Some specific solutions of a generalized Emden equation, embracing Thomas-Fermi-like theories

2001 J. Phys. A: Math. Gen. 34 L341

(http://iopscience.iop.org/0305-4470/34/23/101)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) L341–L345 www.iop.org/Journals/ja PII: S0305-4470(01)21210-4

LETTER TO THE EDITOR

Some specific solutions of a generalized Emden equation, embracing Thomas–Fermi-like theories

N H March[1,2] **and L M Nieto**[3,4]

[1] Department of Physics, University of Antwerp (RUCA), Antwerpen, Belgium
[2] Oxford University, Oxford, UK
[3] Departamento de Física Teórica, Universidad de Valladolid, 47005 Valladolid, Spain

E-mail: luismi@metodos.fam.cie.uva.es

Received 17 January 2001, in final form 27 April 2001

Abstract
Recently, a generalization of Emden's equation has been proposed by one of us in a form which embraces Thomas–Fermi-like theories. Here some specific solutions are presented and discussed.

PACS numbers: 0530F, 0230H, 3115B

Recently [1], a generalization of Emden's equation has been proposed, namely

$$\frac{\mathrm{d}^2\phi_n^{(\lambda)}(x)}{\mathrm{d}x^2} = \frac{\left(\phi_n^{(\lambda)}(x)\right)^n}{x^{n-1}}\left[1+\lambda\,\frac{\phi_n^{(\lambda)}(x)}{x}\right]^n. \qquad (1)$$

The motivation for the generalization (1) was to embrace equations arising in the simplest self-consistent density functional theory: namely the Thomas–Fermi (TF) statistical method [2]. More precisely, for $n = 3/2$ and $\lambda = 0$, equation (1) is the usual dimensionless TF equation designed to describe the screening of the nuclear potential energy $-Ze^2/r$ by the electron density distribution in heavy atoms and positive ions. This is readily seen from the electron gas relation between density $\varrho(\boldsymbol{r})$ and Fermi momentum $p_{\mathrm{F}}(\boldsymbol{r})$ that becomes, when used locally [2]

$$\varrho(\boldsymbol{r}) = \frac{8\pi}{3h^3}\,p_{\mathrm{F}}(\boldsymbol{r}). \qquad (2)$$

This is then to be combined with the equation expressing the constancy of the chemical potential μ throughout the entire inhomogeneous electron density $\varrho(\boldsymbol{r})$

$$\mu = \frac{p_{\mathrm{F}}^2(\boldsymbol{r})}{2m} + V(\boldsymbol{r}) \qquad (3)$$

where $V(\boldsymbol{r})$ is the self-consistent potential energy experienced by an electron in the atomic ion. Eliminating $p_{\mathrm{F}}(\boldsymbol{r})$ between equations (2) and (3) and invoking self-consistency through Poisson's equation

$$\nabla^2 V(\boldsymbol{r}) = 4\pi e^2 \varrho(\boldsymbol{r}) \qquad (4)$$

[4] Corresponding author.

then yields, for spherically symmetric atomic ions, and writing $\mu - V(\boldsymbol{r}) = (Ze^2/r)\,\phi^{(0)}_{3/2}(x)$, $r = \text{const}\, Z^{-1/3}\, x$, with Z the atomic number, equation (1) with $\lambda = 0$ and $n = 3/2$. The introduction of a non-zero value of λ embraces the relativistic generalization of this TF equation, which goes back to Vallarta and Rosen [3]. This is readily verified by replacing the non-relativistic kinetic energy $p^2_{\mathrm{F}}(\boldsymbol{r})/2m$ by the special relativity relation $\sqrt{c^2\, p^2_{\mathrm{F}}(\boldsymbol{r}) + m_0^2\, c^4} - m_0\, c^2$, where the electron rest mass energy $m_0\, c^2$ has been subtracted out in order to recover equation (3) in the non-relativistic limit $c \to \infty$. In addition, it should also be noted that, for the choices $n = 1/2$ and $\lambda = 0$ in equation (1) one is led back to the equation of Kadomtsev [4] describing heavy atomic ions subjected to an intense external magnetic field. For this same value of n, and $\lambda \neq 0$, one obtains the relativistic generalization of the Kadomtsev treatment derived by Hill *et al* [5].

Let us begin with solutions for $\lambda = 0$, i.e. the non-relativistic limit of equation (1). Then (see also [1]),

$$\phi^{(0)}_n(x) = A\, x^{\beta} \tag{5}$$

is a solution, provided A and β are chosen as

$$A = (\beta(\beta - 1))^{\frac{1}{n-1}} \qquad \beta = \frac{n-3}{n-1}. \tag{6}$$

Coulson and March [6] generalized the form (5) for $n = 3/2$, namely $\phi^{(0)}_{3/2}(x) = 144/x^3$ going back to Sommerfeld [7], to read at sufficiently large x:

$$\phi^{(0)}_{3/2}(x) = \frac{144}{x^3}\left[1 - \frac{F_1}{x^c} + \frac{F_2}{x^{2c}} - \cdots\right] \tag{7}$$

where the exponent c is given by

$$c = \frac{-7 + \sqrt{73}}{2} \approx 0.772. \tag{8}$$

The first achievement of this letter is to obtain the exponent c as a function of n appearing in equation (1) for the non-relativistic limit in which λ tends to zero. Taking into account the fact that equation (5), with A and β given by (6), is a solution of equation (1) for $\lambda = 0$, we can find a more general solution near the point of infinity in the form

$$\phi^{(0)}_n(x) = A\, x^{\beta}\, g(x^{-c}) \tag{9}$$

where $c > 0$ is a parameter to be determined, and $g(z)$ is an analytic function. It is easy to prove that the function $g(z)$ satisfies the differential equation

$$g''(z) + \left(\frac{c + 1 - 2\beta}{c\, z}\right) g'(z) + \left(\frac{\beta(\beta - 1)}{c^2\, z^2}\right)(g(z) - g^n(z)) = 0. \tag{10}$$

If $n \geqslant 0$, $z = 0$ is a regular singular point of the equation. We can try to find a solution of (10) as a Taylor series

$$g(z) = \sum_{\ell=0}^{\infty} g_\ell\, z^\ell \tag{11}$$

and we find from the two lowest order powers of z that $g_0 = 1$ and

$$c^2 + (1 - 2\beta)c + \beta(\beta - 1)(1 - n) = 0. \tag{12}$$

The last equation has two solutions

$$c = \frac{(n-5) \pm \sqrt{1 + 22n - 7n^2}}{2(n-1)}. \tag{13}$$

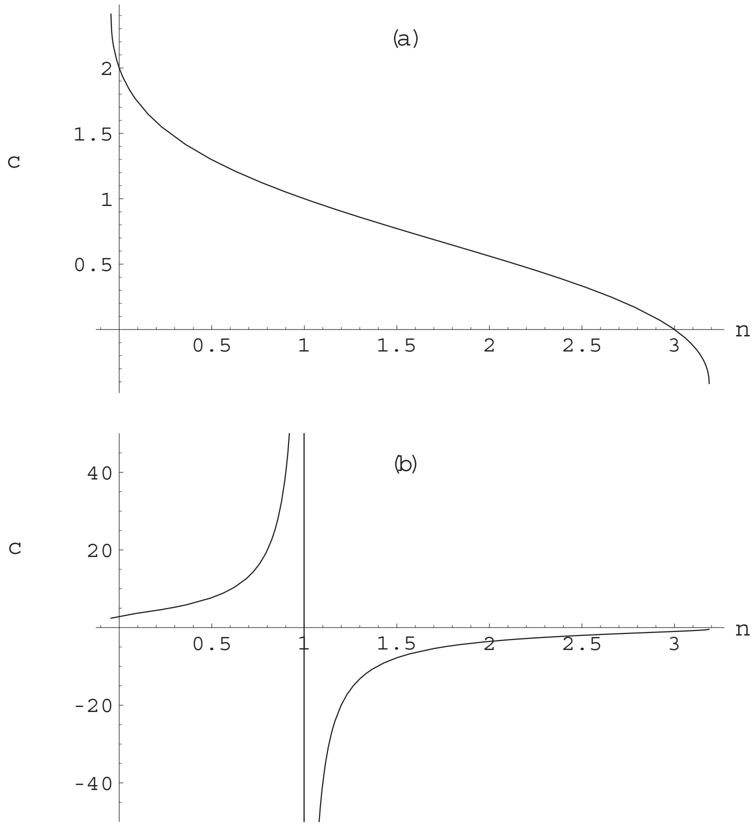

Figure 1. (*a*) A plot of $c_+(n)$ from equation (13) with the positive sign before the square root. (*b*) Same as (*a*) but for $c_-(n)$ from equation (13).

With the positive sign, the solution, c_+ say, is $c_+ > 0$ if $n \leqslant 3$, and it has the form shown in figure 1(*a*). The range of n over which c_+ is purely real is given by

$$-0.05 \approx \frac{11 - 8\sqrt{2}}{7} < n < \frac{11 + 8\sqrt{2}}{7} \approx 3.19. \tag{14}$$

For the solution, c_-, corresponding to the negative sign in equation (13), there is also a region of positive c_-, but then c_- has singular behaviour at $n = 1$, as shown in figure 1(*b*).

In principle, given F_1 in equation (7), the coefficients $F_\ell,\ \ell > 1$, can be derived, but we shall not present that degree of detail here. The same is true for the coefficients g_ℓ of $g(z)$ in equation (11).

Rather, we turn to the modifications that are induced in the solution (5) by the retention of $\lambda \neq 0$ in equation (1). As discussed in detail by Senatore and March [8] for the case $n = 3/2$, the Sommerfeld solution $\phi^{(0)}_{3/2}(x) = 144/x^3$ corresponding to $\lambda = 0$ is modified to read

$$\phi^{(\lambda)}_{3/2}(x) = \frac{144}{x^3}\, f\left(\frac{\lambda}{x^4}\right) \tag{15}$$

where $f(s)$ satisfies another non-linear differential equation, $f(0)$ being equal to unity to regain the Sommerfeld solution. It turns out that $f(s)$ has a simple pole, at $x = x_c$ say, and x_c depends on λ as $x_c \propto \lambda^{1/4}$. Thus, figure 2 shows how non-zero λ affects the non-analyticity in the ϕ–x plane for this specific case $n = 3/2$, $\lambda \neq 0$.

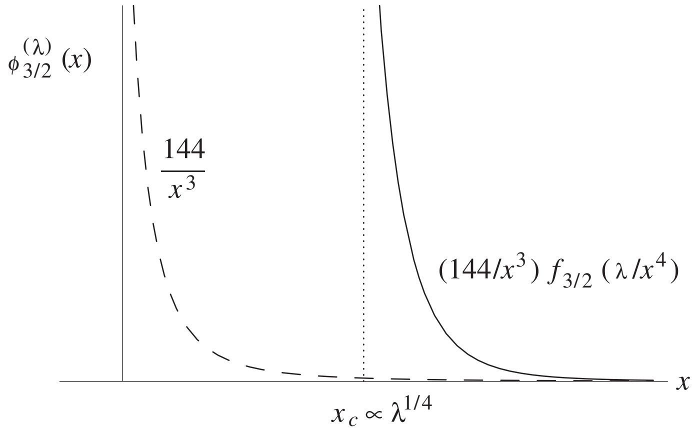

Figure 2. This plot depicts the $\phi_n^{(\lambda)}(x)$ plane 'divided' by the non-relativistic solution in equation (5). For $n = 3/2$, $\phi_{3/2}^{(\lambda)}(x) = (144/x^3)\ f_{3/2}(\lambda/x^4)$ and $f_{3/2}(s)$ has a simple pole at $s = s_c \sim 10^{-2}$.

Our second objective below is to mathematically describe the way the $\lambda = 0$ solution given by equations (5) and (6) is altered by relativistic effects characterized by $\lambda \neq 0$. In order to do that, we will try to find a solution of equation (1) in a form similar to those already considered, like for example (15)

$$\phi_n^{(\lambda)}(x) = A\, x^{\beta}\ f_n(\lambda/x^{\gamma}). \tag{16}$$

The parameters A, β, γ are chosen in such a way as to have a relatively simple differential equation for the function $f_n(s)$, satisfying $f_n(0) = 1$. If we take A, β depending on n as given in equations (6), and $\gamma = 1 - \beta$, we obtain the following equation:

$$2s^2\ f_n''(s) + (7-n)s\ f_n'(s) + (3-n)\ f_n(s) = (3-n)\,(f_n(s) + As\ f_n^2(s))^n. \tag{17}$$

This equation reduces to the form given by Senatore and March [8] for the particular case $n = 3/2$. In order to investigate if the non-linear differential equation (17) has a singularity at a finite value of $s = \lambda/x^{\gamma}$, say s_c, we try to find a solution of it which in the neighbourhood of s_c behaves like

$$f_n(s) \sim \alpha(s_c - s)^{-\mu} \qquad \mu > 0. \tag{18}$$

After a simple calculation we can see that the parameter μ depends on n as

$$\mu = \frac{2}{2n-1} \tag{19}$$

and α, s_c are related through

$$\alpha^{2n-1}\, s_c^{n-2} = \frac{2\mu(\mu+1)}{(3-n)A^n}. \tag{20}$$

From these results we can see that for different values of n, the singular solution near s_c is of a different type; for example, it is a simple pole for $n = 3/2$ (the example analysed by Senatore and March in [8]), a triple pole for $n = 5/6$, etc. For $n = 1/2$ (the case of heavy positive atomic ions in intense applied magnetic fields) the solution seems to present an essential singularity, and for other values of n, s_c will be a branch point. In any case, the singularity on the variable x, say x_c, depends on λ as $x_c \propto \lambda^{(n-1)/2}$.

Another possibility we can explore is to find a solution of (17) as a power series solution around $s = 0$, taking into account that $f_n(0) = 1$. The radius of convergence of this series depends on n and determines the position of the singularity s_c. We show here the first terms of the series

$$f_n(s) = 1 + a_1 s + a_2 s^2 + \cdots = 1 + \left[\frac{n(3-n)A}{n^2 - 5n + 10}\right] s + \left[\frac{2A^2 n(n^5 - 12n^4 + 63n^3 - 173n^2 + 220n - 75)}{(n^2 - 5n + 10)^2 (n^2 - 6n + 21)}\right] s^2 + \cdots .$$

Again, for the special case $n = 3/2$, this solution coincides with the result of Senatore and March [8].

In summary, the main results are embodied in equation (13), and the corresponding figure 1, which generalizes the shape (only) of the Coulson–March solution (7) of the generalized TF equation (1) in the non-relativistic limit to have a dependence of the exponent c on the power n in equation (13). For the case when relativistic effects are included, the principal findings are that the solution (15) appropriate to $n = 3/2$ and non-zero λ generalizes to

$$\phi_n^{(\lambda)}(x) = A\, x^{\beta}\, f_n\,(\lambda/x^{\gamma})\,. \tag{21}$$

The other case of immediate physical interest corresponds to $n = 1/2$, which applies to heavy positive atomic ions (plus neutral atoms) in intense applied magnetic fields. However, $\beta = 3$ in this case, and the physical significance of (21) appears to be quite different. We shall therefore not pursue further the case of atoms in huge magnetic fields here (see, however, Lieb *et al* [9] for a discussion of the limits of validity of the Kadomtsev treatment [4] of positive ions in magnetic fields).

It is a pleasure for NHM to thank Professor J A Alonso for his most generous hospitality during a visit to the University of Valladolid, which made possible this collaborative study. This work has been supported by the Spanish DGES (PB98-0370) and Junta de Castilla y León (CO2/199). Finally we wish to thank the referees for constructive comments which have improved the presentation of this letter.

References

[1] March N H 2000 submitted
[2] See e.g. March N H 1992 *Electron Density Theory of Atoms and Molecules* (New York: Academic)
[3] Vallarta M S and Rosen N 1932 *Phys. Rev.* **41** 708
[4] Kadomtsev B B 1970 *Sov. Phys.–JETP* **31** 945
[5] Hill S H, Grout P J and March N H 1985 *J. Phys. B: At. Mol. Phys.* **18** 4665
[6] Coulson C A and March N H 1950 *Proc. Phys. Soc. Lond.* A **63** 367
[7] Sommerfeld A 1932 *Z. Phys.* **78** 283
[8] Senatore G and March N H 1985 *Phys. Rev.* A **32** 3277
[9] Lieb E H, Solovej J P and Yngvasson J 1992 *Phys. Rev. Lett.* **69** 749