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Resolution of two new Thomas–Fermi problems

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Abstract

Using the Thomas–Fermi (TF) model we describe the electron density distribution that neutralizes two static positive charge distributions, one being planar and the other linear. The first case admits an analytical solution, the second solution is numerical. The various energy terms are calculated and the virial theorem verified. These results are compared with the electron distribution that neutralizes a point-like positive charge, i.e. the familiar TF model for the atom.

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1. Introduction

From an academic point of view, due to its simplicity and elegance, the Thomas–Fermi (TF) model [1, 2] is an almost obligatory first step in atomic physics courses [3–5] previous to more accurate descriptions of the structure of the heavy atoms such as the Hartree–Fock equations [6] or the density functional methods [7, 8]. In addition, the TF equation continues to attract the attention of researchers as a testing ground for new mathematical strategies and refinements [9–16].

In this paper we present and solve two new and interesting TF problems which, in a sense, are complementary to the habitual case in which a degenerate electron distribution neutralizes a point-like fixed positive charge. Here we analyse the electron distribution that neutralizes the other basic geometrical entities in three dimensions, i.e. an infinite uniform planar distribution and an infinite uniform straight-line distribution.

A real system amenable to an approximate description such as a planar distribution of positive charge immersed in a electron sea, is a graphite layer, i.e. a surface inlaid with regular hexagons at the vertices of which are situated carbon atoms. The distance between nearest-neighbour nuclei is 1.42 Å and the covalent bonds in a layer are much stronger than the forces between layers in a graphite crystal. The interlayer binding in graphite has been calculated in [17] using a method akin to the TF model.

Graphite layers can also adopt the form of a lengthy structure such as a hollow cylinder. This type of structure, referred to as nanotubes [18], is receiving widespread attention from scientists and technologists. The nanotubes can reach tens of micrometres in length, which is several orders of magnitude in excess of their diameters usually ranging from one to several nanometres. Other examples of quasi-one-dimensional materials amenable to a description such as a macromolecular chain of ions surrounded by an electron cloud, are the organic conducting polymers, such as polyacetylene [19].

The paper is organized as follows. In section 2 we recall the basic equations of the TF model and the boundary conditions to be fulfilled by the solution. In section 3, for reference, this model is applied to the atom. In section 4 we describe the planar case, write the corresponding TF equation and obtain its analytical solution. Section 5 is devoted to the linear case, the TF equation is written and its numerical solution obtained. The calculation of the energy terms in the three problems is done in section 6. In section 7 we analyse the specific predictions of the virial theorem (VT) for these three cases. Finally, in section 8 we present a discussion of the results.

2. Hypotheses of the Thomas–Fermi model

The TF model describes electron distributions at zero temperature, and is based on three assumptions.

(i) The electron density, $n(\vec{r})$, and the electrostatic potential, $\phi(\vec{r})$, are related by Poisson's equation

$$\vec{\nabla}^2\phi = 4\pi e n, \tag{2.1}$$

where $e = |e|$ is the elementary positive charge.

(ii) The equation of state of the electron cloud is that of a degenerate Fermi gas

$$n = \frac{p_F^3}{3\pi^2\hbar^3}, \tag{2.2}$$

where $p_F = |\vec{p}_F(\vec{r})|$ is the Fermi momentum of the electrons, and $\hbar = h/2\pi$ is the reduced Planck constant.

(iii) The condition of hydrostatic equilibrium is fulfilled throughout the electron cloud

$$\frac{p_F^2}{2m} - e\phi = C, \tag{2.3}$$

where m is the electron mass and C is an arbitrary constant. For neutral systems, ϕ is considered null at infinity and therefore, from now on, we will take $C = 0$.

By eliminating p_F from equations (2.2) and (2.3) we obtain

$$n = \frac{(2m)^{3/2}}{3\pi^2\hbar^3}(e\phi)^{3/2}, \tag{2.4}$$

and by eliminating n from equations (2.1) and (2.4), we obtain

$$\vec{\nabla}^2\phi = 4\pi e\frac{(2m)^{3/2}}{3\pi^2\hbar^3}(e\phi)^{3/2}. \tag{2.5}$$

In the problems studied here there will be only one relevant spatial coordinate and hence equation (2.5) will be an ordinary second-order differential equation, whose solution requires two initial conditions or two boundary conditions. For these problems, a first boundary condition will come by imposing on the electric field a known behaviour in positions near the naked positive charge distribution. The second boundary condition simply comes from the assumed global neutrality of the system.

It will be useful to express equation (2.5) in dimensionless variables: the non-dimensional relevant distance will be called x and the non-dimensional dependent variable will be called χ. Thus, n and ϕ will be simple functions of χ, and the length unit relating actual distances and x will be called b. This b is the TF scale length of each problem. In terms of χ and x equation (2.5) will adopt a universal aspect and the solution that fulfils the mentioned boundary conditions is applicable to any particular case.

3. TF model for the atom

In this case, we deal with Z electrons neutralizing a point-like static positive charge equal to Ze, which is located at $\vec{r} = 0$. Here it is convenient to use spherical polar coordinates $\vec{r}(r, \theta, \varphi)$ and in this problem r will be the only relevant coordinate.

The first condition to be fulfilled by $\phi(\vec{r})$ is that the resulting electric field must have the following limit:

$$\vec{E}(\vec{r})|_{r\to 0} = \frac{Ze^2}{r^2}\vec{e}_r, \tag{3.1}$$

where $\vec{e}_r$ is the unitary vector in the radial direction. That is, the electric field near the origin must coincide with that created by the naked nuclear charge. The second boundary condition, i.e. that of neutrality, is expressed as:

$$\int n\,\mathrm{d}\vec{r} = Z. \tag{3.2}$$

Bearing in mind equation (3.1), an adequate definition of the dimensionless function χ is

$$e\phi = Ze^2\frac{\chi}{r}, \tag{3.3}$$

and inserting equation (3.3) into (2.5), we obtain

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}r^2} = A\frac{\chi^{3/2}}{r^{1/2}}, \tag{3.4}$$

with

$$A = \frac{4e^3(2m)^{3/2}}{3\pi\hbar^3}Z^{1/2}.$$

Now, by using $r = bx$, with

$$b = \kappa a_B Z^{-1/3}, \tag{3.5}$$

$\kappa = (3\pi)^{2/3}/2^{7/3} = 0.885\,34\ldots$ and a_B the Bohr radius, equation (3.4) converts into

$$\ddot{\chi} = \frac{\chi^{3/2}}{x^{1/2}}, \tag{3.6}$$

which is the dimensionless universal TF equation for this problem [1–6]. Here and henceforth a dot on a variable means a derivation with respect to x. In terms of χ, we have

$$n = \kappa'\frac{Z^2}{a_B^3}\left(\frac{\chi}{x}\right)^{3/2}, \tag{3.7}$$

with $\kappa' = (32/9\pi^3)$.

The first boundary condition (3.1) imposes

$$\chi(0) = 1. \tag{3.8}$$

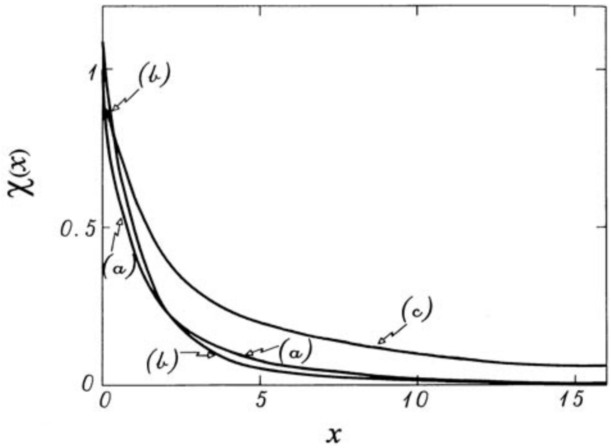

Figure 1. Universal Thomas–Fermi solution, χ, for the three cases studied in the text, (*a*) the atom, (*b*) the plane and (*c*) the line.

If x_a represents the radial distance, expressed in b units, where n vanishes, i.e. from equation (3.7)

$$\chi(x_a) = 0, \tag{3.9a}$$

the second boundary condition (3.2) imposes

$$x_a\dot{\chi}(x_a) = 0. \tag{3.9b}$$

Actually, the conditions (3.9) demand that x_a should be infinite. In fact the asymptotic behaviour of χ is [8, 10, 20]

$$\chi(x)|_{x\to\infty} = \frac{144}{x^3} + \cdots. \tag{3.10}$$

The numerical solution of equation (3.6) fulfilling equations (3.8) and (3.9) appears tabulated in many texts [3–5, 10]. We plot this in figure 1 (curve a) for comparison.

4. Analytic Thomas–Fermi solution for the planar distribution

Consider a homogeneous positive charge distribution located in the plane $z = 0$. The number of positive charges per surface unit will be σ. We will find the electron distribution that neutralizes, at the two sides of the plane, this positive planar distribution. The Cartesian coordinates $\vec{r}(x, y, z)$ are appropriate, and the distance, $|z|$, to the positively charged plane will be the only relevant coordinate.

The first condition to be fulfilled by $\phi(z)$ is that the resulting electric field must have, for example, for $z > 0$, the following limit:

$$\vec{E}(z)|_{z\to 0} = 2\pi\sigma e\vec{e}_z, \tag{4.1}$$

where $\vec{e}_z$ is the unitary vector in the positive z-direction. This is to coincide with the field created by the naked positive distribution (for $z < 0$, the electron distribution is identical). The second condition, i.e. that of global neutrality, is expressed as

$$\sigma = \int n\,\mathrm{d}z. \tag{4.2}$$

Taking into account equation (4.1), an adequate definition of the dimensionless function χ is

$$e\phi = 2\pi\sigma e^2 b\chi, \tag{4.3}$$

where b is the TF scale length. And inserting equation (4.3) into (2.5) we obtain

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}z^2} = B\chi^{3/2}, \tag{4.4}$$

with

$$B = \frac{16}{3\hbar^3}\left(\frac{m^3\sigma}{\pi}\right)^{1/2} e^3 b^{1/2}.$$

Now we pass to non-dimensional distances x, $z = bx$ (note that x is not used as a Cartesian coordinate). Adopting

$$b = \frac{(36\pi)^{1/5}}{4}\sigma^{-1/5} a_B^{3/5}, \tag{4.5}$$

then equation (4.4) converts into

$$\ddot{\chi} = \chi^{3/2}, \tag{4.6}$$

which is the non-dimensional TF equation for this problem. In terms of χ, we have

$$n = \left(\frac{8}{9\pi}\right)^{1/5} \frac{\sigma^{6/5}}{a_B^{3/5}} \chi^{3/2}. \tag{4.7}$$

In terms of χ and x, equation (4.1) imposes that

$$\dot{\chi}(0) = -1. \tag{4.8}$$

Denoting by x_a the distance where the electron density vanishes, from equation (4.7) we obtain

$$\chi(x_a) = 0, \tag{4.9a}$$

and equation (4.2) imposes that

$$\dot{\chi}(x_a) = 0. \tag{4.9b}$$

In a second-order differential equation, the two conditions (4.9), in fact, impose that $x_a \to \infty$. Thus, we have to find a solution of equation (4.6) which fulfils equations (4.8) and (4.9). This nonlinear second-order differential equation is analytically solved: we borrow the solution from another TF problem [16],

$$\chi = \frac{400}{[x + 1600^{1/5}]^4}. \tag{4.10}$$

This function is plotted in figure 1 (curve b), and its asymptotic behaviour is

$$\chi(x)|_{x\to\infty} = \frac{400}{x^4} + \cdots, \tag{4.11}$$

and its value at $x = 0$ is

$$\chi(0) = \left(\tfrac{5}{4}\right)^{2/5} = 1.093\,36\ldots. \tag{4.12}$$

5. Thomas–Fermi solution for the linear distribution

Consider a homogeneous positive charge distribution located along the axis OZ. The number of positive charges per length unit will be called λ. In this problem we will find, in the TF model, the electron distribution that neutralizes this positive straight line distribution. Cylindrical coordinates $\vec{r}(z, \vec{\rho})$ are appropriate, $\vec{\rho} \equiv (\rho, \varphi)$ being the planar polar coordinates, and the distance ρ to the positively charged line will be the only relevant coordinate of this problem.

As in previous sections, the first condition to be fulfilled by $\phi(\rho)$ is that the resulting electric field must have the following limit:

$$\vec{E}(\rho)|_{\rho\to 0} = \frac{2\lambda e}{\rho}\vec{e}_\rho, \tag{5.1}$$

where $\vec{e}_\rho$ is the unitary vector in the planar radial direction. This is in order to coincide with the field created by the naked positive distribution. The second condition, i.e. the condition of global neutrality, reads

$$\lambda = \int n\,\mathrm{d}\vec{\rho}. \tag{5.2}$$

Taking into account equation (5.1), an adequate definition of the dimensionless function χ is

$$e\phi = -2\lambda e^2 \ln(x\chi), \tag{5.3}$$

where $\rho = bx$, and b will be fixed later. It is worth noting at this stage that the electric field resulting from the change of variable (5.3) is

$$\vec{E}(\rho) = \frac{2\lambda e}{b}\left[\frac{1}{x} + \frac{\dot{\chi}}{\chi}\right]\vec{e}_\rho, \tag{5.4}$$

which means that the imposition of equation (5.1), strictly speaking, does not fix the behaviour of $\chi(0)$ nor that of $\dot{\chi}(0)$, as it did in the two cases considered before. However, a simple option fulfilling the requirement of equation (5.1) is to take $\dot{\chi}(0) = 0$ and $\chi(0)$ finite and unknown; the appropriateness of this option will be confirmed later. By inserting equation (5.3) into (2.5) and fixing b as

$$b = \left(\frac{3\pi}{16}\right)^{1/2}\lambda^{-1/4}a_B^{3/4}, \tag{5.5}$$

we obtain the dimensionless TF equation for this problem:

$$\ddot{\chi} = -\frac{\dot{\chi}}{x} + \frac{\dot{\chi}^2}{\chi} - \chi[-\ln(x\chi)]^{3/2}. \tag{5.6}$$

In terms of χ and x, the particle density is

$$n = \frac{8}{3\pi^2}\frac{\lambda^{3/2}}{a_B^{3/2}}[-\ln(x\chi)]^{3/2}. \tag{5.7}$$

Hence the equation (5.2) adopts the form

$$\int_0^{x_a} x[-\ln(x\chi)]^{3/2}\,\mathrm{d}x = 1, \tag{5.8}$$

where x_a represents again the distance where n vanishes, i.e. from equation (5.7)

$$x_a\chi(x_a) = 1. \tag{5.9a}$$

Then, equation (5.8) can be elaborated by using (5.6) leading to

$$x_a\dot{\chi}(x_a) = -1. \tag{5.9b}$$

Conditions (5.9) demand that x_a should be infinite.

Now, directly proceeding from equation (5.6) one can identify the behaviour of the solution that goes asymptotically to zero. It reads

$$\chi(x)|_{x\to\infty} = \frac{1}{x} - \frac{256}{x^5} + \frac{(256)^2}{2x^9} + \cdots. \tag{5.10}$$

Likewise, analysing the behaviour of χ for $x \to 0$ in (5.6) the result is that for $\chi(0)$ finite, $\dot{\chi}(0) = 0$, confirming our above commented option. Thus, we can now apply the Runge–Kutta method to the integration of equation (5.6) by departing from the origin with a null slope and identifying the appropriate $\chi(0)$ such that the asymptotic behaviour is that written in equation (5.10). When this program is carried out one finds the numerical solution plotted in figure 1 as curve (c). The value of $\chi(0)$ is

$$\chi(0) = 0.888\,116\ldots. \tag{5.11}$$

For $x \gtrsim 15$, the values of $\chi(x)$ and that of equation (5.10) are practically coincident.

6. Energy terms

In each of the problems considered, we can distinguish three contributions to the energy of the system: the kinetic energy, the electrostatic attractive term and the electrostatic repulsive term. In this section, we will calculate the value of these nine terms. For the atom, the energy terms represent the contribution of the whole system. For the planar and linear cases, however, due to their infinite extension, we calculate energy per surface unit and energy per length unit respectively. That is, we calculate energy densities.

The kinetic energy term, in general, is given by

$$E_{kin} = \int tn\,\mathrm{d}\vec{r}, \tag{6.1a}$$

with

$$t = \frac{3\hbar^2}{10m}(3\pi^2)^{2/3}n^{2/3} \tag{6.1b}$$

where t is the average kinetic energy of a degenerate Fermi gas.

To calculate the two electrostatic terms we consider the splitting of the electric potential

$$\phi = \phi_+ + \phi_-, \tag{6.2}$$

as a sum of ϕ_+, i.e. the contribution of the positive charge distribution plus ϕ_-, i.e. the contribution of the electron distribution. ϕ_+, is known, and ϕ is deduced from the TF function χ, and hence ϕ_- is also easily deduced. Thus in general, the two electrostatic terms are

$$V_a = -e\int \phi_+ n\,\mathrm{d}\vec{r} \tag{6.3}$$

and

$$V_r = -\frac{e}{2}\int \phi_- n\,\mathrm{d}\vec{r}. \tag{6.4}$$

6.1. The atom

From equation (6.1), in this case we have

$$E_{kin} = 4\pi\frac{3\hbar^2}{10m}(3\pi^2)^{2/3}\int_0^\infty n^{5/3}r^2\,\mathrm{d}r, \tag{6.5}$$

and using equations (3.5)–(3.7) we obtain

$$E_{kin} = \frac{3}{5}\frac{Z^2e^2}{b}\left(-\dot{\chi}(0) - \int_0^\infty \dot{\chi}^2\,\mathrm{d}x\right). \tag{6.6}$$

Besides, from equation (6.3),

$$V_a = -4\pi Z^2 e^2 \int_0^\infty \frac{n}{r} r^2 \, \mathrm{d}r. \tag{6.7}$$

And with equations (3.5)–(3.7) again, we obtain

$$V_a = \frac{Z^2 e^2}{b} \dot{\chi}(0). \tag{6.8}$$

Finally, from equation (6.4),

$$V_r = -4\pi \frac{e}{2} \int_0^\infty \phi_- n r^2 \, \mathrm{d}r, \tag{6.9}$$

using

$$\phi_- = \frac{Ze}{r}\chi - \frac{Ze}{r}, \tag{6.10}$$

and with the same substitutions as before, we obtain

$$V_r = \frac{Z^2 e^2}{2b} \int_0^\infty \dot{\chi}^2 \, \mathrm{d}x. \tag{6.11}$$

The values of $\dot{\chi}(0)$ and $\int_0^\infty \dot{\chi}^2 \, \mathrm{d}x$ can be numerically obtained [3, 10], and amount to

$$\begin{aligned} &\dot{\chi}(0) = -1.588\ldots \\ &\int_0^\infty \dot{\chi}^2 \, \mathrm{d}x = 0.454\ldots. \end{aligned} \tag{6.12}$$

6.2. Planar case

Here we compute energy density terms. Equation (6.1*a*) now reads

$$E_{kin}/S = \frac{3\hbar^2}{10m}(3\pi^2)^{2/3} 2 \int_0^\infty n^{5/3} \, \mathrm{d}z, \tag{6.13}$$

and expressing n in terms of χ, and taking into account equations (4.5)–(4.7), we obtain

$$E_{kin}/S = \tfrac{6}{5} C_{plane} \left(\chi(0) - \int_0^\infty \dot{\chi}^2 \, \mathrm{d}x \right), \tag{6.14}$$

where C_{plane} is defined by

$$C_{plane} = \frac{9\pi^2}{64(36\pi)^{1/5}} \sigma^{6/5} a_B^{12/5} \frac{e^2}{b^3}. \tag{6.15}$$

As

$$\phi_+ = -2\pi\sigma e z, \tag{6.16}$$

we deduce from equation (6.3)

$$V_a/S = 2\pi\sigma e^2 2 \int_0^\infty n(z) z \, \mathrm{d}z, \tag{6.17}$$

and from this, plus equations (4.5)–(4.7), we obtain

$$V_a/S = 2C_{plane}\chi(0). \tag{6.18}$$

Finally, for the repulsion energy, equation (6.4) becomes

$$V_r/S = -\frac{e}{2} 2 \int_0^\infty \phi_- n(z) \, \mathrm{d}z, \tag{6.19}$$

and using the usual substitutions, we obtain

$$V_r/S = -C_{plane}\left(2\chi(0) - \int_0^\infty \dot{\chi}^2\,\mathrm{d}x\right). \tag{6.20}$$

In this problem $\chi(0)$ and $\int_0^\infty \dot{\chi}^2\,\mathrm{d}x$ are analytically calculated, $\chi(0)$ is given in equation (4.12) and the other quantity amounts to

$$\int_0^\infty \dot{\chi}^2\,\mathrm{d}x = \tfrac{4}{9}(\tfrac{5}{4})^{2/5} = 0.485\,938\ldots. \tag{6.21}$$

6.3. Linear case

Here, the calculated energies are per unit length. Therefore, equation (6.1) is given by

$$E_{kin}/L = \frac{3\hbar^2}{10m}(3\pi^2)^{2/3}2\pi\int_0^\infty n^{5/3}\rho\,\mathrm{d}\rho, \tag{6.22}$$

and with the substitutions (5.5) and (5.7), we obtain

$$E_{kin}/L = \tfrac{6}{5}C_{line}I_k, \tag{6.23a}$$

where

$$I_k = \int_0^\infty x[-\ln(x\chi)]^{5/2}\,\mathrm{d}x, \tag{6.23b}$$

and C_{line} is given by

$$C_{line} = \frac{3\pi}{16}\lambda^{3/2}a_B^{3/2}\frac{e^2}{b^2}. \tag{6.24}$$

As from equation (6.3)

$$V_a/L = -2\pi e\int_0^\infty \phi_+ n\rho\,\mathrm{d}\rho, \tag{6.25}$$

and

$$\phi_+ = -2\lambda e\ln x, \tag{6.26}$$

then

$$V_a/L = 2C_{line}I_a, \tag{6.27a}$$

with

$$I_a = \int_0^\infty x\ln x[-\ln(x\chi)]^{3/2}\,\mathrm{d}x. \tag{6.27b}$$

Finally, as

$$\phi = -2\lambda e\ln(x\chi), \tag{6.28}$$

we find, with the habitual substitutions,

$$V_r/L = C_{line}I_r, \tag{6.29a}$$

with

$$I_r = \int_0^\infty x\ln\chi[-\ln(x\chi)]^{3/2}\,\mathrm{d}x. \tag{6.29b}$$

The three integrals I_k, I_a and I_r are numerically calculated. The results are

$$\begin{aligned} I_k &= 0.624\,978\ldots \\ I_a &= 0.091\,402\ldots \\ I_r &= -0.716\,381\ldots. \end{aligned} \tag{6.30}$$

Having obtained the three energy terms for the three problems, we can check that for the atom the relation, $2E_{kin} = -(V_a + V_r)$, is verified but it is not in the other cases. This equation is what one expects in a first instance as the implication of the VT for bound many-particle systems with $1/r^2$ forces. The reason why this relation is not fulfilled in the two extended cases is explained in the next section.

7. Implications of the virial theorem

According to the VT, the total kinetic energy of a bound many-body system, E_{kin}, is given by

$$2E_{kin} = I = -\left\langle \sum_i \vec{r}_i \cdot \vec{F}_i \right\rangle, \tag{7.1}$$

where I is known as the virial of the system. $\vec{F}_i$ denotes the force acting on the ith particle whose position is defined by $\vec{r}_i$, and the brackets denote the time average. In the systems considered here, the force acting on an electron is due to a net electrostatic effect comprising the attraction of the static positive charge and the repulsion of the rest of the electrons. Besides, in the planar (linear) case as we calculate the energy terms per unit surface (length), in the calculus of I one must introduce the pressure effect exerted by the electrons lying just on the other side of the border that defines our subsystem. For this reason, in general, we define

$$I = I_e + I_b, \tag{7.2}$$

where I_e comes from the net electrostatic effect mentioned above and I_b comes from the boundary effect on the subsystem. Passing to the continuum, we have

$$I_e = -e \int n(\vec{r} \cdot \vec{\nabla}\phi)\, \mathrm{d}\vec{r}. \tag{7.3}$$

In the following subsections, we will verify the VT and express I in terms of the energy terms calculated in section 6.

7.1. The atom

In this case $I_b = 0$ and equation (7.3) is

$$I_e = -4\pi e \int_0^\infty n r^3 \left(\frac{\mathrm{d}\phi}{\mathrm{d}r}\right) \mathrm{d}r. \tag{7.4}$$

I_e, in non-dimensional variables, adopts the form

$$I_e = -\frac{N^2 e^2}{b} \int_0^\infty \left\{\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\chi}{x}\right)\right\} \left(\frac{\chi}{x}\right)^{3/2} x^3\, \mathrm{d}x. \tag{7.5}$$

Integrating by parts, one obtains

$$I_e = \frac{6}{5}\frac{N^2 e^2}{b} \int_0^\infty \left(\frac{\chi}{x}\right)^{5/2} x^2\, \mathrm{d}x, \tag{7.6}$$

and using equation (3.6), and integrating by parts again, we obtain

$$I_e = -\frac{6}{5}\frac{N^2 e^2}{b} \left(\dot{\chi}(0) + \int_0^\infty \dot{\chi}^2\, \mathrm{d}x\right). \tag{7.7}$$

Using the energy term expressed in equation (6.6), we can now identify the fulfilment of the VT ($2E_{kin} = I_e$). Besides, considering equations (6.8) and (6.11), we can write

$$I_e = -\tfrac{6}{5}[V_a + 2V_r]. \tag{7.8}$$

On the other hand, if in equation (7.5) we proceed in a different way by acting first with the derivative in the integrand, and then integrating by parts, we finally obtain

$$I_e = -[V_a + V_r]. \tag{7.9}$$

Thus, equations (7.8) and (7.9) permit the expression of the three energy terms as a function of only one of them. For example, V_r,

$$\begin{aligned} E_{kin} &= 3V_r \\ V_a &= -7V_r. \end{aligned} \tag{7.10}$$

7.2. Planar case

Here, our subsystem is, for example, a prism whose axis is coincident with the Oz axis, and its base is a square of unit surface. The origin of coordinates is the centre of that square. And we will apply equation (7.1) to the electron population that lies within this prism.

As mentioned, here I_b/S comes from the pressure existing at the lateral surface of the prism. This effect amounts to

$$I_b/S = 4\int_0^\infty p\,\mathrm{d}z, \tag{7.11}$$

where p denotes pressure. The equation of state of a degenerate Fermi gas is

$$p = \frac{1}{5}(3\pi^2)^{2/3}\frac{\hbar^2}{m}n^{5/3}. \tag{7.12}$$

Inserting this into equation (7.11) and comparing with equation (6.1), we identify the relation:

$$I_b/S = \tfrac{4}{3}E_{kin}/S. \tag{7.13}$$

Thus, having identified I_b/S, the VT relation predicts the following relation

$$\tfrac{2}{3}E_{kin}/S = I_e/S. \tag{7.14}$$

In this problem, we see that equation (7.3) becomes

$$I_e/S = -2e\int_0^\infty nz\left(\frac{\mathrm{d}\phi}{\mathrm{d}z}\right)\mathrm{d}z. \tag{7.15}$$

In dimensionless variables, I_e/S reads

$$I_e/S = -2C_{plane}\int_0^\infty x\dot{\chi}\chi^{3/2}\,\mathrm{d}x. \tag{7.16}$$

After the analytical integration of I_e/S we obtain

$$I_e/S = \tfrac{4}{9}(\tfrac{5}{4})^{2/5}C_{plane}, \tag{7.17}$$

which coincides with the value of the left-hand side of equation (7.14), which was obtained in section 6, and thus the VT is fulfilled. Besides, equation (7.16) can be used to express I_e/S as a function of the energy terms of this problem. Proceeding by first integrating by parts or, alternatively, by differentiating first, then integrating and finally taking into account the behaviour of χ, we obtain

$$I_e/S = V_a/S + V_r/S, \tag{7.18a}$$

or

$$I_e/S = -\tfrac{4}{5}(\tfrac{1}{2}V_a/S + V_r/S). \tag{7.18b}$$

From these results and equation (7.14) we deduce

$$\begin{aligned} E_{kin}/S &= -\tfrac{3}{7}V_r/S \\ V_a/S &= -\tfrac{9}{7}V_r/S. \end{aligned} \tag{7.19}$$

7.3. Linear case

In this case, the analysed subsystem is formed by the electron population contained within a cylinder whose axis coincides with the OZ axis, whose height is unity and the radius of the base is infinity. Thus, the pressure effect exerted by the exterior electrons is calculated by considering the existing pressure on the two bases of the cylinder. Its contribution to the virial is

$$I_b/L = 2\pi \int_0^\infty p\rho \, \mathrm{d}\rho, \tag{7.20}$$

inserting equation (7.12), we obtain

$$I_b/L = \tfrac{2}{3} E_{kin}/L, \tag{7.21}$$

and therefore, in this problem the VT relation is expressed

$$\tfrac{4}{3} E_{kin}/L = I_e/L. \tag{7.22}$$

Here, equation (7.3) becomes

$$I_e/L = -2\pi e \int_0^\infty n\rho^2 \left(\frac{\mathrm{d}\phi}{\mathrm{d}\rho}\right) \mathrm{d}\rho. \tag{7.23}$$

In dimensionless variables equation (7.23) reads as

$$I_e/L = 2C_{line} \int_0^\infty x^2 \left\{ \frac{\mathrm{d}}{\mathrm{d}x}[\ln(x\chi)] \right\} [-\ln(x\chi)]^{3/2} \, \mathrm{d}x. \tag{7.24}$$

Equation (7.24) can be worked out by integration by parts. This leads to

$$I_e/L = \tfrac{8}{5} C_{line} \int_0^\infty x[-\ln(x\chi)]^{5/2} \, \mathrm{d}x, \tag{7.25}$$

which can be identified (6.23) as

$$I_e/S = \tfrac{4}{3} E_{kin}/S, \tag{7.26}$$

and thus the VT is fulfilled. On the other hand, equation (7.25) can be expressed as a function of the electrostatic energy terms (6.27) and (6.29) as

$$I_e/L = \tfrac{8}{5} C_{line} \int_0^\infty x[-\ln(x\chi)]^{3/2}[-\ln x - \ln \chi] \, \mathrm{d}x = -\tfrac{4}{5}[V_a/L + 2V_r/L]. \tag{7.27}$$

Finally, we carry out the integration of equation (7.24) from another perspective

$$I_e/L = 2C_{line} \int_0^\infty \left\{ x \frac{\mathrm{d}}{\mathrm{d}x}[-\ln(x\chi)] \right\} \left\{ \frac{\mathrm{d}}{\mathrm{d}x} \left\{ x \frac{\mathrm{d}}{\mathrm{d}x}[-\ln(x\chi)] \right\} \right\} \mathrm{d}x, \tag{7.28}$$

where we have used the TF equation (5.6) and hence

$$I_e/L = 2C_{line} \int_0^\infty \frac{1}{2} \left\{ \frac{\mathrm{d}}{\mathrm{d}x} \left\{ x \frac{\mathrm{d}}{\mathrm{d}x}[-\ln(x\chi)] \right\}^2 \right\} \mathrm{d}x = \left\{ x \frac{\mathrm{d}}{\mathrm{d}x}[-\ln(x\chi)] \right\}^2 \Bigg|_0^\infty. \tag{7.29}$$

In section 5, we obtained for χ the asymptotic limit (5.10). Hence we deduce

$$I_e/L = C_{line} \lim_{x\to 0} \left[x \left\{ \frac{1}{x} + \frac{\dot{\chi}}{\chi} \right\} \right]^2. \tag{7.30}$$

Therefore, given the behaviour of χ at $x = 0$, we can write

$$I_e/L = C_{line}, \tag{7.31}$$

and with equation (7.26)

$$E_{kin}/L = \tfrac{3}{4} C_{line}. \tag{7.32a}$$

The reader should notice that (7.32*a*) coincides with the numerical result obtained in equations (6.23*a*) and (6.30). Using equations (7.27) and (7.31) we have

$$V_a/L = -\tfrac{5}{4}C_{line} - 2V_r/L. \tag{7.32b}$$

The two relations (7.32*a*) and (7.32*b*) are equivalent to (7.10) and (7.19) obtained for the other problems.

8. Results and discussion

In this paper we have obtained the TF solution for the electron distribution that neutralizes two distributions of static positive charge: one planar and the other straight linear. The classical case of electrons neutralizing a point-like positive charge, i.e. the TF atom, is also discussed as a reference and for comparison. By far, the linear case is the most cumbersome. These solutions are interesting in themselves and besides provide a first approximation to the global field that can be used as a starting point in a Hartree–Fock method. In figure 1 these three solutions are shown. Note that the length scale b is different in each case, equations (3.5), (4.5) and (5.5).

From the asymptotic behaviour of the respective TF solutions, χ, i.e. equations (3.10), (4.11) and (5.10), one deduces the asymptotic behaviour of the electron density, n. We obtain

$$\text{Point: } \lim_{x\to\infty} n(x) \propto \lim_{x\to\infty} \left(\frac{\chi}{x}\right)^{3/2} \propto \left(\frac{1}{x^4}\right)^{3/2} = \frac{1}{x^6}, \tag{8.1a}$$

$$\text{Plane: } \lim_{x\to\infty} n(x) \propto \lim_{x\to\infty} \chi^{3/2} \propto \left(\frac{1}{x^4}\right)^{3/2} = \frac{1}{x^6}, \tag{8.1b}$$

$$\text{Line: } \lim_{x\to\infty} n(x) \propto \lim_{x\to\infty} [-\ln(x\chi)]^{3/2} \propto \left(\frac{1}{x^4}\right)^{3/2} = \frac{1}{x^6}. \tag{8.1c}$$

Thus, in the three cases n has identical behaviour at large distances.

With respect to the small x behaviour of n, we deduce

$$\text{Point: } \lim_{x\to 0} n(x) \propto \frac{1}{x^{3/2}}, \tag{8.2a}$$

$$\text{Plane: } \lim_{x\to 0} n(x) \propto \text{constant}, \tag{8.2b}$$

$$\text{Line: } \lim_{x\to 0} n(x) \propto (-\ln x)^{3/2}. \tag{8.2c}$$

In this paper we have emphasized the use of the electric field (and not the electrical potential) in the vicinity of the naked positive charge to fix an initial condition of the TF solution. In the TF atom this distinction is irrelevant, but especially in the linear case, the use of ϕ leads to unnecessary troubles.

We have shown that the VT theorem is always fulfilled provided the appropriate boundary terms, I_b, are added in the planar and in the linear cases. Along with this discussion, we have also shown that in the three problems the energy terms can be expressed in terms of only one term. This is obviously more restrictive than the VT relation itself.

It is also perhaps worth mentioning that, in the planar and linear cases, the sign of the energy potential terms differs from what our initial intuition suggests for bound Coulomb many-particle systems, i.e. attractive-energy negative, repulsive-energy positive and total energy negative. See equations (6.18), (6.20) and (6.27), (6.29).

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