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On atomic ionization by compression (*)

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Summary. — The Feynman-Metropolis-Teller treatment for compressed atoms is here reexamined in view of the process of *ionization by compression* of atoms.

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1. – Introduction

It is well known that the Fermi-Thomas [1] model of the atom has introduced a drastic modification in the treatment of the many-body electron distribution problem, otherwise analyzed with laborious and detailed Hartree-Fock calculations. The Fermi-Thomas model, describing Z electrons in their ground state in the presence of a point-like nucleus of charge Ze, uses a statistical approach consisting of a fluid description of the electrons fulfilling the Fermi-Dirac statistics at $T = 0$. Surprisingly, it works much better than one should have been reasonably expected.

Feynman, Metropolis and Teller [2] have shown that the standard Fermi-Thomas method can be generalized to treat both ions and compressed atoms as well as their excited states. In sect. **2** we present a brief review of the Fermi-Thomas model of the atom. In sect. **3** we develop the theory of *ionization by compression* giving explicit numerical examples. In sect. **4** we give the corresponding procedure to obtain compressed ions in the framework of the Fermi-Thomas model. Section **5** is devoted to the analogy between the Fermi-Thomas equation and the traditional fluid approximation which leads to a direct estimate of the pressure acting at the boundary of the atom. We give an explicit table (table I), for selected values of the compression, of the Fermi momentum and pressure in the non-relativistic regime, generalizing the results in [2].

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The corresponding relativistic treatment, following the work of Ruffini and Stella [3] will be presented elsewhere.

2. – From the Fermi-Thomas atom to compressed matter

The Fermi-Thomas model assumes that the electrons of an atom constitute a fully degenerate gas of fermions, confined in a spherical region of space by the Coulomb potential of the point-like nucleus of charge $+Ze$. It further assumes that the potential does not change appreciably in a volume containing a statistically significant number of electrons. This assumption, artificial at first sight, is actually well satisfied by almost all atoms and works especially well for heavy atoms and even better for atoms subjected to high pressure. This last circumstance is often encountered in situations of astrophysical interest.

A notable application of the Fermi-Thomas model to the study of compressed atoms is due to Feynman, Metropolis and Teller [2], while a comparison between the predictions of the model and the experimental results can be found in [4]. In the following we will recover the main results of the Feynmann-Metropolis-Teller treatment and we shall apply their work to the process of *ionization by compression*.

The chemical equilibrium condition for an electron inside the atom is expressed by the following relation [5]:

$$E_F = \frac{p_F^2}{2m} - eV = \text{const}\,, \tag{1}$$

where m is the electron mass, V is the electrostatic potential and E_F is the Fermi energy, the maximum energy allowed for an electron. The Fermi momentum p_F is related to the electronic density by

$$n = \frac{p_F^3}{3\pi^2\hbar^3}\,. \tag{2}$$

For neutral atoms and ions the electronic density vanishes at the boundary r_0, corresponding to $p_F = 0$. Correspondingly, the Fermi energy is, obviously, negative or zero and equals the potential energy of the electron at r_0, $E_F = -eV_0$.

In the case of compressed atoms, the density does not vanish at r_0 while the potential energy is zero $-eV_0 = 0$. From eq. (1) it follows that the Fermi energy can be written as $E_F = p_F^2(r_0)/2m$.

Let us now define

$$\phi = V + E_F/e \tag{3}$$

and

$$\phi(r) = \frac{Ze}{r}\chi(r)\,, \tag{4}$$

$$r = bx\,, \tag{5}$$

where

$$b = (3\pi)^{2/3} a_0/2^{7/3} Z^{1/3}\,, \tag{6}$$

$a_0 = \hbar^2/me^2 = 0.53\cdot 10^{-8}$ cm being the Bohr radius. The Poisson equation, expressed in a dimensionless form, becomes

$$\frac{d^2\chi}{dx^2} = \frac{\chi^{3/2}}{x^{1/2}} . \tag{7}$$

The first boundary condition $\chi(0) = 1$ corresponds to a point-like nucleus of charge $+Ze$ at the center, and the second is given by the constraint on the total number of electrons

$$N = \int_0^{r_0} 4\pi n(r)\, r^2 \, dr , \tag{8}$$

which, in terms of the dimensionless quantities, becomes

$$1 - \frac{N}{Z} = \chi(x_0) - x_0 \chi'(x_0), \tag{9}$$

where $x_0 = r_0/b$.

We recall that the second boundary condition of eq. (7) is given by the value of $\chi'(0)$: for every value of $\chi'(0)$ we have a physically relevant solution. If we now numerically integrate eq. (7) we find three different types of solutions for different values of $\chi'(0)$ (see fig. 1):

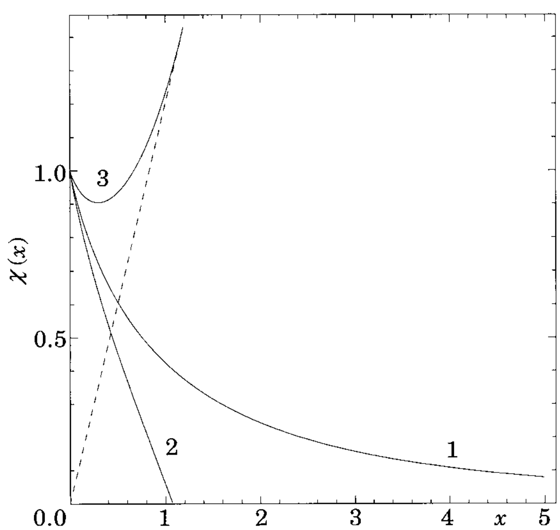

Fig. 1. – Plots of different solutions of the Thomas-Fermi equation. 1) neutral atom, 2) positive ion, 3) compressed atom. The dotted vertical line intersect curve 3) in $(x_0, \chi(x_0))$, where the linear function $\chi = \chi'(x_0)\, x$ is tangent to the curve, corresponding to overall charge neutrality. As explained in the text, the value $\chi'(x_0)$ is directly related to the Fermi energy, see eq. (22). Only the regions $x < x_0$ are physically relevant.

1) The free neutral atom corresponds to an asimptotical solution: $x_0 = \infty$, $\chi(\infty) = \chi'(\infty) = 0$, obtained for $\chi' = -1.57561249$. In this case we have $N = Z$, *i.e.* neutral atom with infinite radius.

2) The free-ions solutions have a $\chi(x)$ vanishing for finite values of x_0: they are obtained for $\chi'(0) < -1.57561249$. In this last case we have $N < Z$, *i.e.* ionized atom with finite radius.

3) In the third family of solutions $\chi(x)$ attains an infinite value when $x \to \infty$. They are obtained for $\chi'(0) > -1.57561249$. In this last case $N = Z$ is reached for an x_0 such that $\chi(x_0) = x_0 \chi'(x_0)$. These solutions correspond to a compressed atom (that is, non-isolated and undergoing external pressure).

3. – Ionization by compression

If a neutral atom is compressed, it is forced to fill in a volume which is smaller than the one that would be naturally occupied by a free atom. As a consequence of the uncertainty principle, the kinetic energy of the electrons raises: this process can enhance the total energy of some electrons to positive values. If an electron possesses a positive energy with respect to the nucleus, it must be considered free; this allows to say that a suitable compression can partially ionize an atom: the more the atoms are compressed the higher is the number of the ionized electrons. The number of electrons per unit volume is given by

$$\frac{\mathrm{d}N}{\mathrm{d}V} = n(r) = \frac{8\pi}{h^3} \int_0^{p_F(r)} p^2 \,\mathrm{d}p \,. \tag{10}$$

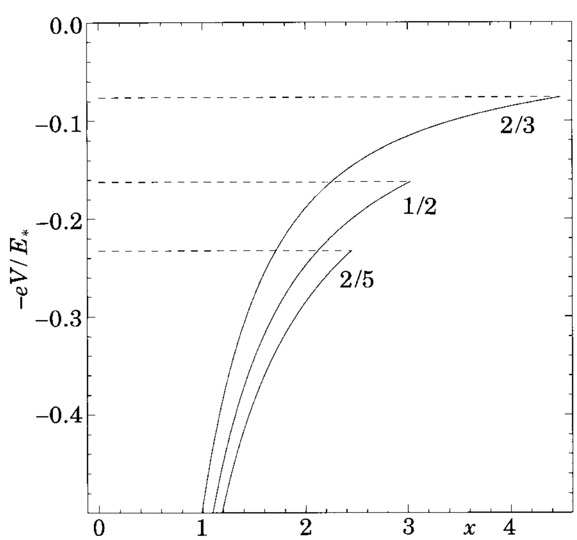

Fig. 2. – The potential energy of an electron inside three different Fermi-Thomas ions. The horizontal dashed lines indicate the level of the Fermi energy, each curve being labeled with the corresponding value of N/Z.

If we want to know the number of electrons per unit volume with positive energy we have

$$\left(\frac{\mathrm{d}N}{\mathrm{d}V}\right)_{\mathrm{ion}} = \frac{8\pi}{h^3}\int_{p_*(r)}^{p_\mathrm{F}(r)} p^2\,\mathrm{d}p\,, \tag{11}$$

where p_* fulfils the equation

$$\frac{p_*^2}{2m} - eV = 0\,. \tag{12}$$

In fig. 2 we plot the potential energy of three different ions.

From (11) it is easy to obtain the total number of ionized electrons:

$$N_{\mathrm{ion}} = \frac{32\pi^2}{3h^3}\int_0^{r_0} r^2(p_\mathrm{F}^3 - p_*^3)\,\mathrm{d}r\,. \tag{13}$$

Let us focus our attention on the general relation between the Fermi energy and the solution of the TF equation (see also fig. 3). From eqs. (3), (4) and (6) we evaluate the Fermi energy

$$E_\mathrm{F} = \frac{Ze^2}{b}\,\frac{\chi(x_0)}{x_0} - eV(r_0)\,. \tag{14}$$

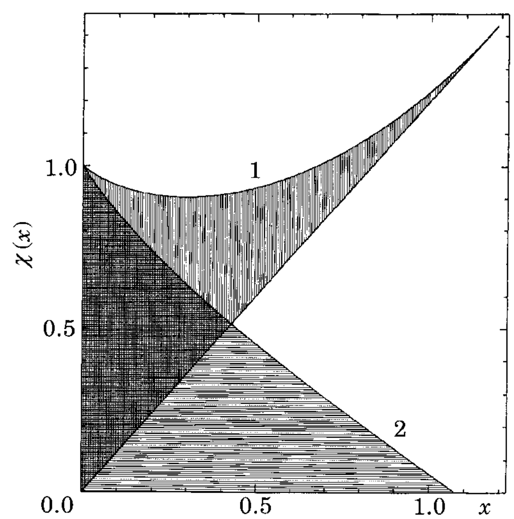

Fig. 3. – The vertically dashed region delimited by the curve 1 (a compressed atom) and its tangent at x_0 is a monotonically increasing function of the number of bound electrons. The same consideration applies to the horizontally dashed region delimited by the curve 2 (an ion) and the x-axis.

From the normalization condition we obtain

$$\frac{\chi(x_0)}{x_0} = \chi'(x_0) + \frac{1}{x_0}\left(1 - \frac{N}{Z}\right). \tag{15}$$

The potential energy at the boundary is

$$-eV(r_0) = -\frac{e^2}{bx_0}(Z - N). \tag{16}$$

If we now insert (15) and (16) in (14) we obtain the relation we were searching for,

$$E_F = \frac{Ze^2}{b}\chi'(x_0). \tag{17}$$

This relation allows a simple geometrical interpretation of formula (13). If we consider the case of compressed atoms we have

$$\frac{\chi(x_0)}{x_0} = \chi'(x_0). \tag{18}$$

and for the number of bound electrons

$$N_{\text{bound}} = Z\int_0^{x_0} x^{1/2}(\chi - x\chi'(x_0))^{3/2}\,dx. \tag{19}$$

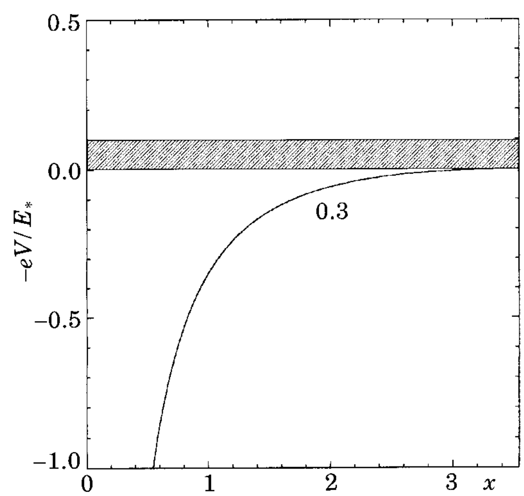

Fig. 4. – The potential energy of an electron as a function of the dimensionless distance from the nucleus. The curve is labeled with the fraction N_*/Z of ionized electrons, which occupies the energy levels corresponding to the dashed region. The radius of the atom is $r_0 = 0.56$ Å.

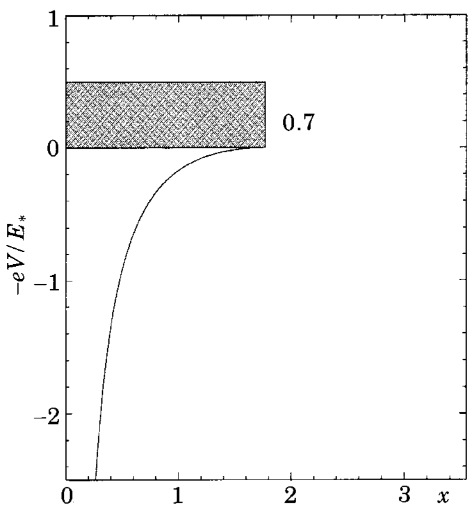

Fig. 5. – The same plot of the previous figure is shown for a compressed atom of radius $r_0 =$ 0.28 Å, with a fraction of ionized electrons equal to $N_*/Z = 0.7$.

The last one is a monotonically increasing function of the area delimited by the solution of the TF equation and its tangent at x_0.

In fig. 4-6 we show three different degrees of compression of an atom. In the last case it is easy to see how the more the atom is compressed the more the Fermi energy (and, consequently, the number of free electrons) increases.

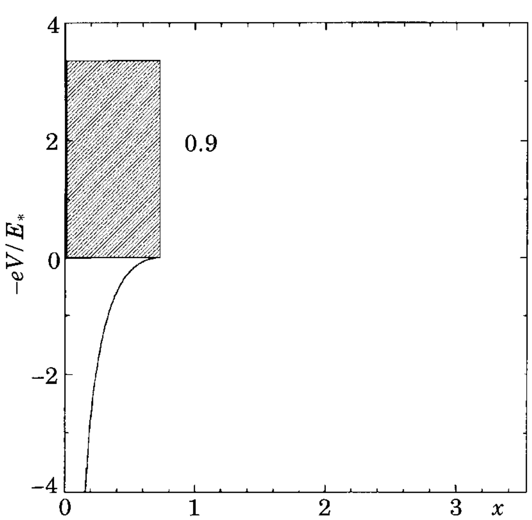

Fig. 6. – The same plot of the previous figure is shown for a compressed atom of radius $r_0 =$ 0.12 Å, with a fraction of ionized electrons equal to $N_*/Z = 0.9$.

4. – Compressed ions

Up to now we have considered three possible solutions of the TF equation, each one representing a different physical system: free ions, free atoms and compressed atoms. It is interesting to note that a fourth possibility exists, namely compressed ions. This picture can be obtained as follows.

Let us consider a particular ion with Z protons, $N > Z$ electrons and boundary at x_0; let us now choose a smaller value of the radius, say x_1. Among all the possible solutions with boundary greater than x_0 we focus our attention on the unique curve that, at x_1, contains the same number of electrons with the same nuclear charge. This solution, in which we have introduced a cut-off, may be interpreted as a compressed ion. It is not possible, *a priori*, to know if the compressed ion will lay on an ion curve or on a compressed-atom curve, nevertheless for x_1 ranging from 0 to x_0 all the possible cut-off will be covered. A structure made of TF ions has no physical meaning in our picture of self-gravitating systems, but it is exactly what one would obtain following Slater [6], because of his different choice of the arbitrary constant in the electrostatic potential.

5. – Fluid analogy

We want to discuss the behaviour of the function $(\mathrm{d}N/\mathrm{d}V)_{\mathrm{ion}}$, in order to explain the difference between the unbound electrons in the Fermi-Thomas compressed atom and a perfect degenerate Fermi gas.

The density of unbound electrons is not constant whithin the atom, as it should be if the electrons had only kinetic energy. It is clear that the most general method for calculating the pressure acting at the boundary of the atom is the application of the virial theorem (see below); nevertheless, in order to estimate the pressure to which the atom is submitted at x_0, we propose a formal analogy, dictated by the structure of the equtions, with a fluid model.

Instead of using the Fermi-Thomas equation we solve the Fermi-Thomas atom treating the electron gas as a fluid. The set of equations is

$$\frac{\mathrm{d}P}{\mathrm{d}r} = en(r)\,\frac{\mathrm{d}\phi}{\mathrm{d}r} = -en(r)\,\frac{q(r)}{r^2}\,, \tag{20}$$

$$\frac{\mathrm{d}q}{\mathrm{d}r} = -4\pi r^2 en(r)\,, \tag{21}$$

where $q(r)$ is the charge contained in the radius r. Equation (20) is analogous to the hydrostatic equation while eq. (21), which represents the charge conservation, is analogous to the mass conservation equation of the hydrostatic equilibrium problem. Inserting $\mathrm{d}\phi/\mathrm{d}r$ from the Fermi-Thomas equation into eq. (20) and using dimensionless quantities we find

$$P(r) = \frac{Z^{5/2}e^5(2m)^{3/2}}{b^{5/2}\hbar^3 3\pi^2}\int \mathrm{d}x\left(\frac{\chi}{x}\right)^{3/2}\left(\frac{\chi'}{x} - \frac{\chi}{x^2}\right). \tag{22}$$

TABLE I. – *Relevant physical quantities derived from the non-relativistic Fermi-Thomas compressed atom. All quantities are calculated assuming $Z = 26$.*

r_0(Å)	p_F (g·cm/2)	P (dyne/cm^2)
2.684	$8.494\cdot 10^{-20}$	$2.794\cdot 10^{10}$
1.857	$1.561\cdot 10^{-19}$	$5.855\cdot 10^{11}$
1.285	$2.651\cdot 10^{-19}$	$8.282\cdot 10^{12}$
$8.887\cdot 10^{-1}$	$4.437\cdot 10^{-19}$	$1.087\cdot 10^{14}$
$6.148\cdot 10^{-1}$	$7.217\cdot 10^{-19}$	$1.237\cdot 10^{15}$
$4.253\cdot 10^{-1}$	$1.138\cdot 10^{-18}$	$1.207\cdot 10^{16}$
$2.810\cdot 10^{-1}$	$1.853\cdot 10^{-18}$	$1.381\cdot 10^{17}$
$1.944\cdot 10^{-1}$	$2.801\cdot 10^{-18}$	$1.090\cdot 10^{18}$
$1.345\cdot 10^{-1}$	$4.175\cdot 10^{-18}$	$8.017\cdot 10^{18}$
$9.305\cdot 10^{-2}$	$6.162\cdot 10^{-18}$	$5.618\cdot 10^{19}$

The integral gives

$$\frac{2}{5}\left(\frac{\chi}{x}\right)^{5/2}. \tag{23}$$

This expression coincides with the pressure of a non-relativistic degenerate Fermi gas [3]. We would have reached the same expression recalling that in the Fermi-Thomas model the virial theorem applies [2] and that the pressure can be derived from

$$2E_{\rm kin} + E_{\rm pot} = 3PV\,. \tag{24}$$

For the system to be in equilibrium, we require the pressure acting on the boundary of an atom to be equal to the pressure exherted by the nearest atoms and hence it is the point pressure in a system containing a large number of atoms. This gives an equation of state which is different from the classical one used in the earliest works on compact stars [7]. In table I we give the relevant quantities calculated for $Z = 26$. For arbitrary Z the results can be obtained by scaling laws. In a forthcoming publication [8] we will examine, for a compressed atom or ion, the effects of the exchange terms intoruced by Dirac [9] in the Thomas-Fermi equation.

6. – Conclusions

We have generalized the Feynman-Metropolis-Teller approach to the analysis of compressed atoms considering explicitly the concept of ionization by compression on much improved range of compression parameters. The generalization of these results to relativistic treatment will be considered elsewhere.

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