Appl. Phys. B 52, 230–233 (1991)

Applied Physics B Photophysics and Laser Chemistry

Energy Equation of State' of High-Density Plasmas

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Received 20 July 1990/Accepted 14 September 1990

Abstract: The equation of state for fully degenerate high-density plasmas is derived using a modified Thomas-Fermi model. Although the classical TF model is adequate to obtain the energy of an atom at very high densities it fails for low densities. A new version of this model for plasmas is presented which addresses this deficiency by including near-nucleus, exchange and correlation corrections. An analytic formula for the equation of state $E(n_i)$ is obtained, valid for all densities ($n_i < 10^{26}$ cm^{-3}). For low densities, Hartree-Fock results are reproduced with less than 1% error, and the classical result is recovered in the high-density limit.

PACS: 31.20Lr, 52.25Kn, 64.10+h

Recently, various experiments have produced high-density plasmas, using, for example, high-energy lasers, particle beams and Z-pinches. High-density is important for inertial confinement fusion experiments as well as in connection with the irradiation of matter by short pulses, ($\simeq$fs). In nature, such densities exist inside planets and stars.

An essential requirement for the analysis of high-density experiments is the equation of state (EOS), which is usually the pressure p or the energy E as a function of density and temperature. In this paper only the fully degenerate or *temperature-independent* energy of the electrons is investigated; this means

$$n_i \geqq 1.4 \times 10^{23} \frac{1}{Z} \left(\frac{kT}{10\,\mathrm{eV}} \right)^{3/2} . \tag{1}$$

In the case of dense plasmas a strong interaction of the ions exists, i.e. the orbits of neighbouring atoms overlap and conducting bands occur. This lowers the binding energy of the electrons, and the energy gap between free and bound electrons decreases, which in turn leads to the lowering of the ionization potentials. If the density is high enough, this can lead to ionization, i.e. pressure ionization.

The Thomas-Fermi (TF) model [1] is used to describe atoms in high-density matter, because in contrast to Hartree-Fock calculations it enables one to investigate the influence of high density in high-Z atoms with relatively little effort. The main problems with numerical simulations using the TF equation occur at low densities and temperatures, because quantum effects are always significant in regions near the nucleus, and on the periphery of the isolated atom. Thus the application of the simple TF model to the calculation of the total energy of a heavy atom will actually lead to substantial errors. Attempts have been made to improve the results by taking into account exchange and correlation effects. The results are not very satisfactory because these effects lead to corrections in the outer region of the atom, but the energy is dominated by the behaviour near the nucleus. Schwinger improved the TF model for free atoms in this region [2]. A comparison of the energy of the free atom calculated by i) TF, ii) TF with two corrections proposed by Schwinger, and iii) measured values, will show that for high-Z atoms the Schwinger equation with both corrections approximates the Hartree-Fock results with less than 1% error. Because the TF model with corrections is an adequate method for free atoms, this result implies that a similiar near-nucleus correction should improve the energy results in the case of dense plasmas too.

In Sect. 2 the energy is calculated using near-nucleus as well as exchange and correlation corrections for high-density matter. An analytic formula for the density dependence of the energy of atoms is obtained, which can be used over a large range of densities.

1. Energy in the Thomas-Fermi Model

The statistical model for atomic electrons was originally derived by Thomas [3] and Fermi [4] to investigate free

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many-electron atoms. Later on it was shown [1] that the model could be used in the case of high-density plasmas, too.

The statistical theory of the atom is based on the assumption that the electrons of the system can be treated as a degenerate electron gas within a self-consistent electrostatic field. The electron gas is described by Fermi-Dirac statistics, which in the case of full degeneracy, see (1), reduces to the Pauli principle. In this paper only the temperature-independent case will be considered. If all effects other than the electrostatic interaction can be neglected, the energies of the atoms and ions are given by: the kinetic energy E_{kin}; the potential energy of the electron gas in the potential field of the core E_{p}^{V}; and the energy of the electrostatic interaction E_{p}^{WW}. Thus

$$E = E_{\text{kin}} + E_{\text{p}}^{\text{V}} + E_{\text{p}}^{\text{WW}} \tag{2}$$

$$= C_1 \int n_{\text{e}}^{5/3} d^3r - e\int V n_{\text{e}} d^3r + \frac{e^2}{2}\iint \frac{n_{\text{e}}(r) n_{\text{e}}(r')}{|r-r'|} d^3r d^3r', \tag{3}$$

where $C_1 = \frac{3}{10}(3\pi^2)^{2/3} e^2 a_o$ and n_{e} is the electron density. Using the Thomas-Fermi equation

$$\Phi'' = \frac{\Phi^{3/2}}{x^{1/2}} \tag{4}$$

with $x = r/\mu$, $C_2 = \frac{8\pi}{3}\left(\frac{2me}{h^2}\right)^{3/2}$, $\mu = [(4\pi C_2)^{2/3} e Z^{1/3}]^{-1}$ and $\Phi = r(V - V_o)/Ze$ and boundary conditions as for atoms in plasmas $\Phi(0) = 1$; and $\Phi(x_o) - x_o \Phi'(x_o) = 0$, where x_o is the boundary of the elementary cell, the electron density is then given by

$$n_{\text{e}}(r) = \frac{Z}{4\pi\mu^3}\left(\frac{\Phi(x)}{x}\right)^{3/2}. \tag{5}$$

Eliezer et al. [5] have shown that the energy of the atom in a plasma using the TF model is

$$E_{\text{AP}} = -\frac{Z^2 e^2}{\mu}\left[-\frac{3}{7}\Phi'(0) + \frac{2}{35} x_o^{1/2} \Phi_o^{5/2}\right], \tag{6}$$

where Φ_o is the abbreviated notation for $\Phi(x_o)$. Approximation formulae for $\Phi(x_o)$ and $\Phi'(0)$ are given by March [6].

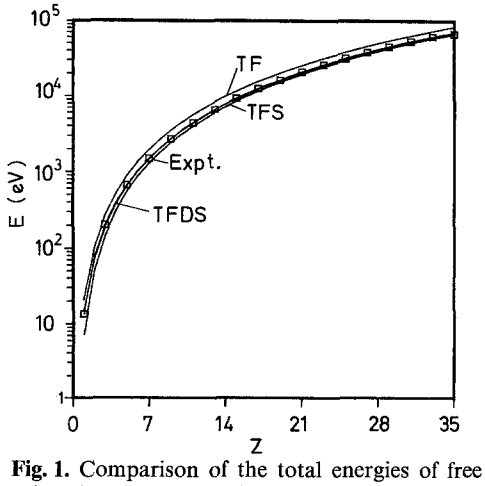

Fig. 1. Comparison of the total energies of free atoms calculated using the TF, TFS, and TFDS model and experimental data as a function of the atomic number Z

2. Energy Corrections

It has been shown [7–9] that the TF model is an adequate description at very high densities ($> 10^{25}$ cm^{-3}), but its use at low densities ($\simeq$ solid density) is problematic. What are the deficiences of the TF model in this region?

In the case of free atoms Schwinger [2] and Englert [10, 11] have shown that the TF model fails because of:

(a) the inner region of strong binding. The basic point of this correction is that the TF description is valid only when the wavelength of the particle is small compared to the radial distance, $\hbar/p \ll r$, which leads to $x \gg Z^{-2/3}$. So for a given x the TF model is only reliable if Z is large enough or, alternatively, there is a inner region where the TF approximation fails.

(b) the neglect of all interactions other than electrostatic. For a more detailed description of the electrons, the exchange and correlation corrections have to be taken into account.

Because of the strong binding energies of the electrons near the nucleus, the first of these is the more important. The energy in the corrected model is given by

$$E_{\text{TFSD}} = E_{\text{TF}} \cdot (1 - 0.6505 Z^{-1/3} + 0.346 Z^{-2/3}). \tag{7}$$

Figure 1 compares the results using the simple TF, the TF with corrections (a) and (b), and experimental data [12] for the energies for free atoms of different Z.

For low-Z elements the error of the simple TF model is up to 25%. A comparison with energies obtained by the TF model with the two Schwinger corrections shows that for $Z > 20$ the discrepancy is less than 1%.

We now consider similar corrections for atoms in high-density plasmas.

2.1. Leading Correction

Scott [13] was the first to present the leading correction of the TF energy. As shown before, the TF model is only valid if $x \gg Z^{-2/3}$. There have been different attempts to improve the result by including a gradient correction. Here a different method is used to avoid the unphysical behaviour of the electron number density at small x. Similar to Schwinger's treatment of free atoms, the integration is stopped at a lower limit $\simeq Z^{-2/3}$. To analyze the density dependence of the energy, the integrals of (3) are solved within different limits.

$$E_{\text{kin}} = -\frac{3}{5}\frac{e^2}{a_o}\frac{(2Z)^{7/3}}{(3\pi)^{2/3}} \int_{\sim Z^{-2/3}}^{x_o} \frac{\Phi^{5/2}}{x^{1/2}} dx$$

$$= \frac{3}{5}\frac{e^2}{a_o}\frac{(2Z)^{7/3}}{(3\pi)^{2/3}}\left(\int_0^{x_o} \frac{\Phi^{5/2}}{x^{1/2}} - \int_0^{\sim Z^{-2/3}} \frac{\Phi^{5/2}}{x^{1/2}}\right) dx \tag{8}$$

with

$$\int_0^{\sim Z^{-2/3}} \frac{\Phi^{5/2}}{x^{1/2}} dx \simeq \int_0^{\sim Z^{-2/3}} \frac{1}{x^{1/2}} dx = C_3 Z^{-1/3}. \tag{9}$$

For moderate densities, $C_3 = 1.03$ as in Schwinger's calculation for the free atom. At high densities C_3 is a function of the density too. Here, and in what follows, it is

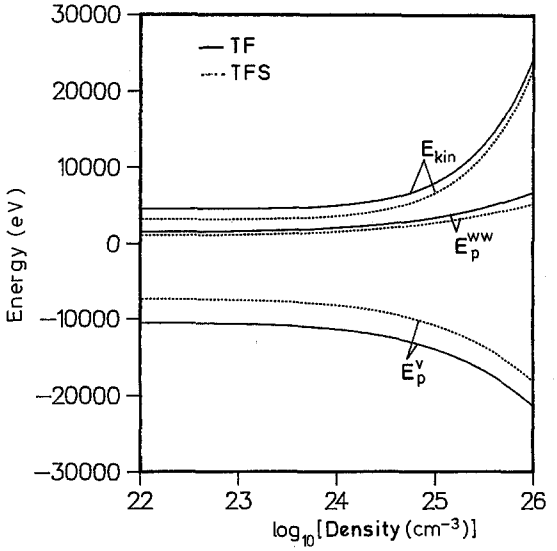

Fig. 2. Comparison of the density dependence of E_{kin}, E_p^V, and E_p^{WW} using the TF and the Thomas-Fermi model with generalized Schwinger correction (TFS)

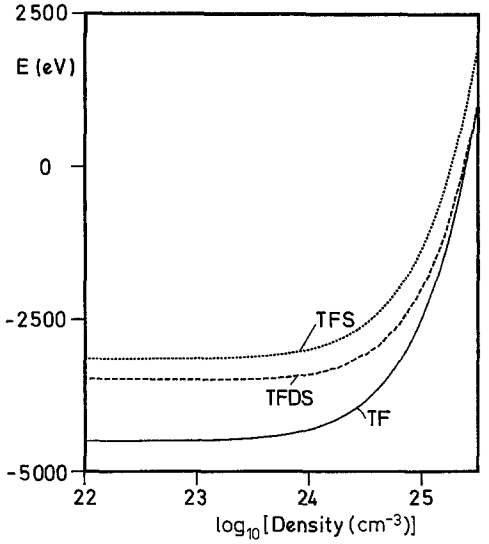

Fig. 3. Comparison of the density dependence of the total energy of an atom using the TF, Thomas-Fermi model with generalized leading (TFS) and exchange and correlation (TFDS) correction

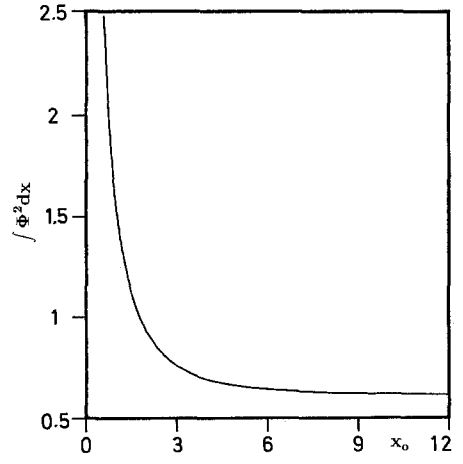

Fig. 4. Numerical solution of (16) as a function of x_o

assumed that $\Phi(x)=1$ near the nucleus. The kinetic energy of ions in high density plasmas is given by

$$E_{kin}=\frac{3}{7}\frac{e^2}{a_o}\frac{(2Z)^{7/3}}{(3\pi)^{2/3}}\left(-\Phi'+\frac{4}{5}x_o^{1/2}\Phi_o^{5/2}-C_3Z^{-1/3}\right). \quad (10)$$

The potential energies are given by

$$E_p^V=-\frac{Z^2e^2}{\mu}\int_{\sim Z^{-2/3}}^{x_0}\frac{\Phi^{3/2}}{x^{1/2}}dx$$
$$=-\frac{Z^2e^2}{\mu}\left(\frac{\Phi_o}{x_o}-\Phi'(0)-C_3Z^{-1/3}\right), \quad (11)$$

$$E_p^{WW}=-\frac{e}{2}\int_{\sim Z^{-2/3}}^{r_o}n_e(r)\left(V(r)-\frac{Ze}{r}\right)d^3r$$
$$=-\frac{Z^2e^2}{\mu}\left\{\frac{1}{7}[\Phi'(0)+C_3Z^{-1/3}]+\frac{2}{7}x_o^{1/2}\Phi_o^{5/2}\right.$$
$$\left.+\frac{\Phi_o}{x_o}\left(1-\frac{1}{3Z}\right)\right\}. \quad (12)$$

Figure 2 shows a comparison of these energies calculated by using the simple TF equation and the TF equation with the first correction.

The total energy is then given by

$$E=\frac{3}{7}\frac{e^2}{a_o}\frac{(2Z)^{7/3}}{(3\pi)^{2/3}}$$
$$\times\left[\Phi(0)+\frac{2}{5}x_o^{1/2}\Phi_o^{5/2}-C_3Z^{-1/3}-\frac{\Phi_o}{x_o}\frac{7}{9Z}\right]. \quad (13)$$

Figure 3 shows a comparison between the TF and the (TFS) result of (13). As expected the main difference occurs at low densities.

2.2. *TFS with Exchange and Correlation Corrections*

Like the Thomas-Fermi model, the TFS model can be improved by taking into account exchange and correlation corrections. The exchange energy is the effect of the antisymmetrization of the electron wavefunctions on the electrostatic interaction energy. This additional energy E_{ex} is [14]

$$E_{ex}=-\frac{e^2}{4\pi^3}(3\pi^2)^{4/3}\int n^{4/3}d^3r, \quad (14)$$

which, using the TF equation, is given by

$$E_{ex}=-\frac{e^2}{a_o}Z^{5/3}\left(\frac{3^2}{2\pi^4}\right)^{1/3}\int\Phi^2dx=-0.3588\frac{e^2}{a_o}Z^{5/3}\int\Phi^2dx. \quad (15)$$

Solving the integral

$$\int_0^{xo}\Phi^2dx \quad (16)$$

numerically, one obtains Fig. 4. The correlation energy E_c is of the same order as the exchange correction. Englert

and Schwinger [10] have shown that

$$E_c = \frac{2}{9} E_{ex}. \tag{17}$$

Therefore, the total correction term is

$$E_\Delta = -0.438 \frac{e^2}{a_o} Z^{5/3} \int \Phi^2 dx. \tag{18}$$

Figure 3 also includes the result of the TF equation including all corrections. So the energies in these three models are given by

$$E_{TF}(n_i) = 1.195 Z^{7/3} \frac{e^2}{a_o} \left[\frac{3}{7} \Phi'(0) - \frac{2}{35} x_o^{1/2} \Phi^{5/2} \right]$$

$$E_{TFS}(n_i) = 1.195 Z^{7/3} \frac{e^2}{a_o} \left[\frac{3}{7} \Phi'(0) - \frac{2}{35} x_o^{1/2} \Phi^{5/2} + \frac{3}{7} C_3 Z^{-1/3} - \frac{\Phi_o}{x_o} \frac{1}{3Z} \right]$$

$$E_{TFDS}(n_i) = 1.195 Z^{7/3} \frac{e^2}{a_o} \left[\frac{3}{7} \Phi'(0) - \frac{2}{35} x_o^{1/2} \Phi^{5/2} + \frac{3}{7} C_3 Z^{-1/3} - \frac{\Phi_o}{x_o} \frac{1}{3Z} - Z^{-2/3} \int \Phi^2 dx \right]. \tag{19}$$

For low densities the result reproduces the Schwinger equation, which means that our result is in good agreement with Hartree-Fock results too. In the case of high densities it reproduces the standard TF results.

3. Conclusions

In this paper the TF model has been modified by including near-nucleus, exchange and correlation corrections for fully degerate high-density plasmas. This model has been used to calculate the energy equation of state, from which we obtain the following:

- Hartree-Fock results are repruduced to within 1% for low densities
- the classical TF model is recovered in the high-density limit ($n_i > 10^{24}\,\mathrm{cm}^{-3}$)
- the equation of state can be expressed by a simple analytic expression (suitable for insertion into fluid codes)

This method could be extended with little effort to the temperature-dependent case.

Acknowledgement. The author wishes to thank Prof. P. Mulser for stimulating this work through many discussions.

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