt{3}} \frac{(\zeta_e + \langle Z^2 \rangle)^{3/2} - \zeta_e^{3/2} - \langle Z^2 \rangle^{3/2}}{\langle Z \rangle^{1/2} \langle Z^{5/3} \rangle^{3/2}}, \quad (160)$$

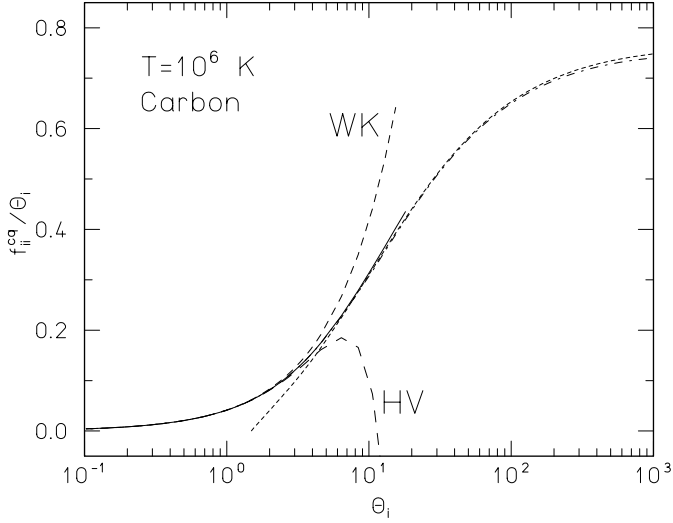


Fig. 5. The free energy contribution of the ionic quantum corrections for carbon at $T = 10^6$ K vs. ionic quantum parameter (Eq. 135). The solid line represents Nagara et al. (1987) (Eq. 137) (shown only within its validity regime), the dashed line refers to Chabrier et al. (1992), and the dashed-dotted line to Iyetomi et al. (1993). The curve labeled by WK refers to the first order in the Wigner-Kirkwood expansion and HV to Hansen & Vieillefosse (1975).

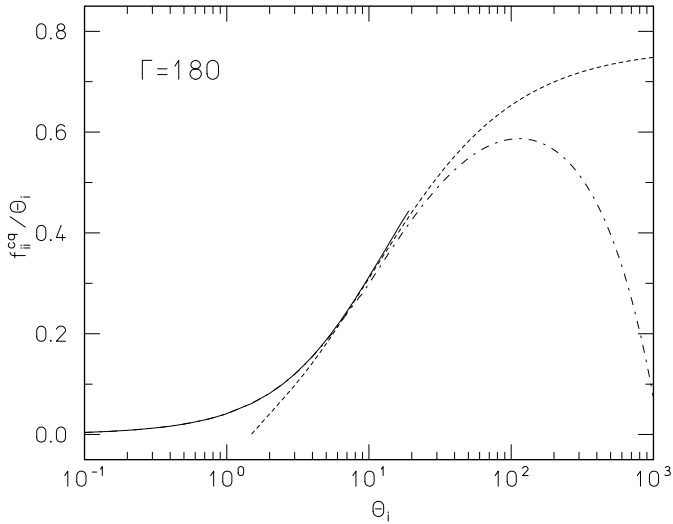


Fig. 6. The free energy contribution of the ionic quantum corrections at $\Gamma_i = 180$ vs. Θ_i . The solid line represents Nagara et al. (1987) (Eq. 137) (shown only within its validity regime), the dashed line refers to Chabrier et al. (1992), and the dashed-dotted line to Iyetomi et al. (1993).

$$c_1 = \frac{3}{2} \frac{1}{c_0 \langle Z \rangle \langle Z^{5/3} \rangle^3} \left[\frac{\sqrt{\pi\tau}}{8} \zeta_e \langle Z^2 \rangle - \sum_{ab} \zeta_a \zeta_b Z_a^3 Z_b^3 \left(\frac{Q_3(-|\xi_{ab}|)}{|\xi_{ab}|^3} - \frac{1}{6} \ln |\xi_{ab}| - C_0 \right) \right] \quad (161)$$

$$c_2 = Z r_s^{-7/4}, \quad c_3 = 0.01, \quad (162)$$

$$c_4 = (2 \cdot 1.786 - 0.9 - 0.9 \Gamma_e / \Gamma_i) \Gamma_i \quad (163)$$

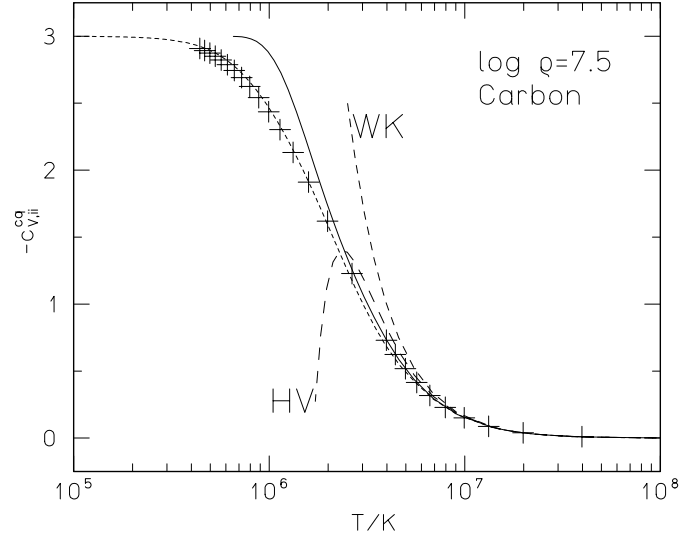


Fig. 7. The isochoric specific heat for the ionic quantum corrections for carbon at $\rho = 10^{7.5}$ g/cm³ vs. temperature. The solid line represents Nagara et al. (1987) (Eq. 147) (shown only within its validity regime), the dashed line refers to Chabrier (1993), and the crosses to Pollock & Hansen (1973). The curve labeled WK refers to the first order in the Wigner-Kirkwood expansion and HV to Hansen & Vieillefosse (1975).

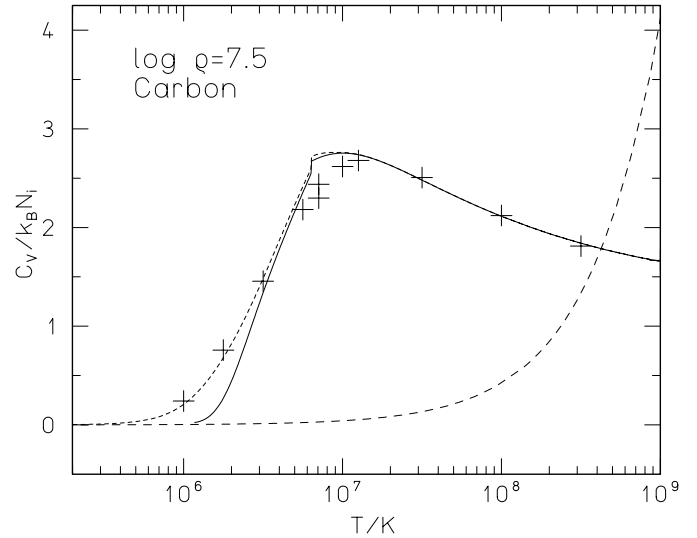


Fig. 8. The electronic and ionic parts of the isochoric specific heat for carbon at $\rho = 10^{7.5}$ g/cm³ vs. temperature. The long-dashed line represents the electronic terms of Eq. (20). The solid line (applies Nagara et al. (1987) for $c_{V,ii}^{cq}$) and the short-dashed line (applies Chabrier (1993) for $c_{V,ii}^{cq}$) represent the ionic terms of Eq. (20). The crosses refer to the ionic contribution calculated by Lamb & Van Horn (1975).

$$\xi_{ab} = -\frac{2Z_a Z_b}{\sqrt{\tau(\gamma_a + \gamma_b)}}, \quad \gamma_k = \frac{m_e}{m_k}, \quad \zeta_e = \frac{n_e}{\sum_i n_i} \quad (164)$$

In Eq. (161) is summed up over $a \neq b$ in contrast to summations made in earlier approaches (Ebeling 1993, paper I). For $\varepsilon_{ie}(r_s, \Gamma_i)$ we apply the expression given by Ebeling & Richert (1985), which consider the high density/large coupling-

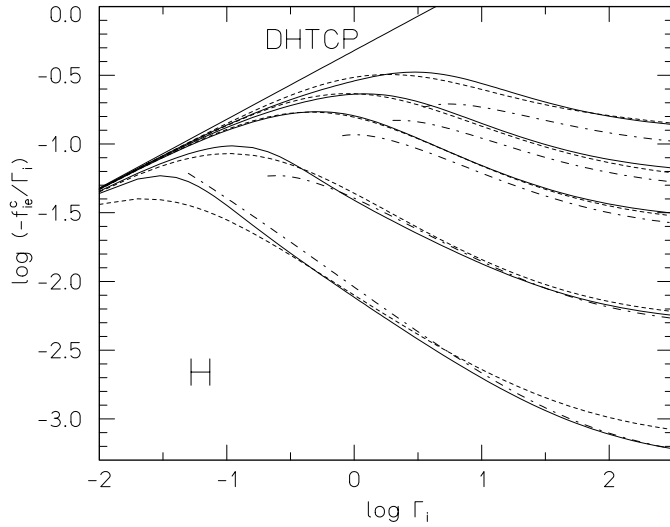


Fig. 9. The free energy contribution of the screening contribution for hydrogen and densities referring to $r_s = 2, 1, 0.5, 0.1, 0.01$ (from top to bottom) compared with the Debye-Hueckel limiting law (DHTCP) (the first term in the nominator of Eq. (159)) and the high density/large coupling-asymptotics from Galam & Hansen (1976) (dashed-dotted lines). The dashed lines refer to Chabrier & Potekhin (1998) and the solid lines correspond to Eq. (159).

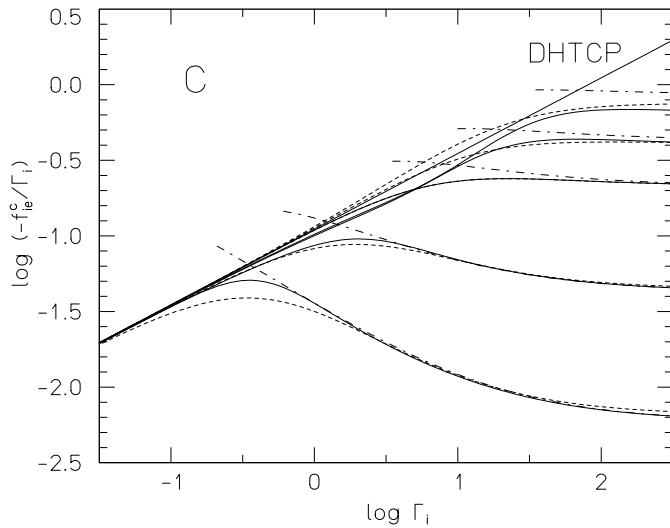


Fig. 10. The free energy contribution of the screening contribution for carbon and densities referring to $r_s = 2, 1, 0.5, 0.1, 0.01$ (from top to bottom) compared with the Debye-Hueckel limiting law (DHTCP) and the high density/large coupling-asymptotics from Galam & Hansen (1976) (dashed-dotted lines). The dashed lines refers to Chabrier & Potekhin (1998) and the solid lines correspond to Eq. (159).

asymptotics from Galam & Hansen (1976) including high-density corrections according to Kagan et al. (1977).

$$\varepsilon_{ie}(r_s, \Gamma_i) = \left(\frac{12Z}{\pi^{5/2}} \right)^{2/3} \Gamma_i r_s [\varepsilon_{ie}^0(r_s, \Gamma_i) + x^2 J(\Gamma)] \quad (165)$$

$$\varepsilon_{ie}^0 = \frac{A + C \Gamma_i^{-1}}{1 + 0.089 r_s^2} + \frac{B \Gamma_i^{-3/4}}{1 + 0.353 \Gamma_i^{-1/4}} \quad (166)$$

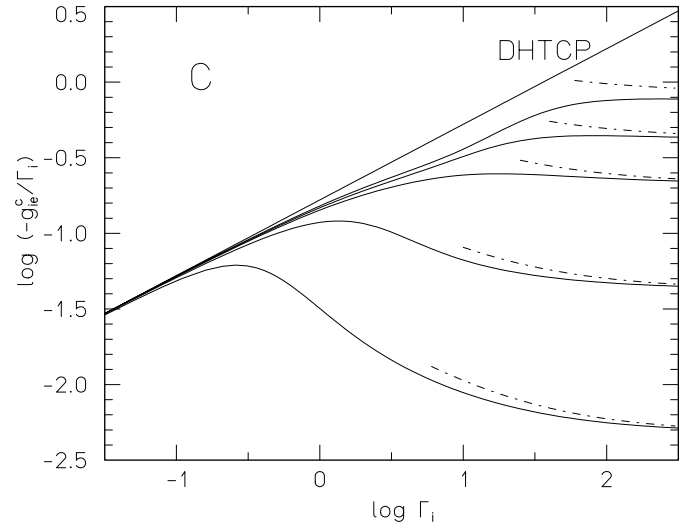


Fig. 11. The free gibbs energy contribution of the screening contribution for carbon and densities referring to $r_s = 2, 1, 0.5, 0.1, 0.01$ (from top to bottom) compared with the Debye-Hueckel limiting law (DHTCP) and the high density/large coupling-asymptotics from Galam & Hansen (1976) (dashed-dotted lines). The solid lines correspond to Eq. (167).

with the relativity parameter $x = 0.014/r_s \cdot J(\Gamma_i)$ as well as A, B and C depending on Z are given by Galam & Hansen (1976). Recently, Chabrier & Potekhin (1998) presented a Padé formula for the screening contribution of the free energy, which includes the Thomas-Fermi approximation in the limit of high densities and large coupling parameters. The results of Chabrier & Potekhin (1998) with Eq. (159) are compared for hydrogen and carbon at five densities in Fig. 9 and Fig. 10.

In the following we proceed in the same manner as in the case of the electron-electron subsystem in Sect. 4.3.1.

For the ion-electron Gibbs energy we use the Padé expression

$$g_{ie}^c = - \frac{\frac{3}{2} c_0 \Gamma_i^{3/2} + c_2 \Gamma_e^{5/2} (\varepsilon_{ie} + \frac{1}{3} (h_{ie} - d_{ie})) + c_3 c_4 \Gamma_e^{5/2}}{1 + c_1 \Gamma_i^{3/2} + c_2 \Gamma_e^{5/2} + c_3 \Gamma_e^{5/2}} \quad (167)$$

with $h_{ie} = \Gamma_i \cdot \partial \varepsilon_{ie} / \partial \Gamma_i$ and $d_{ie} = r_s \cdot \partial \varepsilon_{ie} / \partial r_s$. Fig. 11 illustrates the Gibbs energy for carbon at five densities. The polarization pressure can be determined by $p_{ie}^c = g_{ie}^c - f_{ie}^c$.

5. Numerical results and discussion

This section will be devoted to illustrate the behaviour of the adiabatic temperature gradient ∇_{ad} . The adiabatic temperature gradient is a highly sensitive quantity, because it depends on first and second-order derivations of the model Helmholtz free energy. Therefore it is well suited to test the quality of the explicit expressions derived in Sects. 3 and 4. The adiabatic gradient is a crucial ingredient for many applications. For instance, ∇_{ad} determines the Schwarzschild criterion for convective instability and an accurate evaluation is required for evolutionary calculations of very-low mass stars. We restrict our comparisons

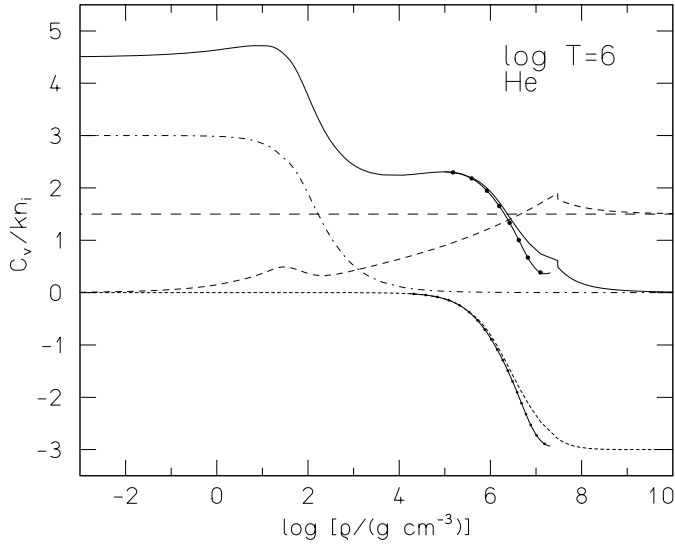


Fig. 12. Contributions of the isochoric specific heat in units of kn_i for helium at $T = 10^6$ K vs. density. The lines refer to the ideal electrons (dashed dotted) and ions (long-dashed), the exchange and correlation (dashed), the ionic quantum correction from Chabrier et al. (1992) (short-dashed), and the sum of those (solid). The curves with dots represent ionic quantum corrections after Nagara et al. (1987).

of the adiabatic temperature gradient to the EOS tables given by Straniero (1988), Saumon et al. (1995), and Rogers et al. (1996). Further detailed comparisons can be found in Saumon et al. (1995) who compared their results for ∇_{ad} with those of Fontaine et al. (1977), Däppen et al. (1988), and Magni & Mazzitelli (1979).

Fig. 12 shows the total isochoric specific heat according to Eq. (20) as well as their various single contributions (in units of $n_i k$), i.e. electronic exchange and correlation terms (electronic, ionic and screening part). We note that the discontinuity in the ionic correlation is caused by the fluid-solid phase transition at $\Gamma = 178$ (Stringfellow et al. 1990), which can also be observed for the adiabatic temperature gradient in the high-density region. The influence of quantum effects on the fluid-solid transition of the OCP is discussed in detail by Pollock & Hansen (1973), Lamb & Van Horn (1975), Nagara et al. (1987), Chabrier (1993) and Iyetomi et al. (1993). We chose for our numerical calculations $\Gamma = 178$, which is based on an simulated OCP without quantum effects (Stringfellow et al. 1990). The specific heat contribution according to the ionic correlation is monotonously increasing until the phase transition of the OCP model. The first maximum at $\log \rho \approx 1.5$ in the dashed curve in Fig. 12 is determined essentially by the electronic exchange and electronic correlation. The influence of electronic exchange and correlation increases with decreasing temperatures. Quantum effects for the specific heat according to the ions after Chabrier (1993) are illustrated by the dotted line in Fig. 12, which can be seen also in Figs. 7 and 8. This contribution is compensated at very high densities by the contributions of the ideal and the correlated ions. Considering ionic quantum corrections calculated

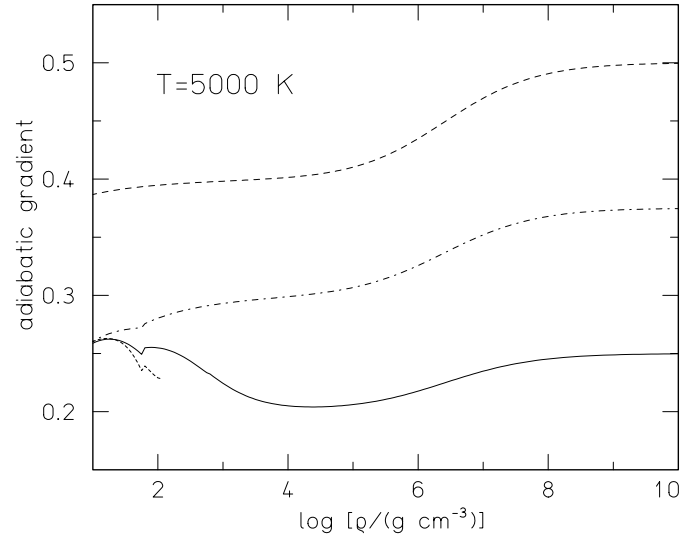


Fig. 13. High-density asymptotics of the adiabatic temperature gradient ∇_{ad} vs. density for hydrogen, demonstrated along the isotherm $T = 5 \cdot 10^3$ K. The dashed line refers to the ideal and exchange terms only. The dashed-dotted (without ionic quantum effects), the solid (with ionic quantum corrections from Chabrier et al. 1992), and the short-dashed (with ionic quantum corrections from Nagara et al. 1987) lines take into account correlations. For more explanation: see text.

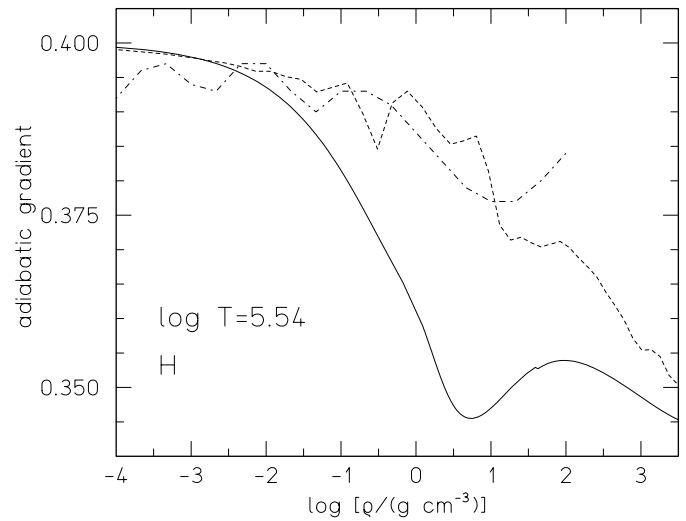


Fig. 14. Adiabatic temperature gradient ∇_{ad} (without radiation and *all* terms in Eq. (20)) for hydrogen (solid line) at $T = 10^{5.54}$ K vs. density. The dashed line refers to Saumon et al. (1995) and the dashed-dotted line to Fontaine et al. (1977).

by Nagara et al. (1987) the isochoric specific heat will be more strongly reduced as shown in Fig. 12.

We point out that the same behaviour appears for the adiabatic temperature gradient as indicated in Figs. 13 and 15-18. Note, that although the ionic quantum correction calculated by Chabrier et al. (1992) and Chabrier (1993) are valid only for the solid phase we considered here also the fluid range in order to illustrate the differences to the result of Nagara et al. (1987).

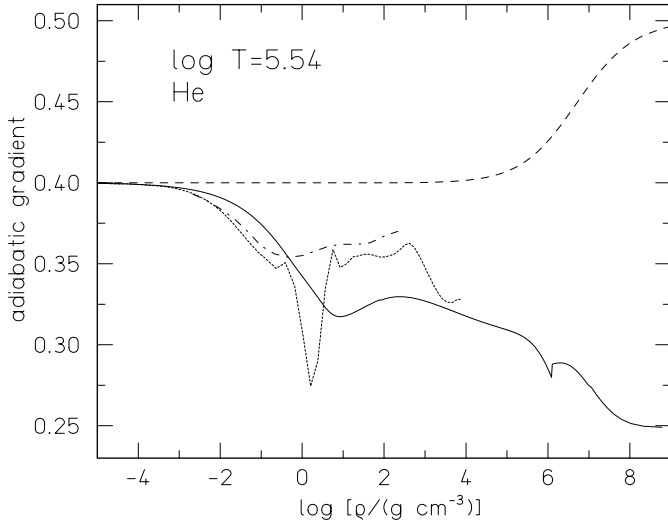


Fig. 15. Adiabatic temperature gradient ∇_{ad} (without radiation and *all* terms in Eq. (20)) for helium at $T = 10^{5.54}$ K vs. density. For the ionic quantum corrections the results from Chabrier et al. (1992) and from Nagara et al. (1987) (solid line) are used. The dotted line refers to Saumon et al. (1995) and the dashed-dotted line to Fontaine et al. (1977). The ideality (long-dashed line) is shown for comparison.

Figs. 13-20 display isotherms of the adiabatic temperature gradient evaluated on the basis our analytic expressions given in Sect. 4 including the photonic contribution (Figs. 16–20) over a broad range of densities. As already mentioned, the representations towards very high densities aimed at the purpose to show the asymptotic behaviour of the potentials given by Eq. (20). The accurate description of plasmas at very high density region requires the consideration of additional effects as electron captures and other processes (cf. Shapiro et al. 1983). Fig. 13 shows the high density asymptotics of the adiabatic temperature gradient calculated by different approximations. Considering ideal and exchange contributions we obtained the well known value $\nabla_{\text{ad}} = 1/2$, according to relativistic considerations. The limiting value $\nabla_{\text{ad}} = 3/8$ is determined by inclusion of the classical ionic correlation and $\nabla_{\text{ad}} = 1/4$ is obtained with ionic quantum corrections given by Chabrier et al. (1992). In Fig. 14-18 we compare our formalism with data from other authors (Lamb 1974, Fontaine et al. 1977, Straniero 1988, Saumon et al. 1995, Rogers et al. 1996) based on analytical as well as numerical methods and valid for various density and temperature ranges. The radiation contribution is dominant at high temperatures and low densities. The well-known limiting case of $\nabla_{\text{ad}} = 0.25$ in the low-density limit depends on the temperature in a strong manner.

The largest deviations for the adiabatic temperature gradient are observed in the intermediate density region, that means for plasma parameter where e.g. correlation effects must be described by accurate expressions. It should be emphasized that the Padé technique is well suited to meet the challenging requirements of this - sometimes poorly known - density regime.

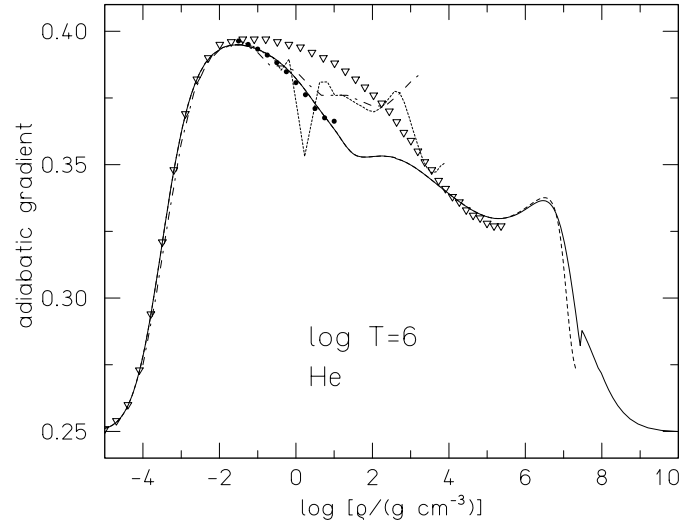


Fig. 16. Adiabatic temperature gradient ∇_{ad} (with radiation and *all* terms in Eq. (20)) for helium at $T = 10^6$ K vs. density. For the ionic quantum corrections the results from Chabrier et al. (1992) (solid line) and from Nagara et al. (1987) (short-dashed line) are used. The dotted line refers to Saumon et al. (1995), the triangles to Straniero (1988), the dashed-dotted line to Fontaine et al. (1977), and the dots to Rogers et al. (1996).

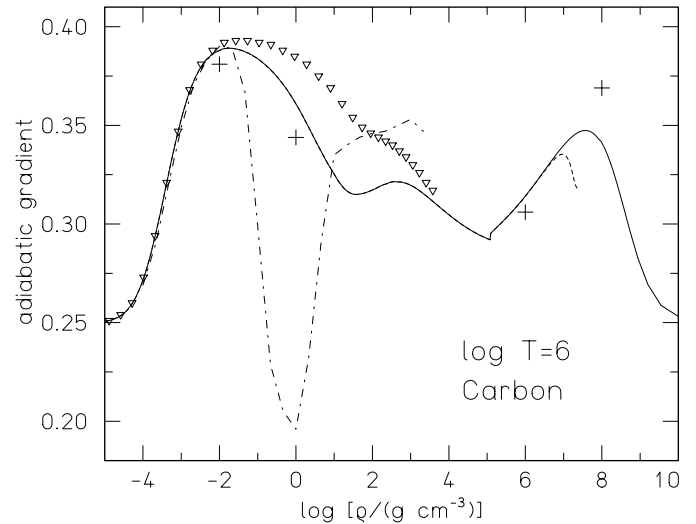


Fig. 17. Adiabatic temperature gradient ∇_{ad} (with radiation and *all* terms in Eq. (20)) for carbon at $T = 10^6$ K vs. density. For the ionic quantum corrections the results from Chabrier et al. (1992) (solid line) and from Nagara et al. (1987) (short-dashed line) are used. The triangles refers to Straniero (1988), the dashed-dotted line to Fontaine et al. (1977), and the crosses to Lamb (1974).

Fig. 19 shows the adiabatic temperature gradient for helium. In Fig. 20 we draw ∇_{ad} for a mixture of carbon and oxygen at high temperatures as appropriate for white dwarf interiors.

The temperatures and densities are chosen here according to the conditions for a fully ionized plasma. Nevertheless, our EOS-formalism can be applied for the conditions of a partially ionized plasma (lower temperatures) provided additional terms in Eq. (20) are considered and are solved in connection with

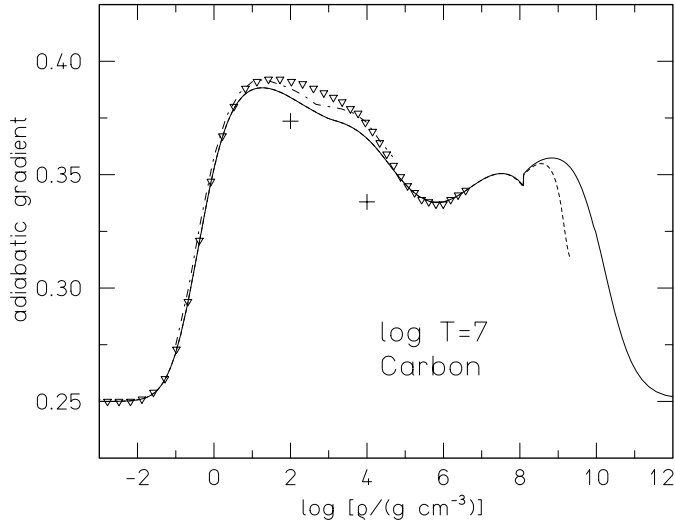


Fig. 18. Adiabatic temperature gradient ∇_{ad} (with radiation and *all* terms in Eq. (20)) for carbon (solid line and short-dashed lines) at $T = 10^7$ K vs. density. For the ionic quantum corrections the results from Chabrier et al. (1992) (solid line) and from Nagara et al. (1987) (short-dashed line) are used. The triangles refers to Straniero (1988), the dashed-dotted line to Fontaine et al. (1977), and the crosses to Lamb (1974).

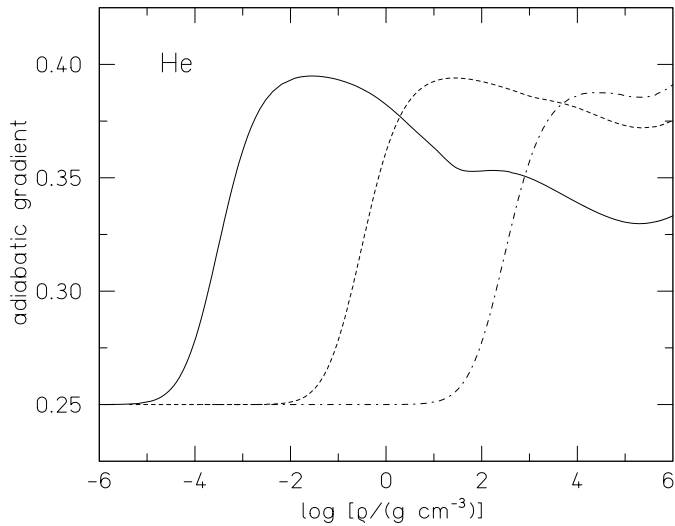


Fig. 19. Adiabatic temperature gradient ∇_{ad} (with radiation and *all* terms in Eq. (20)) for helium along the isotherms $T = 10^6$ (solid), 10^7 (dashed), and 10^8 K (dashed-dotted) vs. density.

the formalism of the dissoziation- and ionization equilibrium (Beule et al. 1999).

6. Summary

Our aim was to provide data for the thermodynamical potentials summarized in Eq. (20) which are applicable to, e.g., stellar interiors (fully ionized regions). For the Helmholtz free energy, the Gibbs free energy, and the pressure (equation of state), expressions for each term in Eq. (20), i.e. ideality, exchange and correlation, have already been presented in paper I. In this pa-

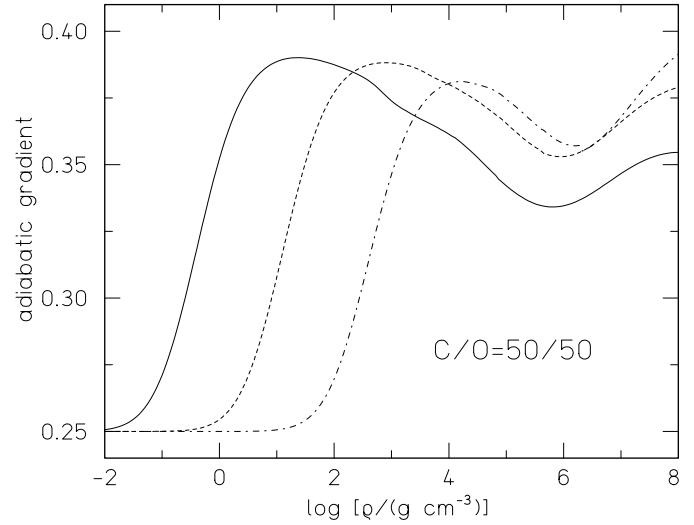


Fig. 20. Adiabatic temperature gradient ∇_{ad} (with radiation and *all* terms in Eq. (20)) for a mixture of C/O=50/50 (mass fractions) along the isotherms $T = 10^7$ (solid), $10^{7.5}$ (dashed), and 10^8 K (dashed-dotted) vs. density.

per we have improved our Padé Approximants for the correlation contributions and continued to present formulae for the explicit calculation of the internal energy, reciprocal compressibility (bulk modulus), coefficient of strain, and the specific heat. Further results using our calculational concept for the adiabatic temperature gradient for fully ionized plasmas are presented by Stolzmann & Blöcker (1998). The extension of our formalism to the partially ionized region is in progress.

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