RELATIVISTIC THOMAS-FERMI MODEL AT FINITE TEMPERATURES

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We briefly review the Thomas-Fermi statistical model of atoms in the classical non-relativistic formulation and in the generalised finite-nucleus relativistic formulation. We then discuss the classical generalisation of the model to finite temperatures in the non-relativistic approximation and present a new relativistic model at finite temperatures, investigating how to recover the existing theory in the limit of low temperatures. This work is intended to be a propedeutical study for the evaluation of equilibrium configurations of relativistic “hot” white dwarfs.

1 Introduction

The Thomas-Fermi statistical model of the atom has been extensively used, since its early formulation in 1927

We first consider the simple Thomas-Fermi model. Let us consider the spherically symmetric problem of a nucleus with Z protons and A nucleons interacting with a fully degenerate gas of Z electrons.
The fundamental equation of electrostatics for this problem is

\[ \Delta V(r) = 4\pi en_e(r) \]  

(1)

where \( V(r) \) is the electrostatic potential and \( n_e(r) \) is the number density of electrons.

The electrostatic potential is related to the Fermi momentum (and thus to the number density of electrons) by the equilibrium condition (see [1])

\[ p_F^2(r)/2m - eV(r) = \text{const} \equiv E_F \]  

(2)

where the name \( E_F \) stands for Fermi-Thomas chemical potential or Fermi Energy of the electrons.

To put the equation in adimensional form we introduce the new function \( \Phi(r) \), related to the coulomb potential by

\[ \Phi(r) = V(r) + E_F/e \]  

(3)

and the corresponding adimensional function \( \chi \), implicitly defined by

\[ \Phi(r) = Ze\chi \]  

(4)

Furthermore we introduce the new independent variable \( x \), related to the radius \( r \) by the relation \( r = bx \), where

\[ b = (3\pi)^{2/3} \frac{\hbar^2}{me^2} \frac{1}{2^{7/3}} \frac{1}{Z^{1/3}} \]  

(5)

It is easy to show that in this case one can write eq.1 in the form

\[ \frac{d^2\chi}{dx^2} = \frac{\chi^{3/2}}{x^{1/2}} \]  

(6)

which is the classical adimensional form of the Thomas-Fermi equation.

The first initial condition for this equation follows from the request that approaching the nucleus one gets the ordinary Coulomb potential

\[ \chi(0) = 1 \]  

(7)

The second condition comes from the normalisation condition

\[ N = \int_0^{\tau_0} 4\pi n_e r^2 dr \]  

(8)

which gives

\[ N = Z [x_0\chi'(x_0) - \chi(x_0) + 1] \]  

(9)

and for neutral atoms \((N = Z)\)

\[ x_0\chi'(x_0) = \chi(x_0) \]  

(10)
3 Temperature Dependent Non-relativistic Model

We introduce now the finite temperature effects in the model. This was already done in 1940 by Marshack and Bethe through a perturbation treatment, while the full adimensional equation is discussed in a successive work of Feynman, Metropolis and Teller.

The density of an electron gas at temperature T can be written as

\[ n_e = \frac{\sqrt{2m_e}^{3/2}}{\pi^2 \hbar^3} \int_0^\infty \frac{\sqrt{\epsilon}}{e^{\frac{\epsilon}{kT}} + 1} d\epsilon = \frac{\sqrt{2m_e}^{3/2}}{\pi^2 \hbar^3} (KT)^{3/2} I_1 \left( \frac{\mu}{kT} \right) \]  

(11)

where

\[ I_1(x) = \int_0^\infty \frac{\sqrt{y}}{e^{y-x} + 1} dy \]  

(12)

Using the same adimensional variables introduced in the previous section and introducing the temperature parameter \( \tau \) as

\[ \tau = \frac{b Z e^2}{Ze^2} KT \]  

(13)

we can rewrite the electron density in adimensional form

\[ n_e = \frac{\sqrt{2m_e}^{3/2} Z^{3/2} e^3}{\pi^2 \hbar^{3/2} b^{3/2}} I_1 \left( \frac{\chi}{\tau x} \right) \]  

(14)

We can thus express the electrostatic equation in the following adimensional form

\[ \frac{d^2 \chi}{dx^2} = \frac{3}{2} \tau^{3/2} x I_1 \left( \frac{\chi}{\tau x} \right) \]  

(15)

This equation is formally different from the one obtained in the case of complete degeneracy, nevertheless it can be easily shown that if one develops the integral which appears in eq. (11) for small temperatures (see appendix for details) one gets the following formula at the first order

\[ \frac{d^2 \chi}{dx^2} = \frac{\chi^{3/2}}{x^{1/2}} \left[ 1 + \frac{\pi^2}{8} \tau^2 x^2 + \ldots \right] \]  

(16)

where we neglect terms of the order \( O(\tau^4) \).

4 Relativistic model at T=0

When considering a relativistic extension of the model the finite size of the nucleus must be taken in account to avoid the central singularity (see e.g. [1]). In this case we have thus to introduce a new term into the fundamental equation of electrostatics, representing the positive distribution of charges in the interior of the nucleus \( n_p(r) \)

\[ \Delta V(r) = 4\pi e n_e(r) - 4\pi e n_p(r) \]  

(17)
The quantities \( V(r) \) and \( n(r) \) are in this case related by
\[
c\sqrt{p_F^2 + m^2c^2} - eV(r) = \text{const} \equiv E_F
\] (18)

Using eq(3) it is possible to put eq. 18 in the form
\[
p_F^2 = \frac{e^2}{b} \Phi^2 + 2me\Phi
\] (19)
which, using 4, becomes
\[
p_F = 2mc \left( \frac{Z}{Z_{cr}} \right)^{2/3} \left( \frac{\chi}{x} \right)^{1/2} \left[ 1 + \left( \frac{Z}{Z_{cr}} \right)^{4/3} \frac{\chi}{x} \right]^{1/2}
\] (20)
where
\[
Z_{cr} = \left( \frac{3\pi}{4} \right)^{1/2} \left( \frac{\hbar c}{e^2} \right)^{3/2} \approx 2462.4
\] (21)

Remembering the relation between the Fermi momentum and the number density of a fermion gas
\[
n_e = \frac{p_F^3}{3\pi^2\hbar^3}
\] (22)
we obtain the following expression
\[
n_e = \frac{Z}{4\pi b^2} \left( \frac{\chi}{x} \right)^{3/2} \left[ 1 + \left( \frac{Z}{Z_{cr}} \right)^{4/3} \frac{\chi}{x} \right]^{3/2}
\] (23)

We can also express the second term of the right-hand side of eq(4) in terms of adimensional quantities: we assume here an homogeneous spherical nucleus, with a radius given by the approximate formula
\[
r_{nuc} = 1.2A^{1/3} \text{ fm}
\] (24)

The number density of protons is therefore
\[
n_p = \frac{3Z}{4\pi r_{nuc}^3} \Theta(x_{nuc} - x)
\] (25)

Finally we can write eq(17) in the form
\[
\frac{d^2\chi}{dx^2} = \frac{\chi^{3/2}}{x^{1/2}} \left[ 1 + \left( \frac{Z}{Z_{cr}} \right)^{4/3} \frac{\chi}{x} \right]^{3/2} - \frac{3x}{x_{nuc}^3} \Theta(x_{nuc} - x)
\] (26)
where \( x_{nuc} \) is the adimensional size of the nucleus (\( r_{nuc} = bx_{nuc} \)).

Equation 6 is what we call ‘Generalised adimensional Fermi-Thomas equation’.

The first initial condition for this equation follows from the fact that \( \chi \propto r\Phi \) and therefore \( \chi \xrightarrow{r \to 0} 0 \), and so
\[
\chi(0) = 0
\] (27)
The second condition comes from the normalisation condition
\[ N = \int_0^{r_0} \frac{4\pi n_e r^2}{2} dr = Z \int_0^{x_{0}} \frac{x^{3/2}}{x^{1/2}} \left[ 1 + \left( \frac{Z}{Z_{cr}} \right)^{4/3} \frac{\chi}{x} \right]^{3/2} x \; dx \] (28)
with \( r_0 = b x_0 \) atom size. Developing this formula we have
\[ N = Z \int_0^{x_{nuc}} x \chi'' \; dx + \frac{3Z}{x_{nuc}^3} \int_0^{x_{nuc}} x \chi' \; dx + Z \int_0^{x_{0}} x \chi'' \; dx \] (29)
which gives again the relation
\[ N = Z \left[ x_0 \chi'(x_0) - \chi(x_0) + 1 \right] \] (30)

Note that the physical quantities such as the coulomb potential and the density of electrons do not show any singularity in the center, neither on the border of the nucleus, being dependent just on the function \( \chi \) and his first derivative. The only discontinuity appears in the second derivative of \( \chi \) due to our rough assumption of homogeneous spherical nucleus.

It is also evident that the scaling properties of the classical Thomas-Fermi equation are lost in this case, where one has to integrate the adimensional equation separately for each value of \( Z \) and different values of \( x_0 \), i.e. for different states of compression.

In figs.1 and 2 we show an example of the applications of this model to the study of equilibrium configurations of cold White Dwarfs. For more details see ref. 4.

5 Temperature Dependent Relativistic Model

We consider now the complete problem of a relativistic and degenerate gas of electrons at temperature \( T \) surrounding a positively charged nucleus.

The number density of such a gas is
\[ n_e = \frac{1}{\pi^2 (ch)^3} \int_{mc^2}^{\infty} \frac{\sqrt{\epsilon^2 - mc^4}}{e^{\frac{\epsilon}{m}} + 1} \; d\epsilon = \frac{(KT)^3}{\pi^2 (ch)^3} I_2 \left( \frac{\mu}{KT} \right) \] (31)
where
\[ I_2(x) = \int_{a}^{\infty} \frac{y \sqrt{y^2 - a^2}}{e^{y^2} + 1} \; dy \] (32)
and \( a = mc^2/(KT) \).

Introducing adimensional variables and the temperature parameter \( \tau \) we can write now
\[ n_e = \frac{1}{b^3 \pi^2} \left( \frac{c^2}{ch} \right)^3 \tau^3 I_2 \left( \frac{\chi}{\tau x} \right) \] (33)

and inserting the previously defined quantity \( Z_{cr} \) we find
\[ n_e = \frac{3Z}{4\pi b^3} \left( \frac{Z}{Z_{cr}} \right)^2 \tau^3 I_2 \left( \frac{\chi}{\tau x} \right) \] (34)
The final and more general expression of the Thomas-Fermi equation is thus found to be

$$\frac{d^2 \chi}{dx^2} = 3\tau^3 x \left( \frac{Z}{Z_{cr}} \right)^2 I_2 \left( \frac{\tau x}{\sqrt{3}} \right) - \frac{3x}{x_{\text{nuc}}^3} \Theta \left( x_{\text{nuc}} - x \right)$$  (35)

This formula is the main result of this paper and will be the point of departure for the evaluation of the equation of state of compressed matter in extreme conditions of high temperatures in a relativistic regime.

We will present elsewhere the numerical integration of this equation and the corresponding equilibrium configurations of hot relativistic white dwarfs.

6 Conclusions

We have first discussed the classical Thomas-Fermi method and the corresponding generalisation to finite temperature or to the relativistic regime. A finite nucleus treatment including both effects has then been presented. This work must be considered as propedeutical to the evaluation of the equilibrium configurations of relativistic hot white dwarfs. The numerical integration of the highly non-linear equation obtained and the application to the equation of state of white dwarfs matter will be presented elsewhere.
Figure 2. Equilibrium configurations curve for Iron WD in the $M/M_\odot - \rho_c$ plane, obtained in Newtonian theory (the General relativistic curve is practically superposed at the Newtonian one at these low densities). For comparison we show the results obtained by Chandrasekhar and Salpeter. Reproduced from Bertone & Ruffini.

Appendix

Following Landau and Lifshitz we recall here how to approximate for low temperatures integrals of the form

$$I = \int_0^\infty \frac{f(\epsilon)}{e^{\mu/\epsilon} + 1} d\epsilon$$

appearing in the statistical treatment of fermions.

Without going into details, we just recall that using the fact that $\mu/T \gg 1$ one can put the former integral in the form

$$I = \int_0^\mu f(\epsilon) d\epsilon + 2(KT)^2 f'(\mu) \int_0^\infty \frac{z}{e^{z} + 1} dz + \frac{1}{3}(KT)^4 f''(\mu) \int_0^\infty \frac{z^3}{e^{z} + 1} dz + ...$$

(37)

These integrals can be evaluated as

$$\int_0^\infty \frac{z^n}{e^{z} + 1} dz = (1 - 2^{1-x}) \Gamma(x) \sum_{n=1}^\infty \frac{1}{n^x}$$

(38)
We thus obtain our approximate result

$$I = \int_{0}^{\mu} f(e)de + \frac{\pi^2}{6} (KT)^2 f'(\mu) + \frac{7\pi^4}{360} (KT)^4 f'''(\mu) + ...$$  \hspace{1cm} (39)$$

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