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Thomas–Fermi method for exponential forces

A F Pacheco† and J Sañudo‡

† Departamento de Física Teórica, Facultad de Ciencias, University of Zaragoza, 50009 Zaragoza, Spain

‡ Departamento de Física, Facultad de Ciencias, University of Extremadura, 06071 Badajoz, Spain

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Abstract. A fourth-order non-linear Thomas-Fermi equation describing an assembly of fermions moving under the action of two-body exponential forces is obtained. Its physical boundary conditions and numerical solutions are discussed.

1. Introduction

The Thomas-Fermi (TF) method has been of general interest since its birth because of the remarkable simplicity and elegance of this formalism. For a rigorous view see, for example, [1]. Its original and most famous application is in atomic physics [2]. With regard to nuclear physics [3], there have been important developments in the last two decades known as extended Thomas-Fermi [4], where the TF predictions are obtained as the lowest-order contribution of a systematic expansion in powers of $\hbar$. This clearly shows the semiclassical nature of the method. Recently [5] we extended the TF method in its most simple presentation to pure Yukawa forces and we also showed how a hard-core effect can be easily included in order to produce an effective saturation in the bound state. Furthermore, the Coulomb nature of the gravitational Newtonian field allows the construction of a TF analysis [6], quite similar to the equations used in astrophysics to describe the equilibrium structure of several stellar objects [7].

The Yukawa potential has long been regarded as the most reasonable way of simulating a static nucleon-nucleon potential, since it is the characteristic radial function of a meson field theory. Notwithstanding, both the exponential force and the Yukawa potential have the property of a short-range, and in fact the former has also been used as a phenomenological nucleon-nucleon interaction [8]. The main difference between them lies in their short-distance behaviour: $V_{\text{Yukawa}} \propto -K_1/r$ and $V_{\text{exp}} \propto -K_2$ (K_1 and K_2 are constants).

In this paper we study what a TF method for exponential forces is like and how it works. In spite of its presumed analogy with the Yukawa case, it is substantially different, in that the exponential force leads to a fourth-order TF equation. Hence, a careful analysis has to be made of the boundary conditions to be imposed.

2. Thomas–Fermi equation for exponential forces

Let us suppose that A identical fermions of individual mass equal to m, form a bound distribution of radius R. The potential created by a particle located at $\boldsymbol{r}_1$ at a distance

$r_{1,2} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is supposed to be

$$\phi_{1,2} = -g \exp(-\mu r_{1,2}) \tag{1}$$

and the potential energy of a pair is given by

$$V_{12} = -g^2 \exp(-\mu r_{1,2}) \qquad g^2 = V_0. \tag{2}$$

Natural units $\hbar = c = 1$ are used throughout the paper. If the number of particles per kinematical state is four, and assuming locally the dependence between kinetic energy and particle density (n) that holds for a non-interacting non-relativistic degenerate gas of fermions, then the average kinetic energy per particle will be

$$\bar{t} = \frac{3}{5}\left(\frac{3\pi^2}{4\sqrt{2}}\right)^{2/3} \frac{n^{2/3}}{m}. \tag{3}$$

Before developing the TF method for an assembly like this, let us understand in simple terms the physics of such a system.

2.1. Simple analysis

In order to evaluate the behaviour of this assembly, let us suppose that the particle density n is a constant from $r = 0$ to $r = R$. The total kinetic energy is thus

$$T = \frac{3}{5}\left(\frac{9\pi}{16\sqrt{2}}\right)^{2/3} \frac{A^{5/3}}{mR^2} \tag{4}$$

and, with the convention $y \equiv \mu R$, the total potential energy is

$$V = -\frac{1}{2} V_0 n^2 \int_0^R \mathrm{d}v_1 \int_0^R \mathrm{d}v_2 \exp(-\mu r_{12}) = -\frac{9}{4} \frac{V_0 A^2}{y^3}\left[\frac{4}{3} - \frac{3}{y} + \frac{5}{y^3} - \mathrm{e}^{-2y}\left(2 + \frac{7}{y} + \frac{10}{y^2} + \frac{5}{y^3}\right)\right]. \tag{5}$$

By minimising the total energy ($E = T + V$) with respect to R ($\mathrm{d}E/\mathrm{d}R = 0$), we find the following condition of stability:

$$\frac{(9\pi)^{2/3}}{30} \frac{\mu^2}{V_0 m A^{1/3}} = G(y) \tag{6a}$$

$$G(y) = \frac{2}{y} - \frac{6}{y^2} + \frac{15}{y^4} - \mathrm{e}^{-2y}\left(2 + \frac{10}{y} + \frac{24}{y^2} + \frac{30}{y^3} + \frac{15}{y^4}\right). \tag{6b}$$

$G(y)$ is a universal (independent of the specific parameters of the particles and the interaction) positive definite function, which is plotted in figure 1(a). We see that for any value of μ, m and V_0, if A is large enough, (6a) is always possible, i.e. there exists a bound system.

The asymptotic behaviour of $G(y)$ is as follows:

$$G(y) = \tfrac{4}{35} y^3 \qquad y \to 0 \tag{7a}$$

$$G(y) = 2/y \qquad y \to \infty. \tag{7b}$$

There are two solutions, denoted by y_m and y_M, for (6a). They correspond to the minimum and to the maximum of the energy. Geometrically, in figure 1(b), we see that y_m and y_M are the two crossing points between $G(y)$ and the horizontal straight line of the constant at the left of (6a). For fixed values of μ, m and V_0, an increasing

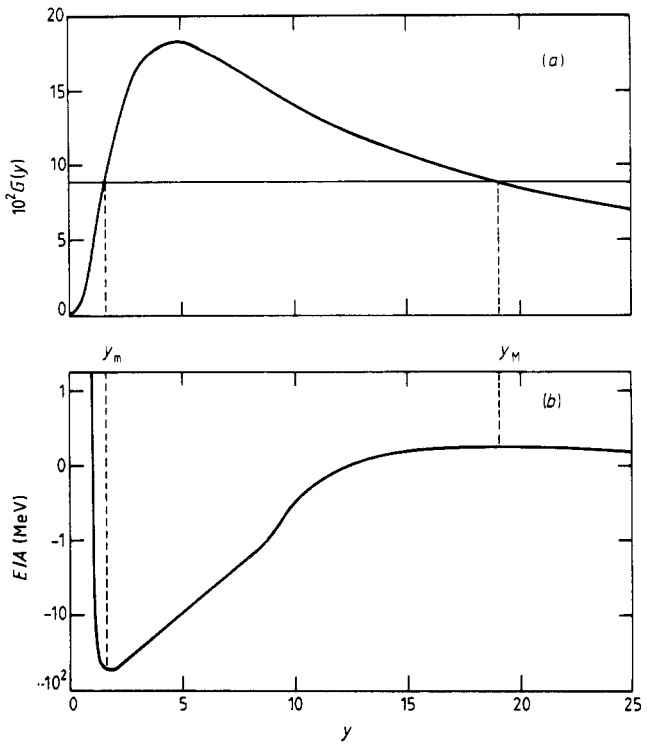

Figure 1. Stability condition for an attractive exponential force. (*a*) y_m and y_M are the solutions of stable and unstable equilibria. (*b*) Energy per fermion as a function of y.

value of A makes y_m and y_M smaller and larger respectively, and eventually they would enter the asymptotic regimes of (7). As can be seen in figure 1(*b*) where the energy per fermion is plotted against y, y_m corresponds to the solution of minimum energy and y_M to the maximum. The existence of a maximum in the energy is a consequence of the short range of the attractive force, because in a very diluted assembly the potential energy is practically null but not the kinetic energy, which increases according to (4). Only when the value $R_M = y_M/\mu$ is crossed, the attraction effect is manifest and the total energy begins to decrease. At very short distances, the kinetic energy repulsion takes over again. The specific parameters used in figure 1 are: $V_0 = 15$ MeV, $m = 939$ MeV, $\mu = 137$ MeV and $A = 100$. The solutions are $y_m = 1.7$ and $y_M = 19$; i.e. $R_m = 2.5$ fm.

If the value of A is very large, the radius of stability may be calculated from (7*a*) and

$$R_m = [\tfrac{7}{24}(9\pi)^{2/3}]^{1/3}(V_0 m\mu)^{-1/3}A^{-1/9} \tag{8}$$

is obtained. This equation illustrates the collapse induced by purely attractive interactions: the greater the value of A, the smaller the radius of stability of a fermion assembly. This property must also appear in the TF method. It is noteworthy that the exponential forces induce a weaker form of collapse ($R_m \propto A^{-1/9}$) than the Yukawa or Coulomb forces ($R_m \propto A^{-1/3}$). Kinematically an assembly like this, if the density is high enough, would eventually enter a relativistic regime, but we will maintain the non-relativistic formulation (3), taking for granted it is always valid.

2.2. Field equation

According to (1), a distribution of particles with a density $n(\bar{r})$ creates a potential at the position $\bar{r}'$ given by

$$\phi(\bar{r}') = -g \int d^3r\, n(\bar{r}) \exp(-\mu|\bar{r}-\bar{r}'|). \tag{9}$$

In order to implement the TF method we need a local equation for the field ϕ, so let us apply the Laplacian operator to both sides of (9). Assuming spherical symmetry for ϕ and for n, we get

$$\Delta'\phi(\bar{r}') - \mu^2\phi(\bar{r}') = 2g\mu \int_0^R d^3r \frac{n(\bar{r})}{|\bar{r}-\bar{r}'|} \exp(-\mu|\bar{r}-\bar{r}'|). \tag{10}$$

This result differs from the Yukawa case in a qualitative way. There, the application of ∇'^2 leads to the massive Poisson equation, which is a second-order differential equation and not a second-order integro-differential equation, as we have obtained here. Building the TF method on (10) would be really very complicated because of its non-locality: the behaviour of ϕ at a point depends on the value of n in all space. Hence it would demand an awkward self-consistency and the model would definitely lose its simplicity. A possible solution to this problem is to apply the ∇'^2 operator again to both sides of (10) obtaining

$$\nabla^4\phi - 2\mu^2\nabla^2\phi + \mu^4\phi + 8\pi g\mu n = 0 \tag{11}$$

thus solving the problem of locality, although at the cost of increasing the order of the field equation from two to four. This poses the question of what are the two additional boundary conditions necessary for a proper solution of (11). Let us postpone this point for the moment.

2.3. TF equation

Now we impose the condition of statistical equilibrium:

$$p_F^2(r)/2m + g\phi(r) = g\phi(R) = -C \tag{12}$$

i.e. the maximum energy of a particle at any location of the distribution is a constant $(-C)$. By definition $-C$ is the potential energy of a fermion at the border of the distribution, where its kinetic energy vanishes, and is equal to

$$-C = \frac{2\pi V_0}{\mu R} e^{-\mu R} \int_0^R nr\, dr[e^{-\mu r}(R + r + \mu^{-1}) - e^{\mu r}(R - r + \mu^{-1})]. \tag{13}$$

Just as in (3) we assume locally

$$n = 2P_F^3/3\pi^2. \tag{14}$$

From (12) and (14) we have

$$n = \frac{2}{3\pi^2}(2m)^{3/2}(-C - g\phi)^{3/2}. \tag{15}$$

Finally, by eliminating n between (15) and (11) we obtain a differential equation only in ϕ:

$$\nabla^4\phi - 2\mu^2\nabla^2\phi + \mu^4\phi = \frac{-16}{3\pi} g\mu(2m)^{3/2}(-C - g\phi)^{3/2}. \tag{16}$$

We now make a change of variable in (16) to the standard TF adimensional variables χ and x.

$$\phi = -\frac{C}{g} - \frac{\chi}{gr} \qquad r = bx \qquad b^{7/2} = \frac{3\pi}{16 \times 2^{3/2} V_0 \mu m^{3/2}} \tag{17}$$

to obtain

$$\dddot{\chi} - 2b^2\mu^2\ddot{\chi} + \mu^4 b^4 \chi + \mu^4 C b^5 x = \chi^{3/2}/x^{1/2}. \tag{18}$$

This is the TF equation for exponential forces. Its novelty lies in its fourth-order nature coming from (11). According to the definition of b in (17), this length scale depends only on m, μ and V_0, that is, it is independent of A. Apart from that, C does depend on A, and its presence in (18) implies that this equation is not universal and consequently it must be solved for a specific value of A. Furthermore, its solution should obviously fulfil a self-consistency condition: the input of C inserted as a parameter in (18) must be exactly reproduced as an output by the integration of (13).

2.4. Boundary conditions

χ must be regular at the origin. Given its MacLaurin development:

$$\chi = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + \ldots \qquad x \to 0 \tag{19}$$

in order to construct a physical solution of (18), we need to know the value of the first four coefficients a_0, a_1, a_2 and a_3, of (19).

Now, as ϕ has to be finite at the origin, from (17) we deduce that χ must be zero there, i.e. $a_0 = 0$.

As (15) implies that

$$n = \frac{2}{3\pi^2} \frac{(2m)^{3/2} g^3}{b^{3/2}} \left(\frac{\chi}{x}\right)^{3/2} \tag{20}$$

n cannot be zero at the origin, and therefore $a_1 > 0$; and besides $\mathrm{d}n/\mathrm{d}y|_{(y=0)} = 0$, which implies $a_2 = 0$. So we only need to know the values of the first two odd coefficients a_1 and a_3 because a_0 and a_2 are zero. Therefore the effective MacLaurin expansion would be as follows:

$$\chi = a_1 x + a_3 x^3 + a_4 x^4 + a_5 x^5 + \ldots. \tag{21}$$

In fact only one of the two unknown coefficients is independent, because one has to remember that the total fermion number A is given, and a_1 is such that the solution χ has to lodge that precise number of particles. It follows therefore that only one additional relation is needed. But where is it?

Let us explore the substitution of (21) in (18). For small x we have

$$(24a_4 + 120a_5 x + \ldots) - 2b^2\mu^2(6a_3 x + \ldots) + \mu^4 b^4 (a_1 x + \ldots) + \mu^4 C b^5 (x + \ldots) = a_1^{3/2}(x + \ldots) \tag{22}$$

which implies

$$a_4 = 0 \qquad 120a_5 - 12b^2\mu^2 a_3 + \mu^4 b^4 a_1 + \mu^4 C b^5 = a_1^{3/2} \tag{23}$$

so we see that the next even coefficient is also zero. Unfortunately a_1 and a_3 appear linked with a_5, which stops us obtaining a_3 in terms of only lower coefficients (or

parameters of the model). Successive higher powers in the x expansion of (18) link higher coefficients which are of no use for our purposes. So far our discussion has been based on the search for a solution for (18), which requires the knowledge of the first four coefficients of the expansion of χ near the origin. We realise that the usual two boundary conditions of $n'(r=0)=0$ and an $n(0)$ value such that the solutions lodge A, are apparently insufficient to establish a single solution. On the other hand, from a physicist's point of view this is meaningless: we are sure that specifying $n(0)$ and $n'(0)=0$ should define the physics uniquely. What then is missing in our analysis?

The key to this consists in realising that in order to obtain a local equation like (16) we have been forced to increase the order of differentiation from two to four. In doing that we have lost information, in the sense that not all the solutions of (11) are solutions of (10) whereas all the solutions of (10) are solutions of (11). In order to implement TF we need to work with (11) because of its locality, but (10) is necessary to reduce the extra freedom induced by the operation of differentiation. Let us examine this more closely. Substituting (17) in (10) we obtain

$$-\frac{1}{g}\frac{\chi'}{b^3x'}-\mu^2\left(-\frac{C}{g}-\frac{\chi'}{gbx'}\right)=2g\mu\int_0^R \mathrm{d}^3r\frac{n(r)}{|\bar{r}-\bar{r}'|}\exp(-\mu|\bar{r}-\bar{r}'|). \tag{24}$$

When $r'\to 0$, it leads to

$$\frac{-6a_3}{\mu b^2}-\mu(-Cb-a_1)=2V_0b\int_0^R \mathrm{d}^3r\frac{n(r)}{r}\mathrm{e}^{-\mu r}. \tag{25}$$

Let us call the right-hand side D, i.e.

$$D=2bV_0\int_0^R \mathrm{d}^3r\frac{n(r)}{r}\mathrm{e}^{-\mu r}. \tag{26}$$

This function is loosely related to the potential energy at the origin, and in that sense is a counterpart of C. Equation (25) constitutes the new condition we are looking for, linking a_1 and a_3:

$$C\mu b+\mu a_1-(6a_3/\mu b^2)=D. \tag{27}$$

The horizon is now free, and we are able to perform a numerical integration of (18).

3. Numerical solutions and conclusions

The procedure is as follows. Given the set of parameters that define the problem, i.e. m, μ, V_0 and A, we apply the Runge-Kutta method to (18). As b is known, we need to specify C, which appears in the equation, plus the χ function and its first three derivatives at the origin, i.e. a_0, a_1, a_2 and a_3. As previously stated a_0 and a_2 are zero, so our task is to explore an initial set of three parameters a_1, a_3 and C, in such a way that, from the resulting χ, the following three conditions are fulfilled:

(i) Through (20) and (13), the C obtained from χ must neccessarily coincide with the C used as input in the equation.

(ii) The A obtained by integrating n must coincide with our assumed fermion number of the assembly.

(iii) The self-consistent C, and the D obtained from (25) must match in (27).

Our numerical integration is performed using the following set of parameters

$$m=939\text{ MeV}\qquad \mu=137\text{ MeV}\qquad V_0=15\text{ MeV}. \tag{28}$$

Although they remind us of the scales proper for nuclear physics, this system is clearly not a model of the nucleus, because there is no repulsive agent which can induce saturation.

We have obtained two independent solutions to exemplify how this method works. In the first case we used $C = 132$ MeV. This required $a_1 = 1.011$ and $a_3 = -0.1088$ in order to fulfil the three previously stated conditions. The solution corresponds to $A = 77$, with $R = 3.14$ fm and an average binding of $E/A = -50.5$ MeV. In the second case, $C = 300$ MeV, $a_1 = 1.889$, $a_3 = -0.254$, $R = 2.73$ fm, $A = 137$ and $E/A = -120.6$ MeV. In figure 2, the two TF solutions are plotted. Our results agree with our expectations, namely the greater the value of A the more closely packed the system is, and there is an increase in the binding energy per fermion.

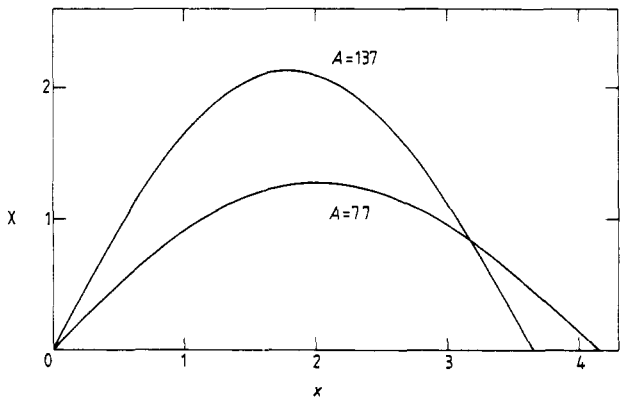

Figure 2. TF solutions for an attractive exponential interaction.

To fix the extra freedom of (11), we have used (10) in the limit $r' \to 0$. It is important to remark that we could alternatively have used (9). In that case the condition obtained would have been as follows:

$$a_1 + b(C + F) = 0 \tag{29}$$

where F is defined as

$$F = g^2 \int_0^R d^3r\, n\, e^{-\mu r}. \tag{30}$$

This procedure must lead, of course, to the same physical solutions. This has been numerically checked in the two solutions explained above.

To conclude, we have shown how the TF method as used in atomic physics can be easily and elegantly extended to the case of exponential forces. It leads to a fourth-order differential equation, but in fact the two usual physical inputs $n(0)$ and $n'(0) = 0$ alone are sufficient to specify the solutions, because the intermediate second-order integro-differential equation provides the additional condition required. Once the procedure for dealing with the attractive exponential force is understood, one can easily introduce a short-range infinite repulsion, by working with an effective kinetic energy just as we did in [5].

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