# AN ITERATIVE TECHNIQUE FOR SOLUTION OF THE THOMAS-FERMI EQUATION UTILIZING A NONLINEAR EIGENVALUE PROBLEM*

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**Abstract.** Development of an iterative solution technique for a certain nonlinear eigenvalue problem supplies an iterative solution technique for the ion case and isolated neutral atom case boundary-value problems for the Thomas-Fermi equation.

**1. Introduction.** In appropriate units, the Thomas-Fermi equation, developed independently by L. H. Thomas [1] and E. Fermi [2] in 1927, may be written

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

This nonlinear second-order differential equation arose in Thomas' and Fermi's studies of potentials and charge densities in atoms. The differential equation (1.1) is still used for atomic calculations (see, for example, [3,4,5]) and the related Thomas-Fermi theory is still a subject of research (see [6,7]). An idea of the extent of the literature on the Thomas-Fermi and related theories can be obtained by consulting the extensive reviews [8,9,10].

There are three sets of boundary values of interest for the Thomas-Fermi equation. They are:

(a) the neutral atom

$$y(0) = 1 \qquad by'(b) = y(b); \tag{1.2}$$

(b) the isolated neutral atom

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

(c) the ionized atom

$$y(0) = 1 \qquad y(a) = 0. \tag{1.4}$$

In this paper we are not concerned with the physical ramifications of Eq. (1.1), but wish only to consider the mathematical aspects of showing that a certain sequence of functions does converge to a solution of Eq. (1.1) subject to the boundary values (1.4).

Solution techniques for the boundary-value problems (a), (b), and (c) and other mathematical aspects of Eq. (1.1), with or without the boundary conditions, have been and continue to be subjects of research. Briefly, the solution history is as follows: Thomas used Adam's method of numerical integration of the differential equation to obtain

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approximate solutions to problem (b), while Fermi used graphical methods. In fact, Fermi obtained the approximation for small $x$ of

$$y(x) = 1 - 1.58x + (4/3)x^{3/2} + \cdots \tag{1.5}$$

Baker [11] later improved this result to

$$y(x) = 1 + b_2x + b_3x^{3/2} + \cdots \tag{1.6}$$

with $b_2 = -1.588588\cdots$. At about the same time, Sommerfeld [12] developed an approximate solution to (b):

$$y(x) = y_1(x)\{1 + [y_1(x)]^{\lambda_1/3}\}^{\lambda_2/3} \tag{1.7}$$

where $\lambda_1$, $\lambda_2$ are zeros of the polynomial $\lambda^2 + 7\lambda - 6$, $\lambda_1 > 0 > \lambda_2$, and

$$y_1(x) = 144/x^3. \tag{1.8}$$

Sommerfeld's approximation is quite accurate for large $x$ but underestimates the solution near the origin [13]. Analogue computers have been used to find numerical solutions [14]. More recently Ramnath [15] has used a technique known as multiple scales to obtain an approximate solution for (b).

Since all three problems (a), (b), and (c) have the same boundary conditions at zero, much computational use has been made of the series expansion

$$y(x) = 1 + b_2x + b_3x^{3/2} + \cdots + b_kx^{k/2} + \cdots \tag{1.9}$$

which is regarded as semiconvergent [16]. The value of $b_2$, the slope of $y$ at the origin, falls into three classes: $b_2 > -1.588\cdots$, $b_2 = -1.588\cdots$, and $b_2 < -1.588\cdots$ which correspond respectively to solutions of problem (a), (b), and (c). Hille [17] answers questions concerning the convergence of the series (1.9).

Other mathematical work that has been done includes the early work of Mambriani [18] and Scorza-Dragoni [19], in which the existence and uniqueness of the solution to problem (b) was established, and the more recent work of Reid [20] and Reid and Depuy [21]. The work of Ramnath [15], Reid [20] and Reid and Depuy [21] also applies to the more general Emden-type equations.

Most of the solution techniques fall into the two categories: (1) machine-computational and (2) approximations via series, multiple scales, or particular solution methods. The technique we exhibit in this paper does not fall into either of these categories. We first transform Eq. (1.1) with boundary conditions (c) into an eigenvalue problem. We then demonstrate an iteration scheme, based on eigenpairs of linear self-adjoint integral operators of Hilbert-Schmidt type, which is shown to converge to a solution. We can also use the iteration to obtain a uniform approximation to the solution of problem (b). In the last section we outline a way that the iterative scheme may be implemented through the use of Galerkin methods. For completeness, we also include some uniqueness results for problem (c).

More specifically, we consider the nonlinear eigenvalue problem

$$\begin{aligned} u'' &= \nu x^{-1/2}u^{3/2}, \ 0 < x < 1, \\ u(1) &= 0, -\alpha u(0) + u'(0) = 0, \\ u(0) &= 1. \end{aligned} \tag{1.10}$$

If $u$ is a positive solution of (1.10) with corresponding eigenvalue $\nu > 0$, then $y(x) = u(\nu^{-}$

${}^{2/3}x)$ is the solution of problem (c) for $a = \nu^{2/3}$. The initial condition $u(0) = 1$ is essentially a normalizing condition for if $u_1$ is a solution of (1.10) with corresponding eigenvalue $\nu_1$, then a solution satisfying $u(0) = b$, $b > 0$, is obtained from $u_1$ by $u_b = bu_1$ and the corresponding eigenvalue is then $\nu b = b^{-1/2}\nu_1$.

In this paper we give an iterative scheme based upon a linearization of (1.10) and eigenpairs of self-adjoint linear integral operators of Hilbert-Schmidt type. The integral operators are obtained from Green's functions for certain boundary-value problems. The iteration generates a sequence of eigenfunctions $\{u_k\}$ and corresponding eigenvalues $\{\nu_k\}$ which satisfy

$$\begin{aligned} u_k'' &= \nu_k x^{-1/2} u_{k-1}^{1/2} u_k \qquad 0 < x < 1, \\ -\alpha u_k(0) + u_k'(0) &= 0 \qquad u_k(1) = 0, \end{aligned} \tag{1.11}$$

normalized by $u_k(0) = 1$. It is shown that there is a solution $(u, \nu)$ of (1.10) such that $\nu_k \to \nu$ and $u_k \to$ u uniformly in [0, 1].

We use the following notation and terminology: $\Gamma(z)$ and $I_\nu(z)$ denote respectively the gamma function and the modified Bessel function of order $\nu$. All needed properties of these functions may be found in [22]. The characteristic function of the interval $[a, b]$ is denoted by $\chi_{[a,b]}$. That is,

$$\begin{aligned} \chi_{[a,b]}(x) &= 1, \; x \in [a, b]; \\ &= 0, \; x \notin [a, b]. \end{aligned}$$

In Sturm-Liouville min-max computations, the set of admissible functions are those functions $\phi$ which satisfy the boundary conditions, are continuous and have piecewise continuous derivatives (see [23]).

**2. Preliminaries.** Before we prove the convergence theorem, we need some results about a class of linear Sturm-Liouville problems. We consider

$$\begin{aligned} u'' - \lambda^2 x^{-1/2} u + \nu x^{-1/2} \rho(x) u &= 0, \quad 0 < x < 1 \\ -\alpha u(0) + u'(0) &= 0, \; u(1) = 0 \end{aligned} \tag{2.1}$$

where

$$1 - (1 - x)^{1/2} \leq \rho(x) \leq 1 - \chi_{[0,-\alpha^{-1}]}(x)(1 + \alpha x)^{1/2}$$

and $\alpha < -1$. The term $\lambda^2 x^{-1/2} u$ is introduced in order to make the kernel of the integral operator to be introduced later a square-integrable positive function. This insures the existence of positive eigenfunctions and positive eigenvalues. The Green's function for

$$\begin{aligned} L(u) &= u'' - \lambda^2 x^{-1/2} u, \; 0 < x < 1 \\ -\alpha u(0) + u'(0) &= 0, \; u(1) = 0 \end{aligned} \tag{2.2}$$

is

$$\begin{aligned} K(x, t; \lambda) &= c_\lambda v_2(x; \lambda) v_1(t; \lambda) \;\; 0 \leq t \leq x, \\ &= c_\lambda v_1(x; \lambda) v_2(t; \lambda) \;\; x \leq t \leq 1, \end{aligned} \tag{2.3}$$

where

$$v_1(x;\lambda) = \alpha\Gamma(5/3)(2\lambda/3)^{-2/3}x^{1/2}I_{2/3}([4\lambda/3]x^{3/4}) + \Gamma(1/3)(2\lambda/3)^{2/3}x^{1/2}I_{-2/3}([4\lambda/3]x^{3/4}),$$

$$v_2(x;\lambda) = I_{2/3}(4\lambda/3)x^{1/2}I_{-2/3}([4\lambda/3]x^{3/4}) - I_{-2/3}(4\lambda/3)x^{1/2}I_{2/3}([4\lambda/3]x^{3/4}),$$

$$c_\lambda = \Gamma(1/3)\Gamma(5/3)/v_1(1;\lambda).$$

Let $H_\rho$ be the Hilbert space

$$H_\rho = \left\{u: \int_0^1 x^{-1/2}\rho(x)|u(x)|^2\,dx < \infty\right\}, \qquad (2.4)$$

$$\|u\|_\rho = \left[\int_0^1 x^{-1/2}\rho(x)|u(x)|^2\,dx\right]^{1/2},$$

and on $H_\rho$ define the linear operator $T_\lambda$ by

$$(T_\lambda u)(x) = \int_0^1 K(x,t;\lambda)t^{-1/2}\rho(t)u(t)\,dt. \qquad (2.5)$$

We now give some properties of the kernel $K(x, t; \lambda)$ and the operator $T_\lambda$.

LEMMA 1: If $\alpha < -1$ then $v_2(x;\lambda) > 0$, $0 \le x < 1$, all $\lambda$, and $\inf\{\lambda > 0: v_1(x;\lambda) > 0, 0 \le x < 1\} > 0$.

*Proof:* Since $v_2(0;\lambda) > 0$, $v_2'(0;\lambda) < 0$ and $v_2$ satisfies $y'' = \lambda^2 x^{-1/2}y$, $y(1) = 0$, it follows that if $v_2(x_1;\lambda) = 0$ for some $x_1$, $0 < x_1 < 1$, then $v_2'(x_1;\lambda) < 0$ and $v_2(x;\lambda) < 0$ for $x > x_1$, contradicting $v_2(1;\lambda) = 0$.

If $\alpha_1 < \alpha_2$ and $y_1$, $y_2$ are corresponding positive eigenfunctions of

$$\begin{gathered} y'' - \gamma x^{-1/2}y = 0,\ 0 < x < 1, \\ -\alpha_i y(0) + y'(0) = 0,\ y(1) = 0,\ i = 1, 2 \end{gathered} \qquad (2.6)$$

with $y(0) = 1$, then $y_1'(0) < y_2'(0)$ and by continuity there is a neighborhood of zero in which $y_1'(x) < y_2'(x)$, $y_1(x) < y_2(x)$. In order to satisfy $y_1(1) = y_2(1) = 0$ there must be a point $x_1$, $0 < x_1 < 1$, at which $y_2''(x_1) < y_1''(x_1)$ and $y_1(x_1) < y_2(x_2)$ which yields $\gamma_1 > \gamma_2$ for the corresponding eigenvalues. Since for $\alpha = -1$, the greatest eigenvalue of (2.6) is $\gamma_0 = 0$, it follows that for $\alpha < -1$, the greatest eigenvalue $\gamma_0 > 0$. Moreover,

$$(\gamma_0)^{1/2} = \inf\{\lambda > 0: v_1(x;\lambda) > 0, 0 \le x \le 1\}. \qquad (2.7)$$

We note that $v_1(x;\lambda) > 0$, $0 \le x \le 1$, if and only if $v_1(1;\lambda) > 0$. Thus $c_\lambda > 0$ if and only if $v_1(x;\lambda) > 0$, $0 \le x \le 1$.

LEMMA 2: If $\lambda_1 > \lambda_2$ then $v_1(x;\lambda_1) > v_1(x;\lambda_2)$, $0 < x \le 1$.

*Proof:* Since $v_1(x;\lambda)$ satisfies $y'' = \lambda^2 x^{-1/2}y$, $0 < x < 1$, $y(0) = 1$, $y'(0) = \alpha$, there is a neighborhood of zero in which $v_1''(x;\lambda_1) > v_1''(x;\lambda_2)$ and in which $v_1(x;\lambda_1) > v_1(x;\lambda_2)$. If there is an $x_1$, $0 < x_1 \le 1$, for which $v_1(x_1;\lambda_1) = v_1(x_1;\lambda_2)$ then there is an $x_2$, $0 < x_2 < x_1$, for which $v_1(x_2;\lambda_1) > v_1(x_2;\lambda_2)$ and $v_1''(x_2;\lambda_1) < v_1''(x_2;\lambda_2)$, contradicting the differential equation.

We will now restrict our considerations to $\alpha < -1$ and $\lambda > \lambda_0$ where

$$\lambda_0 = \inf\{\lambda > 0: v_1(x;\lambda) > 0, 0 \le x < 1\}. \qquad (2.8)$$

Thus $K(x, t; \lambda) > 0$, $(x, t) \in [0, 1) x [0, 1)$.

LEMMA 3: $T_\lambda$ is a selfadjoint Hilbert-Schmidt operator on $H_\rho$.

*Proof:* $(T_\lambda u, w)_\rho = (u, T_\lambda w)_\rho$ follows directly from the definitions of the inner product in $H_\rho$ and the linear operator $T_\lambda$. $T_\lambda$ is a Hilbert-Schmidt operator in $H_\rho$ if and only if the linear integral operator with kernel $U(x, t; \lambda) = x^{-1/4}\rho^{1/2}(x)K(x, t; \lambda)t^{-1/4}\rho^{1/2}(t)$ is a Hilbert-Schmidt operator in $L_2[0, 1]$; that is, if and only if

$$\int_0^1 \int_0^1 |U(x, t; \lambda)|^2 \, dt \, dx < \infty.$$

This follows immediately since $\rho^{1/2}(x)K(x, t; \lambda)\, \rho^{1/2}(t)$ is bounded on $[0, 1] \times [0, 1]$.

Since $T_\lambda$ is a selfadjoint Hilbert-Schmidt operator in $H_\rho$, it has a complete orthonormal system of eigenfunctions $\{\phi_n\}$ in $H_\rho$. The smoothness of the kernel of the integral operator $T_\lambda$ allows us to assume that $\phi \in C^1[0, 1]$.

If $\phi$ is a $C^1[0, 1]$ eigenfunction of $T_\lambda$, i.e. $T_\lambda\phi = \mu\phi$, then

$$\begin{aligned} \phi'' - \lambda^2 x^{-1/2}\phi + \mu^{-1}x^{-1/2}\rho(x), \phi = 0, 0 < x < 1, \\ -\alpha\phi(0) + \phi'(0) = 0, \phi(1) = 0. \end{aligned} \tag{2.9}$$

We then, of course, have $\phi(0) \neq 0$, for otherwise we would also have $\phi'(0) = 0$ and $\phi(x) \equiv 0$, $0 \le x \le 1$. We normalize the eigenfunctions $\{\phi_n\}$ of $T_\lambda$ by $\phi_n(0) = 1$.

It is well known that $T_\lambda$ has at least one positive eigenvalue and that the normalized $C^1[0, 1]$ eigenfunction corresponding to the largest positive eigenvalue is a positive function on $[0, 1)$ (see [24]). Of course by the orthogonality of the eigenfunctions there can be at most one positive $C^1[0, 1]$ eigenfunction of $T_\lambda$. We denote this unique positive $C^1[0, 1]$ normalized eigenpair by $(\phi_0, \mu_0)$.

LEMMA 4: There is a unique $\lambda > 0$ such that $K(x, t; \lambda) > 0$, $(x, t) \in [0, 1) \times [0, 1)$ and $\mu_0(\lambda) = \lambda^{-2}$.

*Proof:* If $\lambda^* > \lambda_0$ and $\lambda \to \lambda^*$ then $K(x, t; \lambda) \to K(x, t; \lambda^*)$ uniformly on $[0, 1] \times [0, 1]$. Thus, since $x^{-1/4}\rho^{1/2}(x)$ is bounded on $[0, 1]$ it follows that

$$\mu(\lambda) = \sup_{\psi \in L_2[0,1]} \int_0^1 \int_0^1 x^{-1/4}\rho^{1/2}(x)K(x, t; \lambda)t^{-1/4}\rho^{1/2}(t)\psi(t)\psi(x)\, dt\, dx, \; \|\psi\|_0 = 1$$

is continuous for $\lambda > \lambda_0$.

Let $\lambda_1^2$ denote the greatest eigenvalue of

$$\begin{aligned} y'' - \lambda^2 x^{-1/2}(1 - x)^{1/2} y = 0, 0 < x < 1, \\ -\alpha y(0) + y'(0) = 0, y(1) = 0. \end{aligned} \tag{2.10}$$

By Sturm-Liouville theory (see [23]),

$$-\lambda_1^2 = \min \frac{\int_0^1 (y'(x))^2\, dx + \alpha y^2(0)}{\int_0^1 x^{-1/2}(1 - x)^{1/2} y^2(x)\, dx} \tag{2.11}$$

where the minimum is taken over all admissible functions $y$. Thus

$$0 < \lambda_0^2 = \frac{\int_0^1 (\phi_0'(x))^2\,dx - \alpha}{\int_0^1 x^{-1/2}\phi_0^2(x)\,dx} < \frac{-\int_0^1 (\phi_0'(x))^2\,dx - \alpha}{\int_0^1 x^{-1/2}(1-x)^{1/2}\phi_0^2(x)\,dx}$$

$$\leq \max \frac{-\int_0^1 (y'(x))^2\,dx - \alpha y^2(0)}{\int_0^1 x^{-1/2}(1-x)^{1/2}y^2(x)\,dx} = \lambda_1^2 .$$

Since the kernel of $T_\lambda$ comes from the Green's function of Eq. (2.2) it follows that ($\phi_0$, $\nu_0(\lambda) = \mu_0^{-1}(\lambda)$) is the first eigenpair for the Sturm-Liouville problem (2.1). Moreover, if $\lambda_0 < \lambda < \lambda_1$ then $\nu_0(\lambda) < \lambda^2$, for otherwise it would follow that for $x \in (0, 1)$

$$\phi_0''(x) = x^{-1/2}(\lambda^2 - \nu_0(\lambda)\rho(x))\phi_0(x) < \lambda_1^2 x^{-1/2}(1 - x)^{1/2}\phi_0(x)$$

and $\phi_0$ would not satisfy the boundary condition $\phi_0(1) = 0$.

We now show that for large values of $\lambda$, $\nu_0(\lambda) > \lambda^2$ and thus, by the continuity of $\mu_0(\lambda)$, there must be at least one value of $\lambda \geq \lambda_1$ such that $\nu_0(\lambda) = \lambda^2$. Let $(a, b)$ denote the point of intersection of the functions $f_1(x) = 1 - (1 + \alpha x)^{1/2}$ and $f_2(x) = 1 + \alpha x$, $0 < a < 1$, $0 < b < 1$. If $\nu_0(\lambda) \leq \lambda^2$ for all $\lambda$ then $\lambda^2 - \nu_0(\lambda)\rho(x) \geq 0$, $0 \leq x \leq 1$ and $\phi_0''(x) \geq 0$, $0 < x \leq 1$. Moreover,

$$\phi_0''(x) = x^{-1/2}(\lambda^2 - \nu_0(\lambda)\rho(x))\phi_0(x) \geq \lambda^2(1 - b)b, \quad 0 < x < a$$

$$\phi_0'(a) \geq \alpha + \lambda^2 a(1 - b)b \geq 0 \quad \text{for } \lambda^2 \geq \frac{-\alpha}{a(1 - b)b}$$

from which we conclude $\phi_0$ could not satisfy $\phi_0(1) = 0$.

For each admissible function $y$, if we let

$$\nu_0(\lambda; y) = \frac{\int_0^1 (y'(x))^2\,dx + \lambda^2 \int_0^1 x^{-1/2}y^2(x)\,dx + \alpha y^2(0)}{\int_0^1 x^{-1/2}\rho(x)y^2(x)\,dx}$$

then $\nu_0(\lambda) = \min \nu_0(\lambda; y)$. The uniqueness of $\lambda$ such that $\nu_0(\lambda) = \lambda^2$ then follows directly from

$$\frac{d}{d\lambda}\nu_0(\lambda; y) = \frac{2\lambda \int_0^1 x^{-1/2}y^2(x)\,dx}{\int_0^1 x^{-1/2}\rho(x)y^2(x)\,dx} \geq 2\lambda. \tag{2.12}$$

**3. The iteration and its convergence.** We now give the iteration scheme for generating the sequence of eigenfunctions $\{u_k\}$ and corresponding eigenvalues $\{\nu_k\}$ which converge to the solution of

$$u'' = \nu x^{-1/2}u^{3/2}, \; 0 < x < 1, \qquad -\alpha u(0) + u'(0) = 0, \; u(1) = 0, \; u(0) = 1 \tag{3.1}$$

where $\alpha < -1$. Let $u_0(x) = \chi_I(x)(1 + \alpha x)$, $0 \leq x \leq 1$, where $I = [0, -\alpha^{-1}]$ and let $\rho_0 = 1 - u_0^{1/2}$. For $k \geq 1$ the eigenfunction $u_k$ and corresponding eigenvalue $\nu_k$ are defined as the unique positive solution of

$$u'' - \lambda^2 x^{-1/2}u + \nu x^{-1/2}\rho_{k-1}(x)u = 0, \qquad -\alpha u(0) + u'(0) = 0, \; u(1) = 0 \tag{3.2}$$

where $u_k$ is normalized by $u_k(0) = 1$, $\lambda$ is chosen so that $\nu_k = \lambda^2$, and $\rho_k = 1 - u_k^{1/2}$. Thus for each $k \geq 1$

$$u_k'' = \nu_k x^{-1/2}u_{k-1}^{1/2}u_k \, , \; 0 < x < 1. \tag{3.3}$$

Our main result can now be stated as

THEOREM 1: If $\{u_k\}_{k=0}^{\infty}$ and $\{\nu_k\}_{k=1}^{\infty}$ are as above then for each $k \geq 1$, $0 < \nu_{2k} < \nu_{2k+2} < \nu_{2k+1} < \nu_{2k-1}$ and $u_0(x) < u_{2k}(x) < u_{2k+2}(x) < u_{2k+1}(x) < u_{2k-1}(x)$, $0 < x < 1$. Moreover there is a positive solution $(u, \nu)$ of (3.1) such that $\nu_k \to \nu$ and $u_k \to u$ uniformly on [0, 1].

The proof of Theorem 1 is developed through a series of lemmas. We start with a technical lemma. Let $h_1$ and $h_2$ be continuous positive functions on [0, 1] satisfying

(i) there is a $\delta > 0$ such that $h_1(x) < h_2(x)$, $0 \leq x < \delta$;

(ii) if there is an $x_0 \in (0, 1)$ such that $h_1(x_0) > h_2(x_0)$, then $h_1(x) > h_2(x)$, $x_0 \leq x < 1$.

LEMMA 5: If $h_1$ and $h_2$ are as above and if for $i = 1, 2$, $v_i$ is a continuous positive solution of

$$y'' = x^{-1/2}h_i(x)y, \qquad y(0) = 1, \; y'(0) = \alpha, \; y(1) = 0 \tag{3.4}$$

then $v_1(x) < v_2(x)$, $0 < x < 1$.

*Proof:* By the assumptions on $h_1$ and $h_2$ we have $h_1(0)v_1(0) < h_2(0)v_2(0)$. By utilizing the continuity and the initial values it follows that there is an $\epsilon > 0$ such that $h_1(x)v_1(x) < h_2(x)v_2(x)$, $0 < x < \epsilon$ and thus $v_1''(x) < v_2''(x)$, $v_1'(x) < v_2'(x)$, $v_1(x) < v_2(x)$, $0 < x < \epsilon$. Assume $x_1 \in (0, 1)$ exists such that $v_1(x_1) = v_2(x_1)$ and $v_1(x) < v_2(x)$, $0 < x < x_1$. Then $v_1'(x_1) \geq v_2'(x_1)$ and since $v_1'(x) < v_2'(x)$, $0 < x < \epsilon$, there must exist $x_2$, $0 < x_2 < x_1$ such that $v_1''(x_2) > v_2''(x_2)$, from which we conclude $h_1(x_2) > h_2(x_2)$. Thus by the assumption $h_1(x) > h_2(x)$, $x_2 \leq x < 1$. It now follows that $v_1''(x) > v_2''(x)$, $x_1 \leq x < 1$ and thus $v_1'(x) > v_2'(x)$ and $v_1(x) > v_2(x)$, $x_1 < x \leq 1$. This of course contradicts $v_1(1) = v_2(1) = 0$. Thus $x_1$ does not exist and $v_1(x) < v_2(x)$, $0 < x < 1$.

LEMMA 6: For $k \geq 1$, $u_k(x) > u_0(x)$, $0 < x < 1$, $0 < \nu_2 < \nu_1$, $\nu_2 u_1^{1/2}$ can intersect $\nu_1 u_0^{1/2}$ at most once in (0, 1) and $u_2(x) < u_1(x)$, $0 < x < 1$.

*Proof:* Since $u_k''(x) > 0$, $0 < x < 1$, $u_k'(0) = \alpha$, $u_k(0) = 1$ and $u_k(x) > 0$, $0 < x < 1$, it follows by integrating $u_k''$ that $u_k(x) > u_0(x)$, $0 < x < 1$. It has already been shown that $\nu_k$

$> 0$, $k \geq 1$. Since $u_1(x) > u_0(x)$, we have from Sturm's second comparison theorem ([23], theorem 7, p. 411) that $0 < \nu_2 < \nu_1$. Since $\nu_2^2 u_1(0) < \nu_1^2 u_0(0)$ and since $\nu_2^2 u_1'(x)$ is increasing and $\nu_1^2 u_0'(x) = \alpha\nu_1^2 \chi_I(x)$, $I = [0, -\alpha^{-1}]$, it follows that $\nu_2^2 u_1(x)$ can intersect $\nu_1^2 u_0(x)$ at most once in (0, 1). Thus $\nu_2 u_1^{1/2}(x)$ can intersect $\nu_1 u_0^{1/2}(x)$ at most once in (0, 1). We can now apply lemma 5 with $h_1(x) = \nu_2 u_1^{1/2}(x)$ and $h_2(x) = \nu_1 u_0^{1/2}(x)$ to conclude $u_2(x) < u_1(x)$, $0 < x < 1$.

LEMMA 7: $\nu_2 < \nu_3 < \nu_1$, $\nu_2 u_1^{1/2}$ can intersect $\nu_3 u_2^{1/2}$ at most once in (0, 1), $\nu_3 u_2^{1/2}$ can intersect $\nu_1 u_0^{1/2}$ at most once in (0, 1) and $u_2(x) < u_3(x) < u_1(x)$, $0 < x < 1$.

*Proof:* $\nu_2 < \nu_3 < \nu_1$ is a direct consequence of $u_0(x) < u_2(x) < u_1(x)$, $0 < x < 1$ and Sturm's second comparison theorem. We have $\nu_2 u_1^{1/2}(0) < \nu_3 u_2^{1/2}(0) < \nu_1 u_0^{1/2}(0)$. Thus $u_2(x) < u_3(x) < u_1(x)$, $0 < x < 1$, follows from lemma 5 as soon as it is shown that $\nu_2 u_1^{1/2}$ can intersect $\nu_3 u_2^{1/2}$ at most once in (0, 1) and $\nu_3 u_2^{1/2}$ can intersect $\nu_1 u_0^{1/2}$ at most once in (0, 1). The proof that $\nu_3 u_2^{1/2}$ can intersect $\nu_1 u_0^{1/2}$ at most once in (0, 1) is virtually the same as the proof in lemma 6 that $\nu_2 u_1^{1/2}$ can intersect $\nu_1 u_0^{1/2}$ at most once in (0, 1). Thus the proof will be completed when it is shown that $\nu_3^2 u_2$ and $\nu_2^2 u_1$ cross at most once in (0, 1).

Assume there are points $a_0$, $a_1$ such that $0 < a_0 < a_1 < 1$ and $\nu_2^2 u_1(a_0) = \nu_3^2 u_2(a_0)$, $\nu_2^2 u_1(a_1) = \nu_3^2 u_2(a_1)$, $\nu_2^2 u_1(x) \leq \nu_3^2 u_2(x)$, $0 \leq x < a_0$, $\nu_2^2 u_1(x) > \nu_3^2 u_2(x)$, $a_0 < x < a_1$. Let $z_1(x) = \nu_2^2 u_1(x)$, $z_2(x) = \nu_3^2 u_2(x)$. Then

$$\begin{aligned} z_1''(x) &= \nu_1 x^{-1/2} u_0^{1/2}(x) z_1(x), \qquad 0 < x < 1, \\ z_2''(x) &= \nu_2 x^{-1/2} u_1^{1/2}(x) z_2(x), \\ z_1(a_0) &= z_2(a_0),\ z_1'(a_0) \geq z_2'(a_0), \\ z_1(a_1) &= z_2(a_1),\ z_1'(a_1) \leq z_2'(a_1), \\ z_1(1) &= z_2(1) = 0. \end{aligned}$$

There is an $x_1 \in (a_0, a_1)$ such that $z_1''(x_1) < z_2''(x_1)$. Thus $\nu_1^2 u_0(x) < \nu_2^2 u_1(x)$, $x > x_1$ and $z_2(x) > z_1(x)$, $a_1 < x < 1$. In order to satisfy $z_2(1) = z_1(1) = 0$ there would have to be an $x_2 \in (a_1, 1)$ such that $z_1''(x_2) > z_2''(x_2)$, contradicting $\nu_1^2 u_0(x_2) < \nu_2^2 u_1(x_2)$. We thus have the required behavior of the functions $\nu_2^2 u_1(x)$ and $\nu_3^2 u_2(x)$, which concludes the proof of the lemma.

LEMMA 8: For each $k \geq 1$, $\nu_{2k} < \nu_{2k+2} < \nu_{2k+1} < \nu_{2k-1}$ and $u_{2k}(x) < u_{2k+2}(x) < u_{2k+1}(x) < u_{2k-1}(x)$, $0 < x < 1$.

The proof of lemma 8 is accomplished by using a straightforward induction argument and the same type of arguments that were used in the proof of lemma 7.

The sequences $\{\nu_{2k}\}$ and $\{u_{2k}\}$ are increasing bounded sequences whereas the sequences $\{\nu_{2k+1}\}$ and $\{u_{2k+1}\}$ are decreasing bounded sequences, all of which thus have limits. As $k \to \infty$, let $\nu^* = \lim \nu_{2k}$, $u^*(x) = \lim u_{2k}(x)$, $\nu_* = \lim \nu_{2k+1}$ and $u_*(x) = \lim u_{2k+1}(x)$. Of course $\nu^* \leq \nu_*$ and $u^*(x) \leq u_*(x)$. By utilizing the fact that for the functions $u_n$,

$$u_n(x) = \nu_n \int_0^1 K(x, t; \nu_n^{1/2}) t^{-1/2} (1 - u_{n-1}^{1/2}(t)) u_n(t)\, dt \tag{3.5}$$

and by applying the dominated convergence theorem, we have

$$u^*(x) = \lim u_{2k}(x) = \nu^* \int_0^1 K(x, t; \nu^{*1/2}) t^{-1/2} (1 - u_*^{1/2}(t)) u^*(t)\, dt,$$

$$u_*(x) = \lim u_{2k+1}(x) = \nu_* \int_0^1 K(x, t; \nu_*^{1/2}) t^{-1/2} (1 - u^{*1/2}(t)) u_*(t)\, dt. \tag{3.6}$$

Thus $u^{*''} = \nu^* x^{-1/2} u_*^{1/2} u^*$, $u_*'' = \nu_* x^{-1/2} u^{*-1/2} u_*$, $0 < x < 1$, and both $u^*$ and $u_*$ satisfy the boundary conditions $-\alpha u(0) + u'(0) = 0$, $u(1) = 0$ along with the initial condition $u(0) = 1$.

LEMMA 9: $\nu^* = \nu_*$, $u^*(x) = u_*(x)$, $0 \le x \le 1$

*Proof:* If $u^*(x) \neq u_*(x)$ then by Sturm's second comparison theorem $\nu^* < \nu_*$. Thus there is an interval $(0, \epsilon)$ on which $u^{*''}(x) < u_*''(x)$, $u^{*'}(x) < u_*'(x)$, and $u^*(x) < u_*(x)$. In order to satisfy $u^*(1) = u_*(1) = 0$ there must be an $x_0 \in (0, 1)$ such that $u^{*''}(x_0) > u_*''(x_0)$ and $u^*(x_0) < u_*(x_0)$. That is,

$$\nu^* x_0^{-1/2} u_*^{1/2}(x_0) u^*(x_0) > \nu_* x_0^{-1/2} u^{*1/2}(x_0) u_*(x_0), \tag{3.7}$$

from which we conclude $\nu^* u^{*1/2}(x_0) > \nu_* u_*^{1/2}(x_0)$, a contradiction. Thus $u^*(x) = u_*(x)$, $0 \le x \le 1$, and then of course $\nu^* = \nu_*$.

We have shown that the sequence $\{(u_n, \nu_n)\}$ converges to a positive solution of Eq. (3.1). The sequence $\{u_n\}$ is uniformly bounded by $u_0$ and $u_1$ and from (3.5) we have that $\{u_n\}$ is equicontinuous on [0, 1] and thus the convergence of $\{u_n\}$ to $u$ is uniform on [0, 1]; this completes the proof of Theorem 1.

Finally, in order to make the discussion complete and self-contained, we include some uniqueness results for the initial-value problem

$$\begin{aligned} y'' &= \beta x^{-1/2} y^{3/2} \\ y(0) &= 1,\ y'(0) = \alpha \end{aligned} \tag{3.8}$$

for $\beta > 0$, and the eigenvalue problem

$$\begin{aligned} u'' &= \lambda x^{-1/2} u^{3/2}, \quad 0 < x < 1, \\ u(0) &= 1,\ u(1) = 0, \\ u'(0) &= \alpha. \end{aligned} \tag{3.9}$$

LEMMA 10: If $y_0$ and $y_0^*$ are two positive solutions of (3.8) and if there is an $x_0 > 0$ such that $y_0(x_0) > y_0^*(x_0)$, then $y_0(x) > y_0^*(x)$ and $y_0'(x) > y_0^{*'}(x)$ for $x > x_0$.

*Proof:* If there is an $x > x_0$ such that $y_0(x) = y_0^*(x)$, let $x_1 = \{\sup x\colon x < x_0, y_0(x) = y_0^*(x)\}$ and $x_4 = \inf \{x\colon x > x_0, y_0(x) = y_0^*(x)\}$. By continuity, $y_0(x_1) = y_0^*(x_1)$, $y_0'(x_1) \ge y_0^{*'}(x_1)$, $y_0(x_4) = y_0^*(x_4)$, and $y_0'(x_4) \le y_0^{*'}(x_4)$, $y_0(x) > y_0^*(x)$, $x_1 < x < x_4$. Thus there are $x_2, x_3$, $x_1 < x_2 < x_3 < x_4$, such that $y_0^{*'}(x_3) > y_0'(x_3)$ and $y_0^{*''}(x_2) > y_0''(x_2)$ which contradicts $\beta x_2^{-1/2} y_0^{*3/2}(x_2) < \beta x_2^{-1/2} y_0^{3/2}(x_2)$. We conclude that $y_0(x) = y_0^*(x)$, $y_0'(x) = y_0^{*'}(x)$, $0 < x < x_1$, and $y_0(x) > y_0^*(x)$, $y_0'(x) > y_0^{*'}(x)$ for $x > x_1$.

*Theorem* 2: The solution $y_0$ to (3.8) is unique.

*Proof:* Suppose $y_0$ and $y_0^*$ are two solutions of (3.8). If $y_0 \neq y_0^*$, then there is an $x_0 \ge 0$ such that $y_0(x) = y_0^*(x)$, $y_0'(x) = y_0^{*'}(x)$, $x \le x_0$ and $y_0(x) > y_0^*(x)$, $y_0'(x) > y_0^{*'}(x)$, $x > x_0$. We show that this cannot happen. Let $x_2 > x_1$ be fixed such that $y_0(x_2)$, $y_0'(x_2)$, $y_0^*(x_2)$, and $y_0^{*'}(x_2)$ all exist. Then for $0 < x < x_2$

$$\begin{aligned} 0 &\le y_0'(x) - y_0^{*'}(x) + \beta x^{-1/2}(y_0^{3/2}(x) - y_0^{*3/2}(x)) \\ &\le M(y_0(x) - y_0^*(x) + y_0'(x) - y_0^{*'}(x)) \end{aligned} \tag{3.10}$$

for $M \geq (x_2^{1/2} + \beta)([3/2]y_0(x_2)y_0^{-1/2}(x_1) + 1)$. Let $P(x) = y_0(x) - y_0^*(x) + y_0'(x) - y_0^{*\prime}(x)$ and $\rho(x) = P(x_2)\exp(2M(x^{1/2} - x_2^{1/2}))$, $0 < x < x_2$. Then $\rho(x)$ satisfies

$$\begin{aligned} \rho' &= Mx^{-1/2}\rho \qquad 0 < x < x_2 \\ \rho(x_2) &= P(x_2) > 0. \end{aligned} \tag{3.11}$$

Moreover, $\rho(x) \leq P(x)$, $0 < x \leq x_2$, for if not there are $t$ and $h$ such that $0 < t - h < t < x_2$, $\rho(t) = P(t)$, $\rho(x) > P(x)$, $t - h \leq x < t$. However, $P(t) - P(t-h) = \int_{t-h}^{t} P'(x)\,dx = \int_{t-h}^{t} y_0'(x) - y_0^{*\prime}(x) + \beta x^{-1/2}(y_0^{3/2}(x) - y_0^{*3/2}(x))\,dx \leq M\int_{t-h}^{t} x^{-1/2}\rho(x)\,dx = \int_{t-h}^{t}\rho'(x)\,dx = \rho(t) - \rho(t-h) = P(t) - \rho(t-h)$. Thus $\rho(t-h) \leq P(t-h)$, a contradiction. However, $\rho(x) \leq P(x)$, $0 < x \leq x_2$ is obviously a contradiction since $\lim_{x\to 0^+}\rho(x) = P(x_2)\exp(-2Mx_2^{1/2}) > 0$ and $\lim_{x\to 0^+}P(x) = 0$. Thus $y_0 = y^*$.

THEOREM 3: The positive solution $(u_0, \lambda_0)$ of (3.9) is unique.

*Proof:* Suppose $(u_0, \lambda_0)$ and $(u_0^*, \lambda_0^*)$ are two solutions of (3.7). If $\lambda_0 \neq \lambda_0^*$, then we can proceed as in the proof of lemma 9 to arrive at a contradiction. So $\lambda_0 = \lambda_0^*$ and, by Theorem 2, $u_0 = u_0^*$.

## 4. The isolated neutral atom.

The Thomas-Fermi equation with boundary conditions for the isolated neutral atom is

$$\begin{aligned} y'' &= x^{-1/2}y^{3/2}, \\ y(0) &= 1,\ y(+\infty) = 0, \end{aligned} \tag{4.1}$$

and its solution is denoted by $y_\infty(x)$. In this section we consider uniform approximations to $y_\infty(x)$.

Using the same methods as in the proof of lemma 1, it can be shown that as $\alpha$ decreases, the eigenvalues of Eq. (2.1) increase. Moreover, since $0 \leq u(x) \leq 1$, $0 \leq x \leq 1$, we have

$$u(x) = 1 + \alpha x + \nu\int_0^x\int_0^t s^{-1/2}u^{3/2}(s)\,ds\,dt \leq 1 + \alpha x + (4/3)\nu x^{3/2},$$

$$0 = u(1) \leq 1 + \alpha + (4/3)\nu.$$

Thus as $\alpha \to -\infty$ the eigenvalue $\nu \to +\infty$.

Now, for $a = \nu^{2/3}$, we let

$$\begin{aligned} y_a(x) &= u(\nu^{-2/3}x), \qquad 0 \leq x \leq a, \\ &= 0, \qquad x > a, \end{aligned}$$

and consider

$$M \equiv \max_{0 \leq x} |y_\infty(x) - y_a(x)|.$$

Since $y_\infty(x)$ is decreasing, it follows that the maximum is attained at some point $x_0 \leq a$. Moreover since $y_a(x) \leq y_\infty(x)$ and both $y_\infty$ and $y_a$ satisfy $y'' = x^{-1/2}y^{3/2}$, $0 < x < a$, $y(0) = 1$, we have $M = y_\infty(a)$. Thus as $\alpha \to -\infty$, $y_a$ converges uniformly on $[0, \infty)$ to $y_\infty$. Finally we note that Sommerfeld's approximate solution (1.7), which is quite accurate for large $x$, can be used to estimate $y_\infty(a)$ and thus to estimate the maximum difference $M$ between $y_a$ and $y_\infty$.

**5. Remarks.** In summary, it was shown in Sec. 3 that our iteration converges to a solution of the Thomas-Fermi equation with the ion case boundary values. It was shown in Sec. 4 that this solution technique can be used to find a uniform approximant to the solution of the isolated neutral atom boundary-value problem. Existence and uniqueness of the solution was also established for the ion case.

In this section we discuss the possible implementation of the iteration for actual numerical computations. This problem is reasonably well suited for an application of Galerkin methods, a technique for approximately calculating the largest eigenvalue and corresponding eigenfunction of $T_\lambda$ in $H_\rho$ .

From the principle of Galerkin's method [25], if $T$ is a compact selfadjoint linear operator with simple spectrum on a separable Hilbert space $H$, if $\{f_k\}$ is a complete orthonormal system in $H$, and if $P_n$ is the orthogonal projection onto $H_n = \text{span}\ \{f_1, \cdots, f_n\}$, then as $n \to \infty$ the largest eigenvalue and corresponding eigenfunction of $P_n T$ converge to the largest eigenvalue and corresponding eigenfunction of $T$.

In the actual numerical computation of each iteration not only is it necessary to calculate the largest eigenvalue $\mu_0(\lambda)$ and corresponding eigenfunction of $T_\lambda$ , it is also necessary to determine the value of $\lambda$ such that $\mu_0(\lambda) = \lambda^{-2}$. The numerical computations thus require the interweaving of two numerical methods. For a given $\lambda$, we propose to use Galerkin's method to calculate the largest eigenvalue $\mu_0(\lambda)$ of $T_\lambda$ and its corresponding eigenfunction. We then propose to use an averaging method along with Eq. (2.12) which gives the slope of $\mu_0(\lambda)$ go make adjustments in the value of $\lambda$ in order to obtain $\mu_0(\lambda) = \lambda^{-2}$.

We also comment that it is probably not most efficient to calculate the sequence of eigenvalues and eigenfunctions directly from the operator $T_\lambda$ , for we note that after each iteration the inner product in $H_\rho$ changes. This would then necessitate a reorthonormalization of the sequence $\{f_k\}$ before the next iteration can be accomplished. For this reason we introduce the selfadjoint Hilbert-Schmidt operator M defined on $L^2[0, 1]$ by

$$M_{\lambda\rho}\phi = \int_0^1 x^{-1/4}\rho^{1/2}(x)K(x, t; \lambda)t^{-1/4}\rho^{1/2}(t)\phi(t)\, dt \tag{5.1}$$

where $K(x, t; \lambda)$ is defined in (2.3) and of course for the $k$th iteration, $\rho = (1 - u_{k-1})^{1/2}$. It now follows that if $\phi \in L^2[0, 1]$ is an eigenfunction of $M_{\lambda\rho}$ with corresponding eigenvalue $\mu$ then for the function $u$ in $H_\rho$ defined by

$$u = x^{1/4}\rho^{-1/2}(x)\phi \tag{5.2}$$

we have

$$x^{-1/4}\rho^{1/2}(x)T_\lambda(u) = M_{\lambda\rho}(\phi) = \mu\phi = \mu x^{-1/4}\rho^{1/2}(x)u. \tag{5.3}$$

Thus $T_\lambda$ and $M_{\lambda\rho}$ have the same spectrum and their eigenfunctions are related by (5.2). Since $M_{\lambda\rho}$ is defined on $L^2[0, 1]$, the reorthonormalization problem does not arise. The largest eigenvalue of $T_\lambda$ is the same as the largest eigenvalue of $M_{\lambda\rho}$ and the corresponding eigenfunction of $T_\lambda$ can be found by utilizing (5.2).

We note that in the proof of the main theorem the eigenfunctions and eigenvalues of $T_\lambda$ are utilized, whereas in the numerical computations we can only obtain approximations to the eigenvalues and eigenfunctions. Theoretically, the procedure still yields a valid approximation to the solution since the necessary eigenvalues and eigenfunctions depend continuously on $\lambda$ and $\rho$ [23]. We are presently investigating numerical computations utilizing a complete orthnormal sequence of polynomials in $L_2[0, 1]$. The outcomes of these investigations will be published elsewherê.

## References


[1] L. H. Thomas, *The calculation of atomic fields*, Proc. Camb. Phil. Soc. **23**, 542–548 (1927)

[2] E. Fermi, *Un metodo statistico par la determinazione di alcune proprietá dell' atome,* Rend. Accad. Naz. del Lincei. Cl. sci. fis., mat. e nat. (**6**) 6, 602–607 (1927)

[3] P. Csavinszky, *Calculation of diamagnetic susceptibilities of ions using a universal approximate analytical solution of the Thomas-Fermi equation*, Bull. Amer. Phys. Soc. (2) **18**, 726–727 (1973)

[4] P. Csavinszky, *Universal approximate analytical solution of the Thomas-Fermi equation for ions*, Phys. Rev. A(3) **8**, 1688–1701 (1973)

[5] Y. Bae Suh, *Perturbation calculation using Thomas-Fermi model*, Phys. Lett. **49A**, 99–100 (1974)

[6] E. H. Lieb and B. Simon, *Thomas-Fermi theory revisited*, Phys. Rev. Lett. **31**, 681–683 (1973)

[7] E. H. Lieb and B. Simon, *The Thomas-Fermi theory of atoms, molecules, and solids*, Advances in Mathematics, to appear 1976

[8] P. Gombás, *Die statistische Theorie des Atoms*, Springer, Berlin, 1949

[9] N. H. March, *The Thomas-Fermi approximation in quantum mechanics*, Adv. Phys. **6**, 1–101 (1957)

[10] J. S. W. Wong, *On the generalized Emden-Fowler equation*, SIAM Rev. (2) **17**, 339–360 (1975)

[11] E. B. Baker, *The application of the Thomas-Fermi statistical model to the calculation of potential distribution of positive ions*, Phys. Rev. **36**, 630–647 (1930)

[12] A. Sommerfeld, *Asymptotische Integration der Differential-Gleichung des Thomas-Fermischen Atoms*, Z. Phys. **78**, 283–308 (1932)

[13] H. T. Davis, *Introduction to nonlinear differential and integral equations*, Dover, New York, 1962

[14] V. Bush and S. H. Caldwell, *Thomas-Fermi equation solution by the differential analyzer*, Phys. Rev. (2) **38**, 1898–1901 (1931)

[15] R. V. Ramnath, *A new analytical approximation for the Thomas-Fermi model in atomic physics*, J. Math. Anal. Appl. **31**, 285–296 (1970)

[16] R. P. Feynman, N. Metropolis, and E. Teller, *Equations of state of elements based on the generalized Fermi-Thomas theory*, Phys. Rev. **75**, 1561–1573 (1949)

[17] E. Hille, *Some aspects of the Thomas-Fermi equation*, J. d'Analyse Math. **23**, 147–170 (1970)

[18] A. Mambriani, *Su un teorema relativo alle equazioni differenziali ordinarie del 2d ordine*, Rend. Accad. Naz. del Lincei, Cl. sci. fis., mat. e nat. (6) **9**, 620–622 (1929)

[19] G. Scorza-Dragoni, *Su un' equazione differenziale particolare,* Rend. Accad. Naz. del Lincei, Cl. sci. fis., mat. e nat. (6) 9, 623–625 (1929)

[20] J. L. Reid, *Solution to a nonlinear differential equation with application to Thomas-Fermi equations*, Rend. Accad. Naz. del Lincei, Cl. Sci. fis., mat. e nat. **53**, 376–379 (1972)

[21] J. L. Reid and R. J. Depuy, *Derivation of modified Thomas-Fermi and Emden equations*, Atti. Accad. Naz. del Lincei **54**, 529 (1973)

[22] M. Abramowitz and I. Stegun, *Handbook of Mathematical functions*, Dover, New York, 1965

[23] R. Courant and D. Hilbert, *Methods of mathematical physics*, Wiley, New York, 1953

[24] S. Karlin, *Positive operators*, J. Math. Mech. 8, 907–937 (1959)

[25] M. Krasnoselskii, *Topological methods in nonlinear integral equations*, Pergamon, New York, 1964