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The relativistic Thomas-Fermi treatment for compressed atoms at finite temperatures

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Summary. — The degenerate relativistic Feynman, Metropolis and Teller treatment of compressed atoms is extended to finite temperatures. We present numerical calculations of the equation of state for dense matter as well as profiles of the electron density as a function of distance from the atomic nucleus for selected values of the total matter density and temperature. Marked differences appear especially in the low-density regimes.

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1. – Introduction

In [1] we have generalized to the relativistic regime the classic work of Feynman, Metropolis and Teller, solving a compressed atom by the Thomas-Fermi equation in a Wigner-Seitz cell. In this relativistic generalization the equation to be integrated is the relativistic Thomas-Fermi equation, also called the Vallarta-Rosen equation [2]. The integration of this equation does not admit any regular solution for a point-like nucleus and both the nuclear radius and the nuclear composition have necessarily to be taken into account [3, 4]. This introduces a fundamental difference from the non-relativistic Thomas-Fermi model where a point-like nucleus was adopted.

The relativistic Feynman-Metropolis-Teller treatment allows to treat globally and in generality the electrodynamical interaction within the atom and the relativistic corrections. As a result it is then possible to derive a consistent equation of state for compressed matter which overcomes some of the difficulties of existing treatments often adopted in

the literature. The equation of state has been applied to the study of the general relativistic white-dwarf equilibrium configurations [5].

In this paper we extend our previous work [1] on the degenerate relativistic generalization of the Feynman, Metropolis and Teller treatment by including the effects of temperature.

The paper is organized as follows: first (sect. **2**) we describe the classical Thomas-Fermi model, *i.e.* the non-relativistic and completely degenerate case and the finite-temperature formulation of this problem, giving the corresponding exact equation and its approximated version. Then (sect. **3**) we will pass to the relativistic theory in the completely degenerate case and to the relativistic treatment at finite temperatures. Finally conclusions are presented in sect. **4**.

2. – The Thomas-Fermi model for compressed atoms

2˙1. *The degenerate case*. – The Thomas-Fermi model assumes that the electrons of an atom constitute a fully degenerate gas of fermions confined in a spherical region by the Coulomb potential of a point-like nucleus of charge $+eN_p$ [6,7]. Feynman, Metropolis and Teller have shown that this model can be used to derive the equation of state of matter at high pressures by considering a Thomas-Fermi model confined in a Wigner-Seitz cell of radius R_{WS} [8].

We recall that the condition of equilibrium of the electrons in an atom, in the non-relativistic limit, is expressed by

$$\frac{(P_e^F)^2}{2m_e} - eV = E_e^F, \tag{1}$$

where m_e is the electron mass, V is the electrostatic potential and E_e^F is their constant Fermi energy.

The electrostatic potential fulfills, for $r > 0$, the Poisson equation

$$\nabla^2 V = 4\pi e n_e, \tag{2}$$

where the electron number density n_e is related to the Fermi momentum P_e^F by

$$n_e = \frac{(P_e^F)^3}{3\pi^2\hbar^3}\,. \tag{3}$$

For neutral atoms and ions n_e vanishes at the boundary so the electron Fermi energy is, respectively, zero or negative. In the case of compressed atoms n_e does not vanish at the boundary while the Coulomb potential energy eV does. Consequently E_e^F is positive.

Defining

$$eV(r) + E_e^F = e^2 N_p \frac{\phi(r)}{r}\,, \tag{4}$$

and introducing the new dimensionless radial coordinate η as

$$r = b\eta \qquad \text{with} \qquad b = \frac{(3\pi)^{2/3}}{2^{7/3}} \frac{1}{N_p^{1/3}} \frac{\hbar^2}{m_e e^2}\,, \tag{5}$$

we obtain the following expression for the electron number density:

$$n_e(\eta) = \frac{N_p}{4\pi b^3}\left(\frac{\phi(\eta)}{\eta}\right)^{3/2}, \tag{6}$$

and then eq. (2) can be written in the form

$$\frac{\mathrm{d}^2\phi(\eta)}{\mathrm{d}\eta^2} = \frac{\phi(\eta)^{3/2}}{\eta^{1/2}}, \tag{7}$$

which is the classic Thomas-Fermi equation [7]. A first boundary condition for this equation follows from the point-like structure of the nucleus

$$\phi(0) = 1. \tag{8}$$

A second boundary condition comes from the conservation of the number of electrons $N_e = \int_0^{R_{WS}} 4\pi n_e(r) r^2 \mathrm{d}r$

$$1 - \frac{N_e}{N_p} = \phi(\eta_0) - \eta_0\phi'(\eta_0), \tag{9}$$

where $\eta_0 = R_{WS}/b$ defines the radius R_{WS} of the Wigner-Seitz cell. In the case of compressed atoms $N_e = N_p$ so the Coulomb potential energy eV vanishes at the boundary R_{WS}.

2˙2. *The non-degenerate case.* – We introduce now the finite temperature effects in the model (see, *e.g.*, [8]).

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

$$n_e = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_0^\infty \frac{\sqrt{\epsilon}\,\mathrm{d}\epsilon}{1 + e^{\frac{\epsilon-\mu_e}{kT}}} = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}(kT)^{3/2} I_1\left(\frac{\mu_e}{kT}\right), \tag{10}$$

where μ_e is the electron chemical potential, k is the Boltzmann constant, T is the temperature and

$$I_1(x) = \int_0^\infty \frac{\sqrt{y}\,\mathrm{d}y}{1 + e^{y-x}}. \tag{11}$$

Using the same dimensionless variables introduced in the previous sub-section and introducing the temperature parameter τ as

$$\tau = \frac{b}{N_p e^2} kT, \tag{12}$$

we can write the electron density as

$$n_e = \frac{\sqrt{2}m_e^{3/2} Z^{3/2} e^3 \tau^{3/2}}{\pi^2\hbar^3 b^{3/2}} I_1\left(\frac{\phi}{\tau\eta}\right). \tag{13}$$

As a result the Poisson equation can be written in the following dimensionless form:

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} = \frac{3}{2}\tau^{3/2}\eta I_1\left(\frac{\phi}{\tau\eta}\right). \tag{14}$$

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. (10) for small temperatures one gets the following formula at the first order

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} = \frac{\phi^{3/2}}{\eta^{1/2}}\left[1 + \frac{\pi^2}{8}\frac{\tau^2\eta^2}{\phi^2} + \dots\right], \tag{15}$$

which in the limit $T \to 0$ gives the classic Thomas-Fermi equation (7).

3. – The relativistic Feynman-Metropolis-Teller treatment for compressed atoms

3˙1. *The degenerate case*. – In the relativistic generalization of the Thomas-Fermi equation the point-like approximation of the nucleus must be abandoned [3, 4] since the relativistic equilibrium condition

$$E_e^F = \sqrt{(P_e^F c)^2 + m_e^2 c^4} - m_e c^2 - eV(r), \tag{16}$$

which generalizes eq. (1), would lead to a non-integrable expression for the electron density near the origin. Consequently we adopt an extended nucleus. Traditionally the radius of an extended nucleus is given by the phenomenological relation $R_c = r_0 A^{1/3}$ where A is the number of nucleons and $r_0 = 1.2 \times 10^{-13}\,\mathrm{cm}$. Further it is possible to show from the extremization of the semi-empirical Weizsacker mass-formula that the relation between A and N_p is given by (see *e.g.* Segré [9] and Ferreirinho, Ruffini and Stella [3])

$$N_p \approx \left[\frac{2}{A} + \frac{2a_C}{a_a}\frac{1}{A^{1/3}}\right]^{-1} \approx \left[\frac{2}{A} + \frac{3}{200}\frac{1}{A^{1/3}}\right]^{-1}, \tag{17}$$

where $a_C \approx 0.71\,\mathrm{MeV}$, $a_a \approx 93.15\,\mathrm{MeV}$ are the Coulomb and the asymmetry coefficients respectively. In the limit of small A eq. (17) gives

$$N_p \approx \frac{A}{2}. \tag{18}$$

In [1] we obtain the relation between A and N_p imposing explicitly the beta decay equilibrium between neutron, protons and electrons.

In particular, following the previous treatments (see, *e.g.*, [10]), we have assumed a constant distribution of protons confined in a radius R_c defined by

$$R_c = \Delta \frac{\hbar}{m_\pi c} N_p^{1/3}, \tag{19}$$

where m_π is the pion mass and Δ is a parameter such that $\Delta \approx 1$ ($\Delta < 1$) corresponds to nuclear (supranuclear) densities when applied to ordinary nuclei. Consequently, the proton density can be written as

$$n_p(r) = \frac{N_p}{\frac{4}{3}\pi R_c^3}\theta(R_c - r) = \frac{3}{4\pi}\frac{m_\pi^3 c^3}{\hbar^3}\frac{1}{\Delta^3}\theta(R_c - r), \tag{20}$$

where $\theta(x)$ is the Heaviside function which by definition is given by

$$\theta(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases} \tag{21}$$

The electron density is given by

$$n_e(r) = \frac{(P_e^F)^3}{3\pi^2\hbar^3} = \frac{1}{3\pi^2\hbar^3 c^3}\left[e^2\hat{V}^2(r) + 2m_e c^2 e\hat{V}(r)\right]^{3/2}, \tag{22}$$

where $e\hat{V} = eV + E_e^F$ and V is the Coulomb potential.

The overall Coulomb potential satisfies the Poisson equation

$$\nabla^2 V(r) = -4\pi e\left[n_p(r) - n_e(r)\right], \tag{23}$$

with the boundary conditions $V(R^{WS}) = 0$ (due to global charge neutrality) and finiteness of $V(0)$.

Using eqs. (4), (5) and replacing the particle densities (20) and (22) into the Poisson equation (23) we obtain the relativistic Thomas-Fermi equation

$$\frac{\mathrm{d}^2\phi(\eta)}{\mathrm{d}\eta^2} = -\frac{3\eta}{\eta_c^3}\theta(\eta_c - \eta) + \frac{\phi^{3/2}}{\eta^{1/2}}\left[1 + \left(\frac{N_p}{N_p^{crit}}\right)^{4/3}\frac{\phi}{\eta}\right]^{3/2}, \tag{24}$$

where $\phi(0) = 0$, $\phi(\eta^{WS}) = 0$ and $\eta_c = R_c/b$, $\eta^{WS} = R^{WS}/b$. The critical number of protons N_p^{crit} is defined by

$$N_p^{crit} = \sqrt{\frac{3\pi}{4}}\alpha^{-3/2}, \tag{25}$$

where, as usual, $\alpha = e^2/(\hbar c)$.

It is interesting that by introducing the new dimensionless variable

$$x = \frac{r}{\lambda_\pi} = \frac{b}{\lambda_\pi}\eta, \tag{26}$$

and the function

$$\chi = \alpha N_p \phi, \tag{27}$$

where $\lambda_\pi = \hbar/(m_\pi c)$, eq. (24) assumes a canonical form, the master relativistic Thomas-Fermi equation (see Ruffini [11])

$$\frac{1}{3x}\frac{\mathrm{d}^2\chi(x)}{\mathrm{d}x^2} = -\frac{\alpha}{\Delta^3}\theta(x_c - x) + \frac{4\alpha}{9\pi}\left[\frac{\chi^2(x)}{x^2} + 2\frac{m_e}{m_\pi}\frac{\chi}{x}\right]^{3/2}, \tag{28}$$

where $x_c = R_c/\lambda_\pi$ with the boundary conditions $\chi(0) = 0$, $\chi(x_{WS}) = x_{WS}\chi'(x_{WS})$, $x_{WS} = R_{WS}/\lambda_\pi$.

The neutron density $n_n(r)$, related to the neutron Fermi momentum $P_n^F = (3\pi^2\hbar^3 n_n)^{1/3}$, is determined by imposing the condition of beta equilibrium

$$\begin{aligned} E_n^F &= \sqrt{(P_n^F c)^2 + m_n^2 c^4} - m_n c^2 \\ &= \sqrt{(P_p^F c)^2 + m_p^2 c^4} - m_p c^2 + eV(r) + E_e^F. \end{aligned} \tag{29}$$

Using this approach, it is then possible to determine the beta equilibrium nuclide as a function of the density of the system. In fact, electrons and protons can be converted to neutrons in inverse beta decay $p + e^- \to n + \nu_e$ if the condition $E_n^F < \sqrt{(P_p^F c)^2 + m_p^2 c^4} - m_p c^2 + eV(r) + E_e^F$ holds. The condition of equilibrium (29) is crucial, for example, in the construction of a self-consistent equation of state of high-energy density matter present in white dwarfs and neutron star crusts [5]. In the case of zero electron Fermi energy the generalized $A - N_p$ relation is obtained (see [1]).

3˙2. *The non-degenerate case.* – We consider now the complete problem of a relativistic and non-degenerate gas of electrons at temperature T surrounding a degenerate finite sized and positively charged nucleus. The number density of such a gas is

$$n_e = \frac{1}{\pi^2(c\hbar)^3}\int_{m_e c^2}^{\infty} \frac{\sqrt{\epsilon^2 - m_e^2 c^4}\,\epsilon\,\mathrm{d}\epsilon}{1 + e^{\frac{\epsilon - \mu_e}{kT}}} = \frac{(kT)^3}{\pi^2(c\hbar)^3} I_2\left(\frac{\mu}{kT}\right), \tag{30}$$

where

$$I_2(x) = \int_a^\infty \frac{y\sqrt{y^2 - a^2}\,\mathrm{d}y}{1 + e^{y-x}}, \tag{31}$$

and a is the fixed parameter $a = m_e c^2/(kT)$. Introducing the dimensionless variables ϕ and η given by eqs. (4), (5) and the temperature parameter τ given by eq. (12) we can write

$$n_e = \frac{1}{b^3}\frac{N_p^3}{\pi^2}\left(\frac{e^2}{c\hbar}\right)^3 \tau^3 I_2\left(\frac{\phi}{\tau\eta}\right), \tag{32}$$

and using the definition of N_p^{critic} we obtain

$$n_e = \frac{3N_p}{4\pi b^3}\left(\frac{N_p}{N_p^{critic}}\right)^2 \tau^3 I_2\left(\frac{\phi}{\tau\eta}\right). \tag{33}$$

The final and more general expression of the Thomas-Fermi equation is

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} = 3\tau^3\eta\left(\frac{N_p}{N_p^{critic}}\right)^2 I_2\left(\frac{\phi}{\tau\eta}\right) - \frac{3\eta}{\eta_{nuc}^3}\theta(\eta_{nuc}-\eta). \tag{34}$$

Using eqs. (26), (27), (34) can be rewritten as

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}x^2} = 4\alpha\sqrt{\frac{t}{\pi}}\tau^3 x I_2\left(\frac{\chi}{\hat{\tau}x}\right) - t\frac{3x}{x_{nuc}^3}\theta(x_{nuc}-x), \tag{35}$$

where

$$\hat{\tau} = \frac{\lambda_\pi \alpha N_p}{b}\tau, \qquad t = \sqrt{\frac{3\pi}{16\alpha}}\frac{\lambda_e}{\lambda_\pi}\left(\frac{N_p^{crit}}{N_p}\right)^{1/3}. \tag{36}$$

Equation (35) is the generalization to finite temperatures of the master relativistic Thomas-Fermi equation (28) and has to be integrated with the boundary conditions $\chi(0) = 0$, $\chi(x_{WS}) = x_{WS}\chi'(x_{WS})$, $x_{WS} = R_{WS}/\lambda_\pi$.

The results of our numerical integrations, referred to iron, are summarized in fig. 1 and in table I. Specifically fig. 1 shows three examples of how temperature changes the electron number density inside an iron Wigner-Seitz cell of a given radius. We see that for a given matter density ρ the electron profiles are in general different for different temperatures. Further the positive temperature effects in determining the electron distribution compete with the compressional effects leading to a decreasing differences between different profiles to an increasing value of ρ. In particular for densities larger than $10^3\,\mathrm{g/cm^3}$ the electron profiles for temperatures smaller than 1 keV are practically overlapped. Finally it is found that, for a fixed matter density ρ, to an increasing value of the temperature the electron density at the boundary of the Wigner-Seitz cell increases.

In table I instead we give the pressure P_{FMTrel} for iron in the relativistic generalization of the Feynman, Metropolis, Teller approach for selected temperatures as a function of the matter density ρ. It is possible to conclude that:

a) for a given density the pressure, as expected, is an increasing function of the temperature.

b) the gap between the pressures at different temperatures is a decreasing function of the density.

While in the degenerate case the relativistic generalization of the Feynman, Metropolis, Teller approach exhibits marked differences with respect to the non-relativistic one especially in the high density regimes (see, *e.g.*, [1]), now the generalization to positive temperatures exhibits differences which appear relevant especially in the low-density regimes.

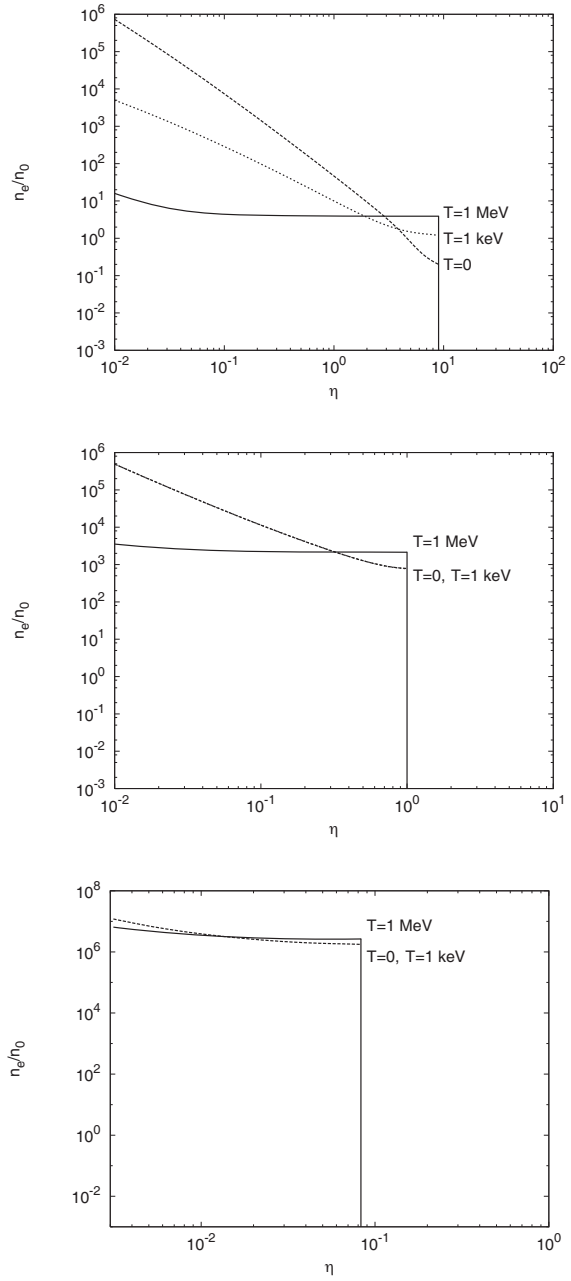

Fig. 1. – The electron number density n_e, in units of the Bohr density $n_0 = 3/(4\pi R^3_{Bohr})$, is plotted as a function of the dimensionless radial coordinate η for selected values of the temperature T in the case of iron at densities $30.0\,\mathrm{g/cm^3}$ (upper panel), $5 \times 10^3\,\mathrm{g/cm^3}$ (middle panel) and $10^7\,\mathrm{g/cm^3}$ (lower panel) using the relativistic generalization of the Feynman, Metropolis and Teller treatment where $R_{Bohr} = \hbar^2/(m_e c^2)$. To an increase of the temperature, the electron number density at the boundary of the atom increases and becomes almost uniform for temperatures larger than 1 keV.

TABLE I. – *Pressure P_{FMTrel} for iron as a function of the density ρ in the relativistic Feynman-Metropolis-Teller approach for selected values of the temperature T.*

ρ (g/cm^3)	P_{FMTrel} (bar) ($T = 0$)	P_{FMTrel} (bar) ($T = 1\,\mathrm{keV}$)	P_{FMTrel} (bar) ($T = 1\,\mathrm{MeV}$)
1.27×10^3	2.25×10^{11}	4.01×10^{11}	1.36×10^{15}
5×10^3	2.79×10^{12}	3.57×10^{12}	4.97×10^{15}
1×10^4	9.62×10^{12}	1.08×10^{13}	9.57×10^{15}
5×10^4	1.57×10^{14}	1.62×10^{14}	4.36×10^{16}
1×10^5	5.10×10^{14}	5.20×10^{14}	8.35×10^{14}
5×10^5	7.25×10^{15}	7.37×10^{15}	3.75×10^{17}
1×10^6	2.20×10^{16}	2.24×10^{16}	7.16×10^{17}
5×10^6	2.53×10^{17}	2.57×10^{17}	3.14×10^{18}
1×10^7	6.90×10^{17}	7.01×10^{17}	5.90×10^{18}
5×10^7	6.24×10^{18}	6.34×10^{18}	2.48×10^{19}
1×10^8	1.54×10^{19}	1.56×10^{19}	4.51×10^{19}
5×10^8	1.12×10^{20}	1.13×10^{20}	2.32×10^{20}
1×10^9	2.49×10^{20}	2.53×10^{20}	4.39×10^{20}

4. – Conclusions

We have generalized the relativistic Feynman-Metropolis-Teller treatment of degenerate compressed atoms [1] to the case of finite temperatures. In particular we have evaluated the equation of state of compressed matter in extreme conditions of high temperatures in a relativistic regime in the case of iron (see, *e.g.*, table I). This work must be considered as propaedeutical to the evaluation of the equilibrium configurations of relativistic *hot* white dwarfs.

The application of this treatment to hot white dwarfs and its extension to nuclear massive cores of stellar dimensions (see, *e.g.*, [1]) will be considered elsewhere.

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