A Semi-relativistic Equation of State for Stellar Interiors

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Abstract

Using the technique of Padé Approximants for the correlation contributions of charged particles we are able to reproduce complex mathematical expressions by simple algebraic formulas. The Padé formulas are analytical expressions, which interpolate between certain density-temperature regions and are characterized by exact asymptotics. We present a semi-relativistic description of the thermodynamics applicable for stellar interiors. Comparisons with equation-of-state data obtained by other calculational schemes are presented.

1. Introduction

The equation of state (EOS) formalism for astrophysical applications requires an accurate calculation of the non-ideal effects in plasmas over a wide range of densities and temperatures. Many successful efforts have been made to provide EOS-tables which are applicable to describe thermodynamical properties of stellar matter. However, detailed comparisons of quantities composed of second-order derivatives of the free Helmholtz energy (e.g. specific heat, adiabatic temperature gradient) reveal considerable discontinuities (see, e.g., [3]). We present an EOS-formalism which avoids such numerical deviations and is well suited for example to evaluate the thermodynamics of stellar interiors.

2. Thermodynamical Functions

We start with the thermodynamical description of a fully ionized plasma

\[
\Sigma = N_e kT \left[ \sigma_{i e}^\text{id} + \sigma_{i e}^\text{x} + \sigma_{i e}^\text{c} \right] + N_i kT \left[ \sigma_{i i}^\text{id} + \sigma_{i i}^\text{q} + \sigma_{i i}^\text{c} \right],
\]

(1)

where \(\Sigma = \{F,G, PV, U, V/K_T, \Phi_S V, C_V T\}\) and \(\sigma = \{f,g,p,u,1/k_T, \phi_S, c_V\}\) symbolize the various thermodynamical functions, as the free Helmholtz energy \(F\), free Gibbs energy \(G\), pressure \(P\), internal energy \(U\), inverse isothermal compressibility \(1/K_T\), strain coefficient \(\Phi_S\), and isochoric specific heat \(C_V\). Quantities given by small letters are the corresponding potentials normalized to \(N_e k_B T\). Terms labeled by id, x, and c denote contributions due to ideality, exchange, and correlation contributions of the plasma species \(a = e, i\). The term labeled by eq takes into account quantum effects of ions.

Furthermore we have to determine the isobaric specific heat \(C_P\) by the relation

\[
\gamma = \frac{C_P}{C_V} = 1 + \frac{V K_T^2}{T C_V} \Phi_S^2, \quad \frac{1}{K_T} = P \chi_\rho = -V \left( \frac{\partial P}{\partial V} \right)_T, \quad \Phi_S = P \chi_T = T \left( \frac{\partial P}{\partial T} \right)_V.
\]

(2)

\(\chi_\rho\) and \(\chi_T\) are the density and temperature exponents in the EOS-formalism. The adiabatic temperature gradient defined by \(\nabla_{ad} = (\partial \ln T/\partial \ln P)_S\) (\(S\) is the entropy) is given by

\[
\nabla_{ad} = \frac{PV}{C_P T} \frac{\chi_T}{\chi_\rho} = \frac{PV}{C_P T} K_T \Phi_S = \frac{\Gamma_2 - 1}{\Gamma_2} = \frac{\Gamma_3 - 1}{\Gamma_1},
\]

(3)
with the adiabatic exponents $\Gamma_1 = \gamma/\text{PK}_T$, $\Gamma_2 = \gamma/(\gamma - \text{PK}_T\gamma_G)$ and $\Gamma_3 = 1 + \gamma_G$, and the generalized Grüneisen coefficient $\gamma_G = V\Phi_S/TC_V$.

The ideal and exchange contributions, $\sigma^\text{id}_e$ and $\sigma^\text{ex}_e$, are calculated in a relativistic approach, which covers the two approximations: a) arbitrary degeneracy ($\psi$) and weak relativity ($\lambda < 1$) and b) strong degeneracy ($\psi > 1$) and arbitrary relativity ($\lambda = kT/mc^2$). Details are given for the free Helmholtz energy, free Gibbs energy, and pressure in [4].

The correlation terms $\sigma^\text{cor}_e$, $\sigma^\text{ii}_e$, and $\sigma^\text{ii}_e$ are taken into account by Padé approximants which are modified versions of those given in [9]. The new Padé approximants are determined by a rearrangement of the quantum virial function which is dominant in the weakly coupled regime. Moreover the Padé formula for the ion-electron subsystem is extended by linear $\Gamma$-asymptotics for the classical region [11]. The ionic quantum correction $\sigma^\text{ii}_e$ is described by [11].

In this paper we present our new Padé approximant for the ion-ion correlation. Starting with the free energy the complete set of the quantities summarized by $\sigma^\text{ii}_e$ will be given. We mention that the Padé formulas for the quantities related by the first and second order derivatives of the free energy are constructed from the analytical limiting laws, which are known to be asymptotically exact. The intermediate region will be fitted by new parameters. Of course, the quality of this procedure with regard to the thermodynamic consistency is determined by comparisons with the numerical data produced from corresponding theories. The advantage is that the Padé approximants for our set of thermodynamic functions are expressed by their correct asymptotics, which cover a wide parameter-region.

For the ion subsystem we use the new formulas for the free Helmholtz- and Gibbs energy with $\Gamma_1 = (2^5/3)e^2(4\pi n_e/3)^{1/3}/k_BT$,

$$f_e^\text{ii} = -\frac{b_0\Gamma_1^{3/2} \left[ 1 + b_3\Gamma_1^{3/2} \left( \ln \Gamma_1 + B_0 \right) \right] + b_2\Gamma_1^6\varepsilon_{\text{ii}}(\Gamma_1)}{1 - b_1\Gamma_1^3 \left( \ln \Gamma_1 + B_1 \right) + b_2\Gamma_1^6}$$ (4)

$$g_{\text{ii}}^e = -\frac{t_0\Gamma_1^{3/2} \left[ 1 + t_3\Gamma_1^{3/2} \left( \ln \Gamma_1 + B_0 + \frac{1}{6} \right) \right] + t_2\Gamma_1^6\mu_{\text{ii}}(\Gamma_1)}{1 - t_1\Gamma_1^3 \left( \ln \Gamma_1 + B_1 + \frac{2}{15} \right) \left[ 1 + \frac{2}{3}\Gamma_1^{3/2} \right] + t_2\Gamma_1^6}$$ (5)

with

$$B_0 = \frac{2}{3} \left( 2C_E + \frac{3}{2} \ln 3 - \frac{11}{6} \right), \quad B_1 = \frac{2}{3} \left( 2C_E + \frac{1}{2} \ln 3 + 2 \ln 2 - \frac{17}{6} \right) - 0.4765$$ (6)

and the coefficients $b_0 = 1/\sqrt{3}, b_1 = 3\sqrt{3}/8b_0$, $b_2 = 100$, $b_3 = b_1/\sqrt{3}$, and $t_0 = 3b_0/2$, $t_1 = 5b_1/3$, $t_2 = b_2$, $t_3 = 4b_3/3$. Eq. (4) is based on the classical $\Gamma_1 < 1$ result from Cohen and Murphy [12] and for $\Gamma_1 \geq 1$ we take into account the Monte-Carlo fits for the free energy $\varepsilon_{\text{ii}}(\Gamma_1)$ of the liquid and solid one-component plasma (OCP) from Stringfellow et al. [13].

The internal energy, the compressibility, and the strain coefficient are determined by [14]

$$u_{\text{ii}}^e = 3 p_{\text{ii}}^e = 3 \left( g_{\text{ii}}^e - f_{\text{ii}}^e \right),$$ (7)

$$\frac{1}{k_{\text{Tii}}^e} = -\frac{1}{9} c_{\text{Vii}}^e + \frac{4}{9} u_{\text{ii}}^e, \quad \phi_{\text{ii}}^e = \frac{1}{3} c_{\text{Vii}}^e.$$ (8)

Note, that a factor $1/3$ is missing in the second term of $1/k_{\text{Tii}}^e$ given by Hansen [14].

For the isochoric specific heat we apply the Padé approximant

$$c_{\text{Vii}}^e = \frac{q_0\Gamma_1^{3/2} \left[ 1 + q_3\Gamma_1^{3/2} \left( \ln \Gamma_1 + B_0 + \frac{5}{6} \right) \right] + q_2\Gamma_1^6\sigma_{\text{ii}}(\Gamma_1)}{1 - q_1\Gamma_1^3 \left( \ln \Gamma_1 + B_1 + \frac{2}{15} \right) \left[ 1 + \frac{2}{3}\Gamma_1^{3/2} \right] + q_2\Gamma_1^6}$$ (9)
with the coefficients \( q_0 = 3b_0/4 \), \( q_1 = 7b_1 \), \( q_2 = 5b_2 \), \( q_3 = 8b_3 \).

\[
\mu_{ii}(\Gamma_i) = \varepsilon_{ii}(\Gamma_i) + \frac{1}{3} \Gamma_i \frac{d\varepsilon_{ii}(\Gamma_i)}{d\Gamma_i}, \quad \rho_{ii}(\Gamma_i) = \Gamma_i^2 \frac{d^2\varepsilon_{ii}(\Gamma_i)}{d\Gamma_i^2}.
\]  

(10)

3. Results and Discussion

In Fig. 1 our new Padé approximants for the internal energy (7) and the isochoric specific heat (9) are compared with other closed-form parametrizations [14, 15, 16]. Obviously, the internal energy is already covered by the asymptotic theories given in [12, 13] over a wide \( \Gamma_i \)-region. A detailed comparison between [15] and the simplified fit formula from Chabrier and Potekhin [16] was carried out by Potekhin [17] recently. Comparisons between the internal energy derived from our earlier Padé approximants for the free energy [9, 18] and a new fit formula from Chabrier and Potekhin [16] are shown in [16]. It is noteworthy, that our former Padé approximant for \( f_{ii}^c \) proposed by Ebeling [18] contains ionic quantum corrections, which deliver in the classical limit the result of Abe [19]. The inclusion of quantum effects (see [9], the coefficient \( b_1 \) in Eq. (65)) implies an additional temperature-dependence besides the pure \( \Gamma \)-dependence. Accordingly, the determination of thermal quantities such as internal energy, strain coefficient, or specific heat from the former Padé formula for \( f_{ii}^c \) must be carried out carefully. Non-thermal derivatives such as pressure did not suffer from this drawback as shown in [9].

In our new calculational scheme all ionic quantum corrections are considered separately. As shown in Fig. 1 the classical interpolation formulas are well in agreement.

Fig. 2 illustrates the course of the adiabatic temperature gradient, \( \nabla_{ad} \), calculated by our new Padé approximants and gives comparisons with numerical results from other authors [16, 14, 20]. \( \nabla_{ad} \) is a highly sensitive quantity, because it depends on first and second-order derivatives of the model free Helmholtz energy as given by Eq. (3). The low-density limes of \( \nabla_{ad} = 0.25 \) (right panel) is a consequence of the photonic contribution in contrast to Fig. 1 (left panel).

We have shown how by means of analytical expressions (see also [9, 10]) the thermodynamics of e.g. stellar interiors can be described over a wide range of densities and temperatures.
Fig. 2: Adiabatic temperature gradient $\nabla_{\text{ad}}$ vs. density for helium at $T = 10^{5.54}$ K without radiation \textit{(left)} and for carbon at $T = 10^{7}$ K with radiation \textit{(right)}. Note, that the discontinuities at $\log \rho \approx 6$ \textit{(left)} and $\log \rho \approx 9$ \textit{(right)} are caused by the fluid-solid phase transition at $\Gamma = 178$ \cite{13}. The solid curves refer to Eqs. \textit{(3)}, \textit{(2)}, \textit{(1)} and the dashed-dotted to \cite{1}. \textit{Left:} The dotted line refers to \cite{6}. For comparision is shown the ideality (long-dashed line). \textit{Right:} The dashed line refers to \cite{21} and the crosses to \cite{20}. Our analytical description leads to a smooth course of $\nabla_{\text{ad}}$ and avoids any numerical noise. Further comparisions are given in detail by \cite{22}.

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