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An exact result for the Thomas–Fermi equation: *a priori* bounds for the potential slope at the origin

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Abstract

We examine the nonlinear boundary value problem formed by the Thomas–Fermi equation $\phi'' = \phi^{3/2}x^{-1/2}$, complemented with the boundary conditions $\phi(0) = 1$ and $\phi(\infty) = 0$. We show that the value of ϕ' at the origin, which plays a crucial role in this problem, can be accurately bounded *a priori*, by exploiting integral properties of the Thomas–Fermi equation, and without any assumption on the functional dependence of $\phi(x)$. Extension of the approach to more general equations of the Emden–Fowler type is also briefly considered.

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1. Introduction

The charge density distribution in neutral atoms of high atomic number is well described by the Thomas–Fermi equation (see, for example, the review [1]), which, using suitable normalizations, can be written as

$$\phi'' = \frac{\phi^{3/2}}{x^{1/2}}. \tag{1}$$

The Thomas–Fermi potential ϕ is a non-negative function of x, which is taken to satisfy the boundary conditions

$$\phi(0) = 1, \qquad \phi(\infty) = 0. \tag{2}$$

Equation (1) is one of the famous equations of mathematical physics (see [2]), and has been the subject of many investigations. By now, the physical implications of this equation, and, more generally, of the Thomas–Fermi atomic theory have been thoroughly explored (see, e.g., [1, 3]). On the other hand, mathematical aspects of (1) are still frequently discussed in the literature, since the equation represents a popular setting for the test of new methods for solving nonlinear ode's.

From a mathematical point of view, (1) and (2) define a difficult nonlinear boundary value problem. The main complications involved, already recognized in earlier work by Hille [4], are clearly expounded in [2, 5]. A key issue is the determination of the slope $\phi_0' \equiv \phi'(0)$, which also has an important physical meaning, being proportional to the energy of the neutral atom. As noted in [5], ϕ_0' can be regarded as an eigenvalue of the problem; the correct value,

$$\phi_0' = -1.588\,0710\ldots, \tag{3}$$

yields a well-posed boundary value problem, with a monotone decreasing solution, while larger or smaller values of ϕ_0' give rise to singular or spatially confined solutions, respectively (see [2]). This makes the construction of a numerical approach to the solution of (1)–(2) a delicate matter.

The quantity ϕ_0' appears difficult to compute by any means (the value in (3) results from an accurate numerical integration by Kobayashi *et al* [6]). Since ϕ_0' represents a global property of the problem, it cannot be computed via a local expansion; when series solutions are sought, as in [7], calculation of ϕ_0' involves an elaborate matching of small-x and large-x expansions. Iterative approaches, such as the δ-expansion method introduced by Bender *et al* [5], and further examined in [8], have provided a good alternative. However, a pretty large number of iterations is required for an accurate solution (and an accurate ϕ_0'), and, except for the very first steps, the approximant linear ode's must be solved numerically. Although other approaches have been proposed in the last two decades (see, e.g., [9] and references therein), these difficulties have not been fully overcome.

A point to be stressed is that in all these works approximations for ϕ_0' are to be computed *a posteriori*, as a part of the solution. It is not clear, however, whether this is mandatory; since ϕ_0' is a global quantity, information on it could be deducible from integral properties of the equation. The main purpose of this paper is to explore this possibility. We shall show that useful integral relations can indeed be derived for (1), and employed to construct accurate *a priori* bounds for ϕ_0'. This will require no assumption on the functional form of $\phi(x)$; we will only need to use the fact that ϕ is a decreasing function of x, which is a simple consequence of the non-negativity of ϕ, and of (1)–(2).

To end the paper, we will briefly examine the extension of the approach to more general equations of the Emden–Fowler type.

2. Derivation of the bounds

Let us show, with a simple example, how integral properties may be used to bound ϕ_0'. Multiplying (1) by $x\phi'^{n-1}$, with $n > 1$ an integer, and integrating on both sides, gives

$$\int_0^\infty \phi'^n = -n \int_0^\infty x^{1/2}\phi^{3/2}\phi'^{n-1}. \tag{4}$$

Integrating twice the term on the rhs by parts, and using (1) and (2), gives rise to a term proportional to $\phi_0'^{n-1}$, and we end up with the identity

$$\phi_0'^{n-1} = -\frac{6n-5}{n}\int_0^\infty \phi'^n + 2(n-1)(n-2)\int_0^\infty \phi^4\phi'^{n-3}. \tag{5}$$

For $n = 2$, this gives

$$\phi_0' = -\frac{7}{2}\int_0^\infty \phi'^2, \tag{6}$$

which is nice, but not very helpful. Instead, for $n = 4$, one finds

$$\phi_0'^3 = -\frac{12}{5} - \frac{19}{4}\int_0^\infty \phi'^4, \tag{7}$$

which is a useful relation. Since the last term is negative definite, (7) implies

$$\phi_0' < -\left(\tfrac{12}{5}\right)^{1/3} = -1.338\,8659. \tag{8}$$

The upper bound (8) differs from the 'true' value (3) by less than 16%, which is not too bad for a first try. As we shall see, with a little effort, it is possible to do much better.

2.1. First step

We now consider the identity

$$\int_0^\infty \frac{\phi'}{\phi^m} = -\frac{1}{1-m}, \tag{9}$$

with $m < 1$. Multiplying and dividing the integrand on the lhs by $x^{1/2}\phi^{-3/2}$, using (1), and integrating by parts, we get

$$\int_0^\infty \frac{\phi'}{\phi^m} = -\frac{1}{4}\int_0^\infty \frac{1}{x^{1/2}}\frac{\phi'^2}{\phi^{m+3/2}} + \frac{1}{2}\left(m+\frac{3}{2}\right)\int_0^\infty x^{1/2}\frac{\phi'^3}{\phi^{m+5/2}}. \tag{10}$$

(Here we have assumed that $x^{1/2}\phi'^2\phi^{-m-3/2}$ vanishes at infinity; since ϕ decays as x^{-3} at large x (see, e.g., [1]), this is certainly verified for $m < 1$.) As in the previous example, we now perform a second integration by parts, which produces a term proportional to $\phi_0'^3$. Placing the result in (9), and solving for $K \equiv \phi_0'^3$, finally gives

$$K = -\frac{12}{1-m} + F(m), \tag{11}$$

with

$$F(m) \equiv \frac{5}{2}\left(m+\frac{21}{10}\right)\int_0^\infty \frac{\phi'^4}{\phi^{m+4}} - \frac{3}{2}\left(m+\frac{3}{2}\right)(m+4)\int_0^\infty x\frac{\phi'^5}{\phi^{m+5}}. \tag{12}$$

Note that the first term on the rhs of (12) is positive for $m > -21/10$, while the second is negative definite for $-4 < m < -3/2$ (ϕ being a monotone decreasing function of x). It follows that

$$K < -\frac{12}{1+21/10} = -\frac{120}{31}, \tag{13}$$

and

$$K > -\frac{12}{1+3/2} = -\frac{24}{5}, \tag{14}$$

which give the bounds

$$-1.686\,8653 < \phi_0' < -1.570\,1453. \tag{15}$$

Another way to look at this result is the following. Since F is negative for $m \leqslant -21/10$, and positive for $m \geqslant -3/2$, there must be a value m^*, in the interval $]-21/10, -3/2[$, such that $F(m^*) = 0$ and $K = -12/(1-m^*)$. Thus, improving the bounds on K is equivalent to narrowing the interval in which m^* is included.

The upper bound in (15) is already quite good. We note, by comparison, that it improves the bound $\phi_0' < -1.563$ derived by Anderson *et al* [10], by using complementary variational principles. The lower bound is not so tight, but can be improved by focusing on the points at which the second term in (12) vanishes. For $m = -3/2$, (11) yields

$$K = -\frac{24}{5} + \frac{3}{2}\int_0^\infty \frac{\phi'^4}{\phi^{5/2}}, \tag{16}$$

while for $m = -4$, it reduces to the expression (7), previously obtained. It follows from (16) that

$$K > -\frac{24}{5} + \frac{3}{2}\int_0^\infty \phi'^4, \tag{17}$$

and, using (7), that

$$K > -\frac{528}{125}. \tag{18}$$

Thus, this first step gives us the bounds

$$-1.616\,4960 < \phi_0' < -1.570\,1453. \tag{19}$$

2.2. *Second step*

To improve the bounds (19), we need to work on the expression of $F(m)$. The basic idea is to keep integrating by parts, as in (10), to bring in higher powers of K, together with integrals involving higher powers of ϕ'. This is done with the help of the identities

$$\begin{aligned}\int_0^\infty \frac{\phi'^p}{\phi^m} &= \frac{\phi_0'^{p+2}}{2(p+1)(p+2)} - \frac{1}{p+1}\left[\frac{m+3}{2(p+2)} + \frac{m+3/2}{p+3}\right]\int_0^\infty \frac{\phi'^{p+3}}{\phi^{m+4}} \\ &\quad + \frac{(m+3/2)(m+4)}{(p+1)(p+3)}\int_0^\infty \frac{x\phi'^{p+4}}{\phi^{m+5}}, \end{aligned}\tag{20}$$

$$\begin{aligned}\int_0^\infty x\frac{\phi'^p}{\phi^m} &= \frac{3}{2(p+1)(p+2)}\left(\int_0^\infty \frac{\phi'^{p+2}}{\phi^{m+3}} - (m+3)\int_0^\infty x\frac{\phi'^{p+3}}{\phi^{m+4}}\right) \\ &\quad + \frac{m+3/2}{p+1}\int_0^\infty x^{3/2}\frac{\phi'^{p+2}}{\phi^{m+5/2}}, \end{aligned}\tag{21}$$

whose derivation parallels that of (10) (note that evaluation of (20) for $p = 1$ directly gives (11) and (12)). Applying (20) and (21) to (11) and (12), we find

$$K = -\frac{12}{1-m} + \frac{1}{24}\left(m + \frac{21}{10}\right)K^2 + G(m), \tag{22}$$

with

$$\begin{aligned}G(m) \equiv &-\frac{1}{6}\left(m^2 + \frac{73}{10}m + \frac{591}{56}\right)\int_0^\infty \frac{\phi'^7}{\phi^{m+8}} \\ &+ \frac{1}{8}\left(m^2 + \frac{67}{10}m + \frac{321}{35}\right)(m+8)\int_0^\infty x\frac{\phi'^8}{\phi^{m+9}} \\ &- \frac{1}{4}(m+\frac{3}{2})(m+4)\left(m + \frac{13}{2}\right)\int_0^\infty x^{3/2}\frac{\phi'^7}{\phi^{m+15/2}}. \end{aligned}\tag{23}$$

It is readily seen that $G(m)$ is negative definite in the range $-3.482\,1562 \leqslant m \leqslant -1.985\,9902$, the upper limit coinciding with the larger root of the coefficient of the first integral. In this range, the following inequality holds,

$$K < -\frac{12}{1-m} + \frac{1}{24}\left(m + \frac{21}{10}\right)K^2, \tag{24}$$

giving the bound

$$K < \frac{12}{m+21/10}\left(1 - \sqrt{1 + 2\frac{m+21/10}{1-m}}\right). \tag{25}$$

Since the rhs of (25) is a monotone decreasing function of m, the best bound,

$$K < -3.944\,8425, \tag{26}$$

is obtained at $m = -1.985\,9902$.

Expressions (22) and (23) can now be used to improve the lower bound, following a procedure similar to that used in the first step. Evaluating (22) at $m = -3/2$ and $m = -4$ yields

$$K = -\frac{24}{5} + \frac{1}{40}K^2 - \frac{173}{560}\int_0^\infty \frac{\phi'^7}{\phi^{13/2}} + \frac{6}{35}\int_0^\infty x\frac{\phi'^8}{\phi^{15/2}}, \tag{27}$$

and

$$K = -\frac{12}{5} - \frac{19}{240}K^2 + \frac{247}{560}\int_0^\infty \frac{\phi'^7}{\phi^4} - \frac{57}{280}\int_0^\infty x\frac{\phi'^8}{\phi^5}, \tag{28}$$

respectively. It follows from (27) that

$$K > -\frac{24}{5} + \frac{1}{40}K^2 - \frac{173}{560}\int_0^\infty \frac{\phi'^7}{\phi^4} + \frac{6}{35}\int_0^\infty x\frac{\phi'^8}{\phi^5}, \tag{29}$$

which, using (28), can be rewritten as

$$420K > -\frac{8004}{5} - \frac{361}{48}K^2 + \left(\frac{1482}{35} - \frac{10089}{2800}\right)\int_0^\infty x\frac{\phi'^8}{\phi^5}. \tag{30}$$

Neglecting the last term, that is positive, we finally obtain a quadratic inequality for K, which gives the bound

$$K > -4.114\,5866. \tag{31}$$

Thus, the result of the second step is

$$-1.6024165 < \phi_0' < -1.580\,0708, \tag{32}$$

with both bounds at less than 1% from the true value.

2.3. *Third step*

The third step is still straightforward, but more laborious. We first need to integrate the last term in (23) by parts, which produces another term containing the integral of $x\phi'^8\phi^{-m-9}$, plus an additional term. Then, we use (20) and (21) to get

$$K = -\frac{12}{1-m} + \frac{1}{24}\left(m + \frac{21}{10}\right)K^2 - \frac{1}{864}\left(m^2 + \frac{73}{10}m + \frac{591}{56}\right)K^3 + H(m), \tag{33}$$

with

$$\begin{aligned} H(m) \equiv{}& \frac{11}{1728}\left(m^3 + \frac{78}{5}m^2 + \frac{49\,031}{700}m + \frac{1298\,427}{15\,400}\right)\int_0^\infty \frac{\phi'^{10}}{\phi^{m+12}} \\ &- \frac{1}{192}(m+12)\left(m^3 + 15m^2 + \frac{3271}{50}m + \frac{108\,153}{1400}\right)\int_0^\infty x\frac{\phi'^{11}}{\phi^{m+13}} \\ &+ \frac{1}{48}\left(m + \frac{21}{2}\right)\left(m^3 + \frac{69}{5}m^2 + \frac{7807}{140}m + \frac{2167}{35}\right)\int_0^\infty x^{3/2}\frac{\phi'^{10}}{\phi^{m+23/2}} \\ &- \frac{1}{32}\left(m + \frac{3}{2}\right)(m+4)\left(m + \frac{13}{2}\right)(m+9)\int_0^\infty x^2\frac{\phi'^9}{\phi^{m+10}}. \end{aligned} \tag{34}$$

Again, there is a range in which $H(m)$ is negative definite. The upper limit of this range is $m = -1.932\,2569$, which is the largest root of the cubic in the first term. The corresponding upper limit for K resulting from (33) is

$$K < -3.969\,1493. \tag{35}$$

Calculation of the lower bound proceeds as in the previous step, and we end up with the inequality

$$2.069\,011K > -7.365\,6264 - 0.059\,63K^2 + 1.128\,9438 \times 10^{-3}K^3, \qquad (36)$$

which yields

$$K > -4.075\,6506. \qquad (37)$$

Therefore, our final bounds for ϕ_0' are

$$-1.597\,3459 < \phi_0' < -1.583\,3095. \qquad (38)$$

As a comparison, we may note that the upper bound in (38) is closer to (3) than the [20, 20] homotopy–Pade' approximation computed in [9] (see their table 2).

3. Conclusions

In this work, we have analysed the classical boundary value problem (1)–(2), and shown that very accurate *a priori* bounds on the slope ϕ_0' can be obtained, by exploiting integral properties of the Thomas–Fermi equation.

Since the procedure can be iterated, the best bounds we have obtained can presumably be refined, although at the expense of lenghty calculations. Examination of (33) and (36) indicates that the terms containing powers of K, created in the iteration, are of the same sign, and of rapidly decreasing size. Would this prove true in the subsequent steps, one would expect the iteration to converge. If so, one might then wonder if the procedure would actually converge towards the true value of the slope (this would be remarkable, since the slope would then be solely determined by the global structure of the boundary value problem). Answering these questions does not seem easy, since at each step terms of both signs are created, which combine in ways that become more and more complicated as the iteration progresses.

Leaving the convergence problem as an open issue, we shall conclude by pointing out an easy extension to more general equations of the Emden–Fowler type. Clearly, our approach relies on the $1/2$ power of x appearing in (1), which makes it possible to construct polynomial inequalities for K. On the other hand, there appears to be no constraint on the exponent of ϕ. Consider the Emden–Fowler equation

$$\phi'' = \frac{\phi^s}{x^{1/2}}. \qquad (39)$$

When $s > 1$, the solution of (39) decays as $x^{-q}, q = 3/(2(s-1))$, at large x (see [11]), and we may consider the same boundary value problem just discussed for the Thomas–Fermi equation.

Bounds on ϕ_0' can be found as in the previous section. The identity (20) is now replaced by

$$\int_0^\infty \frac{\phi'^p}{\phi^m} = \frac{{\phi_0}'^{p+2}}{2(p+1)(p+2)} - \frac{1}{p+1}\left[\frac{m+2s}{2(p+2)} + \frac{m+s}{p+3}\right]\int_0^\infty \frac{\phi'^{p+3}}{\phi^{m+2s+1}} + \frac{(m+s)(m+2s+1)}{(p+1)(p+3)}\int_0^\infty \frac{x\phi'^{p+4}}{\phi^{m+2s+2}}. \qquad (40)$$

For $p = 1$, this gives (11) again, with the following expression for $F(m)$:

$$F(m) \equiv \frac{5}{2}\left(m + \frac{7}{5}s\right)\int_0^\infty \frac{\phi'^4}{\phi^{m+2s+1}} - \frac{3}{2}(m+s)(m+2s+1)\int_0^\infty x\frac{\phi'^5}{\phi^{m+2s+2}}. \qquad (41)$$

This leads to the bounds

$$-\frac{12}{1+s} < K < -\frac{60}{5+7s}, \tag{42}$$

which reduce to (13)–(14), as they should, when $s = 3/2$. The lower bound can be improved as done for the Thomas–Fermi equation, and we get

$$-\left(\frac{12}{1+s}\frac{1+4s/5}{1+s}\right)^{1/3} < \phi_0' < -\left(\frac{60}{5+7s}\right)^{1/3}, \tag{43}$$

which generalize the bounds (19). Further refinement of these bounds, along the lines previously discussed, appears possible.

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