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MONOTONE METHODS FOR THE THOMAS-FERMI EQUATION*

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Abstract. The boundary-value problem for the ionized atom case of the Thomas-Fermi equation is transformed to a certain convex nonlinear boundary-value problem. Two iterative procedures, previously developed for such problems, are constructed for the ionized atom problem. A comparative analysis of the efficiency of the iteration schemes is presented. The existence and uniqueness of a solution is established and the solution is shown to have monotonic dependence on the boundary conditions. Numerical bounds are obtained for a specific problem.

1. Introduction. Luning and Perry [1] have recently derived an iterative technique for the solution of the Thomas-Fermi equation, which may be written in the form

$$y''(x) = x^{-1/2}[y(x)]^{3/2}. \tag{1.1}$$

The ionized atom case of the Thomas-Fermi equation is prescribed by the boundary conditions

$$y(0) = 1, \qquad y(a) = 0. \tag{1.2}$$

Luning and Perry first transform the nonlinear boundary value problem (1.1), (1.2) into an eigenvalue problem. By linearizing this eigenvalue problem an iterative scheme based on the construction of eigenpairs is shown to converge to a solution. In addition, the isolated neutral atom case in which (1.2) is replaced by

$$y(0) = 1, \qquad \lim_{x\to\infty} y(x) = 0 \tag{1.3}$$

is shown to have a solution which can be uniformly approximated by the iteration scheme for the ionized atom case.

By using an approach very different from that of Luning and Perry we demonstrate two iterative procedures which are shown to converge monotonically to a solution of problem (1.1), (1.2). Our approach is based on the convexity of the nonlinearity $f(x, y(x)) = x^{-1/2}[y(x)]^{3/2}$ appearing in the Thomas-Fermi equation. Iterative procedures for general boundary-value problems with convex nonlinearities have been obtained in Mooney and Roach [2] and are described in the following section. An indication of the physical applications of these problems can be obtained from the references ([6]–[10]). To these applications we now add the ionized atom case of the Thomas-Fermi equation by showing that it can be transformed to one of a class of boundary-value problems described in [2].

The results of Luning and Perry rely on Sturm-Liouville theory for a certain class of

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ordinary linear differential operator and their iterative method is developed specifically for the problem (1.1), (1.2). In contrast, the methods described here can be applied to certain elliptic partial differential operators and to a whole class of nonlinear functions f including, of course, the case $f(x, y(x)) = x^{-1/2}[y(x)]^{3/2}$. The simplicity of our iterative schemes, developed from the Picard and Newton algorithms, complements the unifying aspects already mentioned (see [3]).

Subsequently the schemes developed for the Thomas-Fermi problem are compared and numerical bounds are presented for a particular case. The solutions are also shown to depend monotonically on the interval length a and to be unique for each choice of a.

2. Monotonicity theory. Before we introduce the iterative schemes, we describe the general class of boundary-value problems discussed in [2] and [5]. We restrict our attention to ordinary differential operators.

L is a second-order selfadjoint operator defined for all x in an open real interval D by

$$Lu(x) = -\frac{d}{dx}\left(a(x)\frac{du}{dx}\right) + a_0(x)\,u(x).$$

The coefficient a is continuously differentiable, a_0 is continuous and $a_0(x) \geq 0$, for all $x \in D$.

We are concerned with equations of the form

$$Lu(x) = f(x, u(x)) \tag{2.1}$$

where $x \in D$ and f is a given function.

It is not necessary to consider here the general boundary conditions given in [2]. We require that if $\partial D = \bar{D} - D$, then a solution u of (2.1) must satisfy

$$u(x) = 0 \qquad \text{for all} \qquad x \in \partial D. \tag{2.2}$$

Here $\bar{D}$ represents the closure of D.

To construct our iteration schemes we need some properties for the nonlinearity f in (2.1). Naturally the construction of a Newton iteration scheme involves greater differentiability requirements for f than a Picard scheme (see [2, 12]). Since we will introduce both schemes for the Thomas-Fermi equation it is simplest if we require f to satisfy the following conditions.

(i) $f(x, \phi)$ is continuously differentiable on the two-dimensional space $\{(x, \phi(x)) : x \in D, \phi \in C^2(D) \text{ and } \phi \geq 0 \text{ on } D\}$; (2.3)

(ii) $f(x, 0) > 0$ for all $x \in D$; (2.4)

(iii) $f_u(x, \phi) = \left.\dfrac{\partial}{\partial u} f(x, u)\right|_{u=\phi} > 0$ for all $x \in D$ and $\phi \geq 0$ (monotonicity condition); (2.5)

(iv) $f_u(x, \phi) > f_u(x, \psi)$ for all $x \in D$ and $\phi > \psi \geq 0$ (convexity condition). (2.6)

We can now give our iteration schemes. A sequence of Picard iterates $\{u_n(x)\}$, $n \geq 0$, is formally defined by

$$\begin{aligned} L\,u_{n+1}(x) &= f(x, u_n(x)), \qquad x \in D \\ u_{n+1}(x) &= 0, \qquad x \in \partial D \end{aligned} \tag{2.7}$$

where $u_0(x)$ is a given function defined on $\bar{D}$. For Newton iterates $\{v_n(x)\}$, $n \geq 0$, the corresponding definition is

$$\begin{aligned} L\, v_{n+1} &= f(x, v_n) + f_u(x, v_n)(v_{n+1} - v_n), \qquad x \in D \\ v_{n+1} &= 0, \qquad x \in \partial D \end{aligned} \tag{2.8}$$

where $v_0(x)$ is a given function defined on $\bar{D}$.

The uniform convergence of the iteration schemes (2.7) and (2.8) to a solution of the problem (2.1), (2.2) is discussed in the monotonicity theorems which follow. It is well known (see [2], p. 84, for references) that certain problems of the type (2.1), (2.2) possess positive solutions and that there is a minimal positive solution $\mathbf{u}(x)$ (i.e. $0 \leq \mathbf{u}(x) \leq u(x)$ on D for any solution $u(x)$). These existence theorems do not apply to the Thomas-Fermi problem (1.1), (1.2) for a reason given in the next section. Instead, we use a monotonicity theorem based on the existence of a subsolution and a supersolution for the problem (2.1), (2.2).

If v satisfies the differential inequalities

$$\begin{aligned} L\, u(x) - f(x, u(x)) \leq 0, \qquad x \in D \\ u(x) \leq 0, \qquad x \in \partial D \end{aligned} \tag{2.9}$$

then v is called a subsolution of the problem (2.1), (2.2). By reversing the above inequality signs a supersolution of the problem (2.1), (2.2) is defined.

THEOREM 2.1. If u_0 is a subsolution and U_0 a supersolution of problem (2.1), (2.2), subject to the conditions (2.3) – (2.5), and u_0, U_0 are such that $u_0(x) \leq U_0(x)$ for all $x \in \bar{D}$, then problem (2.1), (2.2) has at least one solution $u(x)$ with $u_0(x) \leq u(x) \leq U_0(x)$ and

(i) the Picard iterates (2.7) beginning with $u_0(x)$ converge uniformly and monotonically upwards to the least solution of (2.1), (2.2) which lies above $u_0(x)$ and below $U_0(x)$;

(ii) the Picard iterates (2.7) beginning with $U_0(x)$ converge uniformly and monotonically downwards to the greatest solution of (2.1), (2.2) which lies below $U_0(x)$ and above $u_0(x)$.

This existence theorem is used in [2] (Lemma 2.2), and a more general form of the theorem is proved in [12] (Theorem 1). Many extensions of Theorem 2.1 can be found in the literature (see, for example, [14] and [15]). In particular, $u_0 \equiv 0$ is a subsolution of (2.1), (2.2) since $L\, u_0 \equiv 0$ and $f(x, u_0) > 0$, using (2.4).

We now state a uniqueness theorem contained in Mooney and Roach ([2], Theorem 4.1). This result is applicable to problem (2.1), (2.2) when f satisfies the conditions (2.3) – (2.6).

THEOREM 2.2. If $U_0 \geq u_0 \equiv 0$ is a supersolution of problem (2.1), (2.2), subject to the conditions (2.3) – (2.6), then the Picard iterates (2.7) with initial iterate $U_0(x)$ converge uniformly and monotonically downwards to the least solution of (2.1), (2.2) above $u_0 \equiv 0$ and below U_0 provided U_0 is not a solution. The proof of this is essentially contained in [2, Lemma 4.2].

Comparing this result with Theorem 2.1(ii), it follows that there is a unique $u(x)$ satisfying $0 \equiv u_0(x) \leq u(x) \leq U_0(x)$ on $\bar{D}$ where $U_0(x)$ is a supersolution of problem (2.1), (2.2) and $u(x)$ is a solution of (2.1), (2.2) subject to the conditions (2.3) – (2.6) on f. This unique solution can be approximated from above or below using the monotonic Picard schemes described in Theorem 2.1(i), (ii) above.

We complete our monotonicity theorems with a result on the Newton iterates (2.8).

THEOREM 2.3. If $U_0 \geq 0$ is a supersolution of problem (2.1), (2.2) subject to the above conditions on f, then the Newton iterates (2.8) beginning with $v_0(x) \equiv 0$ converge uniformly and monotonically upwards to the unique solution $u(x)$ of (2.1), (2.2) satisfying $0 \leq u(x) \leq U_0(x)$.

This result is a consequence of [2, Theorem 3.1]. To see this we use the existence of U_0 which guarantees by Theorem 2.1 that a unique solution $u(x)$ exists with $0 \leq u(x) \leq U_0(x)$. $u(x)$ is clearly a positive function since $u(x) \equiv 0$ is not a solution of (2.1), (2.2) subject to (2.3) – (2.6). If another positive solution $U(x)$ exists, then $U(x)$ is a supersolution. Consequently the Picard iterates (2.7) starting at $u_0(x) \equiv 0$ converge to $u(x)$ and $0 \leq u(x) \leq U(x)$. $u(x)$ can therefore be described as the minimal positive solution and the result for the Newton iterates follows immediately from [2, Theorem 3.1].

It would appear that the conditions (2.3) – (2.6) for f and the boundary condition (2.2) are restrictive. In practice these conditions can be weakened and suitable transformations used to obtain a problem of type (2.1) – (2.6) (see examples in [3]).

In the following section we consider a suitable transformation for the Thomas-Fermi problem (1.1), (1.2).

3. Iteration procedures. The ionized atom case of the Thomas-Fermi equation clearly has no real solution $y(x)$ for which $y(x) < 0$ on $\bar{D} = [0, a]$.

Since $y''(x) = x^{-1/2}[y(x)]^{3/2}$ on $(0, a)$ and $y(0) = 1$, $y(a) = 0$ then the graph of any solution is concave upwards on $[0, a]$ and so is bounded above by the line $y = 1 - (x/a)$. Consequently any solution y must be a positive solution satisfying

$$y(x) \leq 1 - \frac{x}{a} \text{ on } [0, a].$$

Let $u(x) = (1 - (x/a)) - y(x)$. Then $0 \leq u(x) \leq 1 - (x/a)$ on D and problem (1.1), (1.2) is transformed to the problem

$$-u''(x) = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - u(x)\right]^{3/2}, \qquad x \in (0, a),$$

$$u(x) = 0 \text{ at } x = 0 \text{ and } x = a.$$

This problem is of the type (2.1), (2.2) and it is easy to show that $f(x, u(x)) = x^{-1/2}[(1 - (x/a)) - u(x)]^{3/2}$ satisfies (2.3), (2.4) but does not satisfy (2.5) where $0 \leq u(x) \leq 1 - (x/a)$.

However, since the coefficient $a_0(x)$ in the operator L defined in Sec. 2 is any continuous positive function of $x \in D$, we write problem (3.1) in the form

$$-u''(x) + k^2x^{-1/2}u(x) = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - u(x)\right]^{3/2} + k^2x^{-1/2}u(x), \qquad x \in (0, a),$$

$$u(0) = u(a) = 0. \tag{3.2}$$

This problem is of the type (2.1) – (2.4) where $L\,u(x) = -u''(x) + k^2x^{-1/2}u(x)$ and $f(x, u(x)) = x^{-1/2}[(1 - (x/a)) - u(x)]^{3/2} + k^2x^{-1/2}u(x)$, with $0 \leq u(x) \leq 1 - (x/a)$. Since

$$f_u(x, \phi(x)) = k^2x^{-1/2} - \frac{3}{2}x^{-1/2}\,[(1 - (x/a)) - \phi(x)]^{1/2} \geq k^2x^{-1/2} - \frac{3}{2}x^{-1/2}[1 - (x/a)]^{1/2}$$

$$> (k^2 - 3/2)\,x^{-1/2} \geq 0 \quad \text{on} \quad (0, a),$$

provided $k^2 \geq 3/2$ and $0 \leq \phi(x) \leq 1 - (x/a)$, then (2.5) is satisfied. Similarly, (2.6) is satisfied.

Consequently problem (3.2) with $k^2 \geq 3/2$ is of the type (2.1) – (2.6) where $0 \leq \phi(x) \leq 1 - (x/a)$.

The restriction $\phi(x) \leq 1 - (x/a)$ prevents the application of the existence theorems in [16, 17] to problem (3.2). However, we now show that Theorems 2.1 – 2.3 are applicable to this problem.

$u_0 \equiv 0$ is a subsolution for (3.2) and $U_0(x) = 1 - (x/a)$ is a supersolution, since

$$L\, U_0(x) = k^2 x^{-1/2} U_0(x) = f(x, U_0(x)), \qquad x \in (0, a);$$
$$U_0(0) = 1 \geq 0, \qquad U_0(a) = 0.$$

Consequently, Theorems 2.1, 2.2 imply that a unique solution $u(x)$ of (3.2) exists with $0 \leq u(x) \leq 1 - (x/a)$. Thus (3.2) has a unique solution and it follows by Theorems 2.2, 2.3 that

(i) the Picard scheme (2.7) defined by

$$-u_{n+1}''(x) + k^2 x^{-1/2} u_{n+1}(x) = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - u_n(x)\right]^{3/2} + k^2 x^{-1/2} u_n(x), \qquad x \in (0, a),$$
$$u_{n+1}(0) = u_{n+1}(a) = 0 \qquad \left(k^2 \geq \frac{3}{2}\right) \tag{3.3}$$

converges monotonically upwards if $u_0(x) \equiv 0$, and monotonically downwards if $u_0(x) = 1 - (x/a)$, to the unique solution of problem (3.2).

(ii) the Newton scheme (2.8) defined by

$$-v_{n+1}''(x) + k^2 x^{-1/2} v_{n+1}(x) = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - v_n(x)\right]^{3/2} + k^2 x^{-1/2} v_n(x)$$
$$+ \left(k^2 x^{-1/2} - \frac{3}{2} x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - v_n(x)\right]^{1/2}\right)\left(v_{n+1}(x) - v_n(x)\right), \qquad x \in (0, a),$$
$$v_{n+1}(0) = v_{n+1}(a) = 0 \qquad \left(k^2 \geq \frac{3}{2}\right)$$

converges monotonically upwards if $v_0(x) \equiv 0$ to the unique solution of problem (3.2).

The Newton iteration scheme reduces to the form

$$-v_{n+1}''(x) = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - v_n(x)\right]^{3/2}$$
$$- \frac{3}{2} x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - v_n(x)\right]^{1/2} (v_{n+1}(x) - v_n(x)), \qquad x \in (0, a),$$
$$v_{n+1}(0) = v_{n+1}(a) = 0. \tag{3.4}$$

Thus we have constructed three iteration schemes of which two converge monotonically from below and one converges monotonically from above to the unique solution of (3.2).

Consequently the solution y of the original problem (1.1), (1.2) is unique and is obtained from the solution of problem (3.2) by using $y(x) = (1 - (x/a)) - u(x)$.

4. Comparison of iteration schemes. We prove two results which are of practical interest in the selection of an efficient iteration scheme of the form (3.3), (3.4).

THEOREM 4.1. The rate of convergence of the iteration scheme (3.3) to the solution of problem (3.2) is maximized by choosing $k^2 = 3/2$.

Proof: (*a*) We consider (3.3) with $u_0(x) = 0$. Thus

$$-u_1'' + k^2 x^{-1/2} u_1 = x^{-1/2}\left[1 - \frac{x}{a}\right]^{3/2}.$$

For $k^2 = 3/2$, we write

$$-w_1'' + \frac{3}{2} x^{-1/2} w_1 = x^{-1/2}\left[1 - \frac{x}{a}\right]^{3/2}.$$

Thus,

$$-(w_1 - u_1)'' + \frac{3}{2} x^{-1/2} w_1 - k^2 x^{-1/2} u_1 = 0,$$

i.e.

$$-(w_1 - u_1)'' + \frac{3}{2} x^{-1/2}(w_1 - u_1) = \left(k^2 - \frac{3}{2}\right) x^{-1/2} u_1 > 0$$

when $k^2 > 3/2$. It follows from the maximum principle [18] that $w_1 - u_1 > 0$, i.e. $w_1 > u_1$ when $k^2 > 3/2$. Assuming that $w_r > u_r$, we have

$$-w_{r+1}'' + \frac{3}{2} x^{-1/2} w_{r+1} = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - w_r\right]^{3/2} + \frac{3}{2} x^{-1/2} w_r = f(x, w_r), \text{ say;}$$

$$-u_{r+1}'' + k^2 x^{-1/2} u_{r+1} = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - u_r\right]^{3/2} + k^2 x^{-1/2} u_r \left(k^2 > \frac{3}{2}\right).$$

Consequently,

$$-(w_{r+1} - u_{r+1})'' + \frac{3}{2} x^{-1/2}(w_{r+1} - u_{r+1})$$

$$= \left(k^2 - \frac{3}{2}\right) x^{-1/2} u_{r+1} + \left(\frac{3}{2} - k^2\right) u_r + f(x, w_r) - f(x, u_r) > 0$$

since $k^2 > 3/2$, $u_{r+1} > u_r$, $w_r > u_r$ and f satisfies (2.5).

Thus we deduce from the maximum principle that $w_{r+1} > u_{r+1}$. Consequently it follows that the sequence $\{w_r\}$, with $k^2 = 3/2$, converges faster than any other sequence of the form (3.3) with $k^2 > 3/2$.

(*b*) By taking $u_0(x) = 1 - (x/a)$ in (3.3), a similar proof to the one above establishes that the sequence (3.3) with $k^2 = 3/2$ converges faster than any other with $k^2 > 3/2$.

THEOREM 4.2. The rate of convergence of the Newton scheme (3.4) to the solution of problem (3.2) is faster than the rate of convergence of the scheme (3.3) when the same starting iterate $u_0(x) \equiv 0$ is used for both schemes.

Proof: From (3.4), (3.3) with $k^2 = 3/2$, and $v_0 \equiv u_0 \equiv 0$, we have

$$-(v_1 - u_1)'' + \frac{3}{2} x^{-1/2}\left(1 - \frac{x}{a}\right)^{1/2} v_1 - \frac{3}{2} x^{-1/2} u_1 = 0,$$

i.e.

$$-(v_1 - u_1)'' + \frac{3}{2} x^{-1/2}\left(1 - \frac{x}{a}\right)^{1/2}(v_1 - u_1) = \frac{3}{2} x^{-1/2}\left[1 - \left(1 - \frac{x}{a}\right)^{1/2}\right] u_1 > 0,$$

and so $v_1 > u_1$. We now assume $v_r > u_r$. Writing

$$h(x, v_r) = \frac{3}{2} x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - v_r\right]^{1/2},$$

$$g(x, v_r) = x^{-1/2}\left[\left(1 - \frac{x}{a}\right) - v_r\right]^{3/2},$$

we have that

$$-v_{r+1}'' = g(x, v_r) - h(x, v_r)\cdot(v_{r+1} - v_r),$$

$$-u_{r+1}'' + \frac{3}{2} x^{-1/2}u_{r+1} = g(x, u_r) + \frac{3}{2} x^{-1/2}u_r .$$

Putting $f(x, u_r) = g(x, u_r) + (3/2)x^{-1/2}u_r$ and writing the first of above equations in the form

$$-v_{r+1}'' + \frac{3}{2} x^{-1/2}v_{r+1} = g(x, v_r) + \left[\frac{3}{2} x^{-1/2} - h(x, v_r)\right](v_{r+1} - v_r) + \frac{3}{2} x^{-1/2}v_r ,$$

it follows that

$$-(v_{r+1} - u_{r+1})'' + \frac{3}{2} x^{-1/2}(v_{r+1} - u_{r+1}) = [f(x, v_r) - f(x, u_r)]$$
$$+ \left[\frac{3}{2} x^{-1/2} - h(x, v_r)\right](v_{r+1} - v_r) > 0$$

since f satisfies (2.5). Consequently $v_{r+1} > u_{r+1}$, which completes the proof of the theorem.

5. Properties of the solutions. Using the constructive schemes developed in Sec. 3, we derive some properties of the solutions of the ionized atom problem. First we show that there exists a unique solution of this problem for all $a > 0$.

THEOREM 5.1. Problem (1.1), (1.2) has a unique solution for all positive values of a.

Proof: (1.1), (1.2) can be expressed in the form (3.2). Any solution $u(x)$ of (3.2) satisfies $0 \leq u(x) \leq 1 - (x/a)$. It is established in Sec. 3 that $1 - (x/a)$, 0 is a supersolution, subsolution respectively of problem (3.2). Consequently a unique solution for (3.2) is implied, for any $a > 0$, by the results of Theorems 2.1, 2.2. Thus problem (1.1), (1.2) has a unique solution for any $a > 0$ and this solution is positive on $(0, a)$.

On substituting $x = ta$, problem (1.1), (1.2) takes the form

$$\ddot{w}(t) = a^{3/2}t^{-1/2}[w(t)]^{3/2}, \qquad t \in (0, 1)$$
$$w(0) = 1, \qquad w(1) = 0 \tag{5.1}$$

where $w(t) = y(ta)$. Similarly, the transformed problem (3.2) becomes

$$-\ddot{u}(t) + a^{3/2}k^2t^{-1/2}u(t) = a^{3/2}t^{-1/2}[(1 - t) - u(t)] + a^{3/2}k^2t^{-1/2}u(t), \qquad t \in (0, 1)$$
$$u(0) = u(1) = 0 \tag{5.2}$$

where $u(t) = (1 - t) - w(t)$.

Next we prove that the solutions of the Thomas-Fermi problem (5.1) are monotonic with respect to a.

THEOREM 5.2. If $0 < \alpha < \beta$ and $w_\alpha(t)$, $w_\beta(t)$ are solutions of problem (5.1) with $a = \alpha, \beta$

respectively, then $w_\alpha(t) > w_\beta(t)$ for all $t \in (0, 1)$. Furthermore, if $u_\alpha(t) = (1 - t) - w_\alpha(t)$, then

$u_\alpha(t)$ is a subsolution of problem (5.2) with $a = \beta$, and
$u_\beta(t)$ is a supersolution of problem (5.2) with $a = \alpha$.

Consequently the schemes (3.3), (3.4) applied to (5.2) give iteration schemes which converge monotonically upwards (resp. downwards) from $u_\alpha(t)$ (resp. $u_\beta(t)$) to the unique solution of (5.2) with $a = \beta$ (resp. $a = \alpha$).

Proof: In (5.2) we have

$$-\ddot{u}_\alpha(t) = \alpha^{3/2}[(1 - t) - u_\alpha(t)]^{3/2} < \beta^{3/2}[(1 - t) - u_\alpha(t)]^{3/2}.$$

Thus $u_\alpha(t)$ is a subsolution of problem (5.2) with $a = \beta$. Similarly $u_\beta(t)$ is a supersolution of problem (5.2) with $a = \alpha$. Consequently Theorem 2.1 implies that $0 < u_\alpha(t) < u_\beta(t)$. Thus $w_\alpha(t) > w_\beta(t)$ for all $t \in (0, 1)$.

Since the solution $u_\alpha(t)$ is a subsolution of problem (5.2) with $a = \beta$ this solution can be used as a starting iterate in the Newton and Picard schemes to obtain the solution $u_\beta(t)$.

6. Numerical bounds for solutions. From (3.3), we have

$$-u_1''(x) + \frac{3}{2} x^{-1/2} u_1(x) = x^{-1/2}\left(1 - \frac{x}{a}\right)^{3/2}, \qquad x \in (0, a)$$

$$u_1(0) = u_1(a) = 0,$$

on putting $k^2 = 3/2$ and $u_0(x) \equiv 0$. The solution $u_1(x)$ of this problem is a lower bound for the solution of (3.2), by Theorem 3.2. On letting $u_1(x) = (1 - (x/a)) - y(x)$, we have

$$y''(x) - \frac{3}{2} x^{-1/2} y(x) = x^{-1/2}\left(1 - \frac{x}{a}\right)^{3/2} - \frac{3}{2} x^{-1/2}\left(1 - \frac{x}{a}\right), \qquad x \in (0, a)$$

$$y(0) = 1, \qquad y(a) = 0 \tag{6.1}$$

and consequently the solution of this linear boundary-value problem provides an *upper* bound for the solution of (1.1), (1.2).

Theorem 4.2 implies that a tighter *upper* bound is provided by the solution of the problem

$$y''(x) - \frac{3}{2} x^{-1/2}\left(1 - \frac{x}{a}\right)^{1/2} y(x) = -\frac{1}{2} x^{-1/2}\left(1 - \frac{x}{a}\right)^{3/2}{}_1, \qquad x \in (0, a)$$

$$y(0) = 1 \qquad y(a) = 0 \tag{6.2}$$

which is obtained from the first iterate of the Newton scheme (3.4). Again, using (3.3) with initial iterate $u_0(x) = 1 - (x/a)$, we have

$$y''(x) - \frac{3}{2} x^{-1/2} y(x) = 0, \qquad x \in (0, a)$$

$$y(0) = 1, \qquad y(a) = 0 \tag{6.3}$$

where $y(x) = (1 - (x/a)) - u_1(x)$. The solution of (6.3) provides a *lower* bound for the solution of (1.1), (1.2).

Unfortunately there are no known analytic solutions for problems (6.1)–(6.3). The

TABLE 1.

n	0	1	2	3	4	5
a_{3n}	1	2	0.5	0.04761	0.00238	0.00007
a_{1+3n}	0	0	0	0	0	0
a_{2+3n}	a_2	$0.4a_2$	$0.05a_2$	$0.00303a_2$	$0.00011a_2$	0

simplest equation, in (6.3), has the solution

$$u(x) = \exp \int x(x)dx$$

where $z(x)$ is the solution of the Riccati equation $z' + z^2 = (3/2)x^{-1/2}$, and Liouville has shown that this equation has no closed-form solution in terms of elementary functions [19]. In addition, the Liouville-Green approximation [20] which provides an approximate analytic solution for many problems of the form (6.3) fails because the term ϕ neglected in the approximation and given by

$$\phi(x) = -f^{-3/4}(x) \frac{d^2}{dx^2} [f^{-1/4}(x)] \text{ with } f(x) = \frac{3}{2} x^{-1/2} - 1,$$

is not small on $(0, a)$.

The solutions of problems (6.1)–(6.3) can, however, be obtained in the form of power series expanded about the origin. We conclude this section by using Eqs. (6.1) and (6.3) to provide upper and lower bounds for the solution of the problem (1.1), (1.2) in the case when $a = 1$.

We consider a series solution of (6.3), with $a = 1$, of the form

$$y(x) = \sum_{n=0}^{\infty} a_n x^{n/2}.$$

The boundary condition $y(0) = 1$ gives $a_0 = 1$ and the series coefficients are listed in Table 1. The boundary condition $y(1) = 0$ leads to a linear equation in a_2 with solution $a_2 = -2.4430$. The numerical solution $y(x)$ of (6.3) is given in Table 3.

Applying the same form of series to (6.1) with $a = 1$ and using the boundary condition $y(0) = 1$, we obtain the coefficients given in Table 2. A linear equation in a_2 is obtained from the boundary condition $y(1) = 0$. We have $a_2 = -1.8938$. The numerical solution $\bar{y}(x)$ of (6.1) is given in Table 3.

The solution $y(x)$ of (1.1), (1.2) with $a = 1$ is bounded above, below by $\bar{y}(x)$, $y(x)$ respectively. The construction of a series solution for the problem (1.1), (1.2) itself is complicated by the fact that the coefficient a_2 is required to satisfy a nonlinear equation by the boundary condition $y(a) = 0$.

TABLE 2.

n	0	1	2	3	4	5	6
a_{3n}	1	1.33333	0.33333	0.03571	0.00179	0.00020	0
a_{1+3n}	0	0	0.04286	0.00321	0.00046	0.00001	0.00004
a_{2+3n}	a_2	$0.4a_2$	$0.05a_2$	$(0.00303a_2 + 0.00095)$	$(0.00011a_2 + 0.00003)$	0.00007	0

TABLE 3.

x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	
	$\underline{y}(x)$	1	.816	.677	.560	.459	.370	.288	.212	.139	.069	0
	$\bar{y}(x)$	1	.851	.730	.623	.524	.432	.343	.256	.170	.085	0

7. Concluding remarks. Iteration schemes of the type we have described can be constructed in a similar manner for higher-dimensional forms of the Thomas-Fermi equation. Numerical computations employing finite differences and the iteration schemes developed above will be published elsewhere. These methods give much better bounds than those in Table 3; however, the latter were obtained without a computer.

The solution of the isolated neutral atom problem can be approximated uniformly and arbitrarily closely by using solutions of the ionized atom problem. This is discussed in [1].

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