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COMPUTATIONAL METHODS FOR GENERALIZED THOMAS–FERMI MODELS OF NEUTRAL ATOMS*

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1. Introduction. Since 1927 when Thomas [10] and Fermi [3] studied potentials and charge densities in atoms, many mathematicians and physicists have contributed further knowledge in this area concerning the following three models. They are described by the nonlinear singular second-order differential equation,

$$y'' = x^{-1/2} y^{3/2}, \tag{1.1}$$

subject to boundary conditions, corresponding to

(a) the ionized atom:

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

(b) the neutral atom with Bohr radius a:

$$y(0) = 1, \qquad B(y(a)) = 0, \tag{1.3}$$

where $B(y(a))$ denotes $ay'(a) - y(a)$;

(c) the isolated neutral atom:

$$y(0) = 1, \qquad \lim_{x\to\infty} y(x) = 0. \tag{1.4}$$

Recently, we [2] generalized (1.1) to the form,

$$y'' + \frac{b}{x} y' = c x^p y^q, \tag{1.5}$$

where b, c, p, and q are constants such that $0 \le b < 1$, $c > 0$, $p > -2$, and $q > 1$. We studied it under the boundary condition (1.2) for existence, uniqueness, and the dependence of the solution on the size of the interval $[0, a]$. We refer to this paper for further references.

The main purpose here is to study existence and uniqueness results for the problems (1.5) subject to the boundary conditions (1.3) and (1.4), respectively; the dependence of the solution for the problem (1.5) and (1.3) on the size of the interval $[0, a]$ is also established. We give accurate computational methods that allow $b < 1$, and devise the constructive methods such that the monotone iterative techniques can be

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applied. The boundary condition, $ay'(a) - y(a) = 0$ in (1.3), is not of the usual type since the coefficient of $y(a)$ is negative while the domain in the boundary conditions (1.4) is unbounded. Thus for example, the results of Mooney [7] using monotone iterations cannot be applied here. For further references on monotone methods, we refer to his paper, and the book of Ladde, Lakshmikantham, and Vatsala [5].

In Section 2, we use modified Bessel functions of the first kind and the second kind to construct Green's functions of linear problems. These are used in Secs. 3 and 4 respectively to construct successive monotone approximations to the solutions of our problems. The use of the two kinds of modified Bessel functions allows us to consider the cases when their orders, determined by the values of b and p, are integers. In Section 3, we study the problem (1.5) and (1.3). Because of different proofs and constructions, we consider the following three cases separately: (i) $0 < b < 1$, (ii) $b = 0$, and (iii) $b < 0$. In Section 4, we study the problem (1.5) and (1.4). As illustrations, we implement our computational methods in Section 5 to obtain four numerical examples. The first three examples illustrate the three cases of the problem (1.5) and (1.3) while the last one illustrates the problem (1.5) and (1.4). In particular, Example 2 is the Thomas–Fermi model (1.1) and (1.3) for a neutral atom; it also improves Luning's results [6]. Example 4 is Thomas–Fermi model (1.1) and (1.4) for an isolated neutral atom; our numerical data agree with those given, for examples, by Bush and Caldwall [1], Fermi [4], and Roberts [9].

2. Green's functions. Let

$$L_0 v \equiv (x^b v')',$$
$$L_r v \equiv (x^b v')' - r x^{p+b} v, \tag{2.1}$$

where r is a positive constant. Comparing (2.1) with the left-hand side of the equation,

$$x^b \left[w'' + \frac{1 - 2\beta\nu}{x} w' + \alpha^2 \beta^2 x^{2(\beta-1)} w \right] = 0, \tag{2.2}$$

we obtain

$$\alpha = 2r^{1/2} i/(p+2),$$
$$\beta = (p+2)/2,$$
$$\nu = (1-b)/(p+2).$$

Thus, the homogeneous equation,

$$L_r w = 0, \tag{2.3}$$

can be written into the form (2.2). Let I_ν denote the modified Bessel function of the first kind of order ν, and K_ν denote that of the second kind. The general solution (cf. Watson [11, p. 97]) of (2.2) is given by

$$w(x) = k_1 w_1(x) + k_2 w_2(x), \tag{2.4}$$

where k_1 and k_2 are arbitrary constants,

$$w_1(x) = x^{(1-b)/2} I_\nu(|\alpha| x^\beta),$$

and

$$w_2(x) = x^{(1-b)/2} K_\nu(|\alpha| x^\beta).$$

Let

$$F(r) \equiv r^{1/2}a^{\beta}I_{\nu+1}(|\alpha|a^{\beta}) - bI_{\nu}(|\alpha|a^{\beta}),$$
$$H(r) \equiv r^{1/2}a^{\beta}K_{\nu+1}(|\alpha|a^{\beta}) + bK_{\nu}(|\alpha|a^{\beta}).$$

For the generalized neutral atoms with Bohr radii a, we need the following results.

LEMMA 1. For $0 < b < 1$, if r_1 is a positive root of $F(r)$, then the homogeneous problem given by (2.3) with $r = r_1$ subject to the boundary conditions,

$$w(0) = 0, \qquad B(w(a)) = 0, \tag{2.5}$$

has a nontrivial solution of the form

$$w(x) = c_1 w_1(x),$$

where c_1 is an arbitrary constant.

Proof. Let us use the boundary conditions (2.5) to determine the constants k_1 and k_2 in (2.4). Since

$$w_1(x) = \left(\frac{|\alpha|}{2}\right)^{\nu} x^{1-b} \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n+\nu+1)} \left(\frac{|\alpha|}{2}\right)^{2n} x^{2n\beta},$$

$$w_2(x) = \frac{\pi}{2\sin\nu\pi}\left[\left(\frac{|\alpha|}{2}\right)^{-\nu} \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n-\nu+1)} \left(\frac{|\alpha|}{2}\right)^{2n} x^{2n\beta} - \left(\frac{|\alpha|}{2}\right)^{\nu} x^{1-b} \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n+\nu+1)} \left(\frac{|\alpha|}{2}\right)^{2n} x^{2n\beta}\right],$$

where Γ denotes the gamma function, we have $w_1(0) = 0$ and

$$w_2(0) = \frac{1}{2}\left(\frac{|\alpha|}{2}\right)^{-\nu} \Gamma(\nu) \neq 0.$$

The boundary condition $w(0) = 0$ gives $k_2 = 0$. Since

$$hI'_{\mu}(h) = \mu I_{\mu}(h) + hI_{\mu+1}(h), \tag{2.6}$$

we have

$$w'_1(x) = (1-b)x^{(-1-b)/2}I_{\nu}(|\alpha|x^{\beta}) + r^{1/2}x^{(p+1-b)/2}I_{\nu+1}(|\alpha|x^{\beta}).$$

From $B(w(a)) = 0$,

$$k_1 a^{(1-b)/2}F(r) = 0. \tag{2.7}$$

Since r_1 is a root of $F(r)$, the lemma is proved.

LEMMA 2. (i) For $0 < b < 1$, $F(r)$ has exactly one positive root, denoted by r_1. Also, $F(r) > 0$ for $r > r_1$. (ii) For $b < 0$, $H(r) > 0$ when $r \geq b^2/a^{2\beta}$.

Proof. (i) Since $0 < b < 1$ and $p > -2$, it follows that $0 < \nu < \infty$. Also, $I_{\nu}(0) = 0$ for $\nu > 0$ implies $F(0) = 0$. Now,

$$F(r) = \left(\frac{|\alpha|a^{\beta}}{2}\right)^{\nu} \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n+\nu+1)} \left(\frac{|\alpha|a^{\beta}}{2}\right)^{2n} \left[\frac{(p+2)|\alpha|^2 a^{2\beta}}{4(n+\nu+1)} - b\right].$$

Because $|\alpha| = 2r^{1/2}/(p+2)$, it follows that $F(r) < 0$ for $r < b(\nu+1)(p+2)/a^{2\beta}$. For sufficiently large r, $I_{\nu+1}(z)$ and $I_\nu(z)$ are asymptotic to $e^z/(2\pi z)^{1/2}$. Hence, $F(r) > 0$ for sufficiently large r. Because $F(r)$ is continuous for $r \in (0, \infty)$, it has a positive root r_1. If $F(r)$ has another root r_2, we may assume, without loss of generality, that $r_2 > r_1$. By Lemma 1, the problems (2.3) and (2.5) corresponding to r equal to r_1 and r_2 respectively have nontrivial solutions. Let v_1 and v_2 denote positive solutions corresponding to r_1 and r_2 respectively. By Green's identity,

$$\int_0^a [v_1(x^b v_2')' - v_2(x^b v_1')']\,dx = [x^b(v_1 v_2' - v_2 v_1')]_0^a,$$

whose left-hand side is

$$\int_0^a v_1 v_2 x^{p+b}(r_2 - r_1)\,dx > 0,$$

in contradiction to its right-hand side being zero.

(ii) For $\nu > 0$ and $z > 0$, we have $K_{\nu+1}(z) > K_\nu(z)$. It follows that for $b < 0$, $H(r) > 0$ when $r \geq b^2/a^{2\beta}$.

We remark that for $r \in (0, \infty)$, if $b \leq 0$, then $F(r) > 0$, and if $0 \leq b < 1$, then $H(r) > 0$. It then follows from Lemma 2 that r can always be chosen such that both $F(r)$ and $H(r)$ are positive for $b < 1$.

LEMMA 3. Let r be chosen such that both $F(r)$ and $H(r)$ are positive. For $b < 1$, the nonhomogeneous problem,

$$L_r v = f(x), \qquad v(0) = 0, \qquad B(v(a)) = 0, \tag{2.8}$$

has a unique solution,

$$v(x) = \int_0^a G(x;\xi) f(\xi)\,d\xi,$$

where $G(x;\xi)$ is Green's function, given by

$$G(x;\xi) = \begin{cases} w_1(x)[w_1(\xi) + k w_2(\xi)]/(-k\beta), & 0 \leq x \leq \xi, \\ w_1(\xi)[w_1(x) + k w_2(x)]/(-k\beta), & \xi \leq x \leq a. \end{cases}$$

Here, $k = F(r)/H(r)$. If f is continuous, nontrivial, and nonpositive, then $v > 0$ for $0 < x < a$.

Proof. Since the boundary condition $w(0) = 0$ implies $k_2 = 0$, and the boundary condition $B(w(a)) = 0$ implies (2.7), it follows from $F(r) > 0$ that $k_1 = 0$. Thus, the homogeneous problem has the trivial solution only, and hence the nonhomogeneous problem (2.8) has a unique solution.

By using (2.6),

$$hK_\mu'(h) = \mu K_\mu(h) - hK_{\mu+1}(h),$$

and the Wronskian $W(I_\mu(h), K_\mu(h)) = -1/h$ for nonzero μ and h, we obtain Green's function, $G(x;\xi)$. Since w_1, w_2, and k are positive, it follows that $G(x;\xi) < 0$ for $0 < x$, $\xi < a$, and the lemma is proved.

For the generalized isolated neutral atom, we have the following result.

LEMMA 4. For $b < 1$, the nonhomogeneous problem,

$$L_r v_\infty = f(x), \qquad v_\infty(0) = 0, \qquad \lim_{x\to\infty} v_\infty(x) = 0, \tag{2.9}$$

has a unique solution,

$$v_\infty(x) = \int_0^\infty G_\infty(x;\xi) f(\xi)\, d\xi,$$

where $G_\infty(x;\xi)$ is Green's function, given by

$$G_\infty(x;\xi) = \begin{cases} w_1(x)w_2(\xi)/(-\beta), & 0 \le x \le \xi, \\ w_1(\xi)w_2(x)/(-\beta), & \xi \le x < \infty. \end{cases}$$

If f is continuous, nontrivial, and nonpositive, then $v_\infty > 0$ for $0 < x < \infty$.

Proof. From the general solution (2.4) of $L_r w = 0$, $v_\infty(0) = 0$ implies $k_2 = 0$. Since $\lim_{x\to\infty} w_1(x) = \infty$, it follows from $\lim_{x\to\infty} v_\infty(x) = 0$ that $k_1 = 0$. Thus, the homogeneous problem corresponding to (2.9) has the trivial solution only, and hence the nonhomogeneous problem has a unique solution. A direct computation gives Green's function $G_\infty(x;\xi)$. Obviously, it is negative for $0 < x$, $\xi < \infty$, and hence the lemma follows.

Using the same procedure as in the proof of Lemma 3, we have the following lemmas.

LEMMA 5. For $b < 1$, the nonhomogeneous problem,

$$L_0 v_3 = f(x), \qquad v_3(0) = 0, \qquad v_3(\delta) = 0,$$

has a unique solution,

$$v_3(x) = \int_0^\delta G_1(x;\xi) f(\xi)\, d\xi,$$

where $G_1(x;\xi)$ is Green's function, given by

$$G_1(x;\xi) = \begin{cases} x^{1-b}(\xi^{1-b} - \delta^{1-b})/[(1-b)\delta^{1-b}], & 0 \le x \le \xi, \\ \xi^{1-b}(x^{1-b} - \delta^{1-b})/[(1-b)\delta^{1-b}], & \xi \le x \le \delta. \end{cases}$$

If f is continuous, nontrivial, and nonpositive, then $v_3 > 0$ for $0 < x < \delta$.

LEMMA 6. For $b < 0$, the nonhomogeneous problem,

$$L_0 v_4 = f(x), \qquad v_4(0) = 0, \qquad B(v_4(a)) = 0,$$

has a unique solution,

$$v_4(x) = \int_0^a G_2(x;\xi) f(\xi)\, d\xi,$$

where $G_2(x;\xi)$ is Green's function, given by

$$G_2(x;\xi) = \begin{cases} x^{1-b}(\xi^{1-b} - ba^{1-b})/[b(1-b)a^{1-b}], & 0 \le x \le \xi, \\ \xi^{1-b}(x^{1-b} - ba^{1-b})/[b(1-b)a^{1-b}], & \xi \le x \le a. \end{cases}$$

If f is continuous, nontrivial, and nonpositive, then $v_4 > 0$ for $0 < x < a$.

3. Bohr radii. The Thomas–Fermi equation (1.1) has no real negative solution. We confine our attention to finding a real, positive, and bounded solution y for the problem (1.5) and (1.3).

We have the following uniqueness result.

THEOREM 7. The problem (1.5) and (1.3) has at most one positive solution.

Proof. Let y_1 and y_2 be two distinct positive solutions of the problem (1.5) and (1.3), and let $\phi \equiv y_1 - y_2$. Then

$$L_0\phi = cqx^{p+b}\eta^{q-1}\phi, \qquad \phi(0) = 0, \qquad B(\phi(a)) = 0,$$

where η lies between y_1 and y_2.

Suppose $y_1(\sigma) = y_2(\sigma)$ for some σ in $(0, a]$. Let σ be the first x-coordinate such that this happens. Without loss of generality, we may assume $\phi < 0$ on $(0, \sigma)$. This contradicts Lemma 5. Thus for all $x \in (0, a]$, either $y_1(x) < y_2(x)$ or $y_1(x) > y_2(x)$.

Case (i): $0 < b < 1$. Using Green's identity on y_1 and y_2 as in Lemma 2, we obtain a contradiction, and hence uniqueness follows.

Case (ii): $b = 0$. Without loss of generality, suppose $\phi < 0$ in the interval $(0, a)$. By the maximum principle (cf. Protter and Weinberger [8, p. 6]), ϕ attains its negative minimum at $x = a$. From the differential equation, $\phi'' < 0$ implies that the graph for ϕ is concave downwards. Since $\phi'(a) = \phi(a)/a$, the tangent line at $x = a$ must pass through the origin. This gives a contradiction.

Case (iii): $b < 0$. Suppose $\phi < 0$ in $(0, a)$. From the differential equation for ϕ, ϕ cannot attain its local negative minimum. This implies $b\phi'(x)/x > 0$. The rest of its proof is similar to that of case (ii).

To prove the dependence of the solution y on a, let $x = at$, and $\zeta(t) = y(at)$. From (1.5),

$$(t^b\zeta')' = ca^{p+2}t^{p+b}\zeta^q, \qquad \zeta(0) = 1, \qquad B(\zeta(1)) = 0. \tag{3.1}$$

By Theorem 7, the problem (3.1) has at most one positive solution for $0 \leq t \leq 1$.

THEOREM 8. If $0 < \lambda < \tau$, and $\zeta_\lambda(t)$ and $\zeta_\tau(t)$ are positive solutions of the problem (3.1) with a equal to λ and τ, respectively, then $\zeta_\lambda > \zeta_\tau$ for $0 < t \leq 1$.

Proof. From (3.1),

$$\begin{gathered}[t^b(\zeta_\lambda - \zeta_\tau)']' = ct^{p+b}(\lambda^{p+2}\zeta_\lambda^q - \tau^{p+2}\zeta_\tau^q), \\ (\zeta_\lambda - \zeta_\tau)(0) = 0, \qquad B((\zeta_\lambda - \zeta_\tau)(1)) = 0.\end{gathered} \tag{3.2}$$

If $\zeta_\lambda < \zeta_\tau$ somewhere in the interval $(0, 1)$, then from (3.1) and the positivity of ζ_λ and ζ_τ, there exists a subinterval (t_1, t_2) such that the right-hand side of (3.2) is negative, and $\zeta_\lambda(t_1) = \zeta_\tau(t_1)$. If $\zeta_\lambda(t_2) = \zeta_\tau(t_2)$, then by the maximum principle, we have a contradiction unless $t_2 = 1$, and $\zeta_\lambda - \zeta_\tau$, being negative in the interval $(t_1, 1)$, attains its negative minimum at $t = 1$.

Case (i): $0 < b < 1$. By Green's identity,

$$\int_{t_1}^1 [\zeta_\lambda(t^b\zeta_\tau')' - \zeta_\tau(t^b\zeta_\lambda')']\,dt = [\zeta_\lambda t^b\zeta_\tau' - \zeta_\tau t^b\zeta_\lambda']_{t_1}^1.$$

This gives

$$c\int_{t_1}^1 t^{p+b}\zeta_\lambda\zeta_\tau(\tau^{p+2}\zeta_\tau^{q-1} - \lambda^{p+2}\zeta_\lambda^{q-1})\,dt = -\zeta_\lambda(t_1)t_1^b[\zeta_\tau'(t_1) - \zeta_\lambda'(t_1)]. \tag{3.3}$$

Since $\zeta_\lambda'(t_1) \le \zeta_\tau'(t_1)$, the right-hand side of (3.3) is nonpositive. Because $\zeta_\tau > \zeta_\lambda$ for $t \in (t_1, 1)$, the left-hand side of (3.3) is positive. Thus we have a contradiction. Hence, $\zeta_\lambda(t) \ge \zeta_\tau(t)$ for $0 < t < 1$.

Suppose $\zeta_\lambda(t_3) = \zeta_\tau(t_3)$ for some $t_3 \in (0, 1)$. Then there exists an interval such that the right-hand side of (3.2) is nonpositive since $\lambda < \tau$. By the maximum principle, $\zeta_\lambda(t) \equiv \zeta_\tau(t)$ for $0 < t < 1$. This contradicts (3.2).

Case (ii): $b = 0$. Since $(\zeta_\lambda - \zeta_\tau)'(1) = (\zeta_\lambda - \zeta_\tau)(1)$, the tangent line at $t = 1$ must pass through the origin. This contradicts that the graph of $\zeta_\lambda - \zeta_\tau$ is concave downwards for $t \in (t_1, 1)$ since $(\zeta_\lambda - \zeta_\tau)'' < 0$. Thus $\zeta_\lambda \ge \zeta_\tau$ for $0 < t < 1$. By following the last part of the proof in case (i), we have $\zeta_\lambda > \zeta_\tau$ for $0 < t < 1$.

Case (iii): $b < 0$. A proof analogous to that of case (iii) of Theorem 7 gives $b(\zeta_\lambda - \zeta_\tau)'/t > 0$ for $t \in (t_1, 1)$. The rest of the proof is similar to that of case (ii).

Since the behavior and the constructions of the solutions of the problem (1.5) and (1.3) depend on the values of b, we divide the discussion on existence below according to (i) $0 < b < 1$, (ii) $b = 0$, and (iii) $b < 0$.

Case (i): $0 < b < 1$. At a positive local maximum, $y' = 0$ and $y'' < 0$. This gives a contradiction by (1.5). Thus, y cannot attain its positive local maximum, and the maximum value of y must be attained at either one of the boundary points. Let $M \ge \max\{1, y(a)\}$. In Theorem 14 later on, we show that $y(a) \le N$, where N denotes

$$[(b + p + q + 1)/(ca^{p+2})]^{1/(q-1)}.$$

For the purpose of constructing a solution y, M may be taken to be $\max\{1, N\}$.

By using the general solution (2.4), we have the following result.

LEMMA 9. Let $r > r_1$. The solution $W(x)$ of the following problem,

$$L_r W = 0, \qquad W(0) = 1, \qquad B(W(a)) = 0, \tag{3.4}$$

is given by

$$W(x) = \frac{2}{\Gamma(\nu)}\left(\frac{|\alpha|}{2}\right)^{\nu} x^{(1-b)/2}\left[\frac{H(r)}{F(r)} I_\nu(|\alpha| x^\beta) + K_\nu(|\alpha| x^\beta)\right], \tag{3.5}$$

which is positive for $0 \le x \le a$.

We remark that the above lemma is also true for $b = 0$ with $r > 0$, and for $b < 0$ with $r \ge b^2/a^{2\beta}$.

LEMMA 10. If $r \ge cM^{q-1}$, and $r > r_1$, then the solution W of the problem (3.4) is a lower bound for y.

Proof. Since from (1.5), (1.3), and (3.4), we have

$$L_r(y - W) \le x^{p+b} M(cM^{q-1} - r) \le 0,$$
$$(y - W)(0) = 0, \qquad B((y - W)(a)) = 0,$$

it follows from Lemma 3 that $y \ge W$.

Let $\underline{w} \equiv y - W$. From (1.5), (1.3), and (3.4), we obtain

$$L_0 \underline{w} = x^{p+b}[c(W + \underline{w})^q - rW], \qquad \underline{w}(0) = 0, \qquad B(\underline{w}(a)) = 0. \tag{3.6}$$

Let us construct a sequence $\{\underline{w}_n\}$ as follows:

$$\underline{w}_0 \equiv 0 \quad \text{for } 0 \le x \le a; \tag{3.7}$$

for $n = 0, 1, 2, \ldots,$

$$\begin{gathered} L_r \underline{w}_{n+1} = x^{p+b}[c(W + \underline{w}_n)^q - r(W + \underline{w}_n)], \\ \underline{w}_{n+1}(0) = 0, \qquad B(\underline{w}_{n+1}(a)) = 0. \end{gathered} \tag{3.8}$$

Since $M > y \ge W$ for $0 < x < a$, the following result follows immediately from the fact that the derivative of the function with respect to z is negative.

LEMMA 11. For $0 \le z < M - W$, the function

$$c(W + z)^q - rz$$

is decreasing with respect to z, provided $r \ge cqM^{q-1}$.

Let us show that the sequence $\{\underline{w}_n\}$ is bounded above.

LEMMA 12. Let $r \ge cqM^{q-1}$, and $r > r_1$. Then $\underline{w}_n < M - W$ for $0 < x < a$, $n = 0, 1, 2, \ldots.$

Proof. Since $y < M$ for $0 < x < a$, and $y - W = \underline{w}$, it suffices to show that $\underline{w}_n < \underline{w}$ for $n = 0, 1, 2, \ldots.$ It follows from (3.6), (3.7), (3.8), and Lemma 11 that

$$L_r(\underline{w} - \underline{w}_1) = x^{p+b}\{[c(W + \underline{w})^q - r(W + \underline{w})] - (cW^q - rW)\} < 0.$$

Because $(\underline{w} - \underline{w}_1)(0) = 0$, and $B((\underline{w} - \underline{w}_1)(a)) = 0$, we have $\underline{w} > \underline{w}_1$ for $0 < x < a$ by Lemma 3. Let us assume that for a particular value of n, say j (≥ 1),

$$\underline{w} > \underline{w}_j \quad \text{for } 0 < x < a.$$

Again from (3.6), (3.8), and Lemma 11, we have $L_r(\underline{w} - \underline{w}_{j+1}) < 0$, and hence by Lemma 3, $\underline{w} > \underline{w}_{j+1}$. By the principle of mathematical induction, we have

$$\underline{w}(x) > \underline{w}_n(x) \quad \text{for } 0 < x < a, \ n = 0, 1, 2, \ldots.$$

The following result gives lower bounds and existence of a unique positive bounded solution constructively. Its proof is analogous to that of Theorem 1 of Chan and Hon [2], and hence is omitted here.

THEOREM 13. Let $r \ge cqM^{q-1}$, and $r > r_1$. For $n = 1, 2, 3, \ldots,$

$$0 < \underline{w}_n < \underline{w}_{n+1} < \underline{w} \quad \text{for } 0 < x < a;$$

furthermore, the problem (1.5) and (1.3) has a unique positive bounded solution y, to which the sequence $\{W + \underline{w}_n\}$ converges monotonically upwards.

By the maximum principle, y attains its maximum either at x equal to 0 or a. To obtain an upper bound for y, we need to establish one for $y(a)$ since $y(0) = 1$.

THEOREM 14. $y(a) \le N$.

Proof. If there exists a number $a^* \in (0, a)$ such that $B(y(a^*)) = 0$, we have $y(a^*) > y(a)$ by Theorem 8. From $B(y(a^*)) = 0$, we obtain $y'(a^*) > 0$. It follows from $y(a^*) > y(a)$ that y attains its positive local maximum somewhere in (a^*, a).

At this point, $y' = 0$ and $y'' < 0$. From (1.5), we have a contradiction. Thus, $B(y(x)) \neq 0$ unless $x = a$.

Obviously, $y(x) \geq y(a)x/a$ for $x = 0$. To show that this inequality is true for $x \in (0, a]$, let $Y(x) = y(x)/x$ for $x \in (0, a]$. Then,

$$\lim_{x \to 0^+} Y(x) = \infty, \qquad Y(a) = y(a)/a > 0.$$

On the other hand, $Y'(x) = B(y(x))/x^2$, which implies that $Y'(x) \neq 0$ unless $x = a$. Hence, the minimum of $Y(x)$ occurs at $x = a$, and we have

$$y(x) \geq y(a)x/a \quad \text{for } x \in [0, a]. \tag{3.9}$$

To obtain an upper bound for $y(a)$, we rewrite (1.5) as $L_0 y = cx^{p+b} y^q$, and integrate this over the interval $[0, a]$. From $y(0) = 1$, we have

$$a^b y'(a) = \int_0^a cx^{p+b}[y(x)]^q \, dx.$$

Using $B(y(a)) = 0$ and (3.9), we obtain

$$a^{b+q-1} \geq c[y(a)]^{q-1} \int_0^a x^{p+b+q} \, dx.$$

Thus

$$[y(a)]^{q-1} \leq (b + p + q + 1)/(ca^{p+2}),$$

from which the theorem follows.

Case (ii): $b = 0$. Since $b = 0$, we consider below the case $p < 0$ in order that the problem (1.5) and (1.3) is singular at $x = 0$. To obtain an upper bound for y, we consider the nonhomogeneous problem:

$$V'' = 2/a^2, \qquad V(0) = 1, \qquad B(V(a)) = 0. \tag{3.10}$$

Its solution is given by

$$V(x) = \frac{x^2}{a^2} + mx + 1,$$

where m is an arbitrary constant. Let

$$d(x) = \left(\frac{2}{ca^2}\right)^{1/q} x^{-p/q-1} - \frac{x}{a^2} - \frac{1}{x}.$$

It follows from $\lim_{x \to 0^+} d(x) = -\infty$ that $\sup_{0 \leq x \leq a} d(x)$ exists.

LEMMA 15. If $p < 0$, and

$$m \geq \sup_{0 \leq x \leq a} d(x), \tag{3.11}$$

then $V \geq y$ for $0 \leq x \leq a$.

Proof. By (3.11), $m \geq d(x)$. This gives

$$\frac{2}{a^2} \leq cx^p \left(\frac{x^2}{a^2} + mx + 1\right)^q \quad \text{for } 0 < x < a.$$

By (3.10), $V'' \leq cx^p V^q$ for $0 < x < a$. From (3.11),

$$V(x) \geq \left(\frac{2}{ca^2}\right)^{1/q} x^{-p/q} > 0 \quad \text{for } 0 < x < a.$$

Now,

$$(V - y)'' - cqx^p \eta^{q-1}(V - y) \leq 0,$$

where η lies between V and y. Since

$$(V - y)(0) = 0, \qquad B((V - y)(a)) = 0,$$

it follows from a proof analogous to that of case (ii) in Theorem 8 with the use of the maximum principle that $V \geq y$ for $0 \leq x \leq a$.

We note that since $p < 0$, the right-hand side of (3.11) can be computed numerically for each given value of a by using the IMSL (Edition 9.2, Revised November, 1984, IMSL LIB-0009) subroutine ZXMWD (to find, to single precision, the global minimum (with constraints) of a function of n variables). Let us denote this supremum value by m_1. Henceforth, we choose

$$V(x) = \frac{x^2}{a^2} + m_1 x + 1.$$

Let $\bar{v} \equiv V - y$. From (1.5), (1.3), and (3.10), we have

$$\bar{v}'' = \frac{2}{a^2} - cx^p(V - \bar{v})^q, \qquad \bar{v}(0) = 0, \qquad B(\bar{v}(a)) = 0.$$

Let us construct a sequence $\{\bar{v}_n\}$ as follows:

$$\bar{v}_0 \equiv 0 \quad \text{for } 0 \leq x \leq a;$$

for $n = 0, 1, 2, \ldots$,

$$L_r \bar{v}_{n+1} = \frac{2}{a^2} - x^p[c(V - \bar{v}_n)^q + r\bar{v}_n], \qquad \bar{v}_{n+1}(0) = 0, \qquad B(\bar{v}_{n+1}(a)) = 0.$$

The following result gives upper bounds and existence of a unique solution constructively. Its proof is similar to that of Theorem 13, and hence is omitted here.

THEOREM 16. Let $r \geq cq \max\{[V(a)]^{q-1}, 1\}$. For $p < 0$,

$$0 < \bar{v}_n < \bar{v}_{n+1} < \bar{v} \quad \text{for } 0 < x < a, \ n = 1, 2, 3, \ldots;$$

furthermore, the problem (1.5) and (1.3) has a unique solution y, to which the sequence $\{V - \bar{v}_n\}$ converges monotonically downwards.

We can also construct another sequence $\{\underline{v}_n\}$ as follows:

$$\underline{v}_0 \equiv V \quad \text{for } 0 \leq x \leq a;$$

for $n = 0, 1, 2, \ldots$,

$$L_r \underline{v}_{n+1} = \frac{2}{a^2} - x^p[c(V - \underline{v}_n)^q + r\underline{v}_n], \qquad \underline{v}_{n+1}(0) = 0, \qquad B(\underline{v}_{n+1}(a)) = 0.$$

Since its proof is similar to that of Theorem 13, we state without proof the following result, giving lower bounds and existence of a unique solution constructively.

THEOREM 17. Let $r \geq cq \max\{[V(a)]^{q-1}, 1\}$. For $p < 0$,

$$V > \underline{v}_n > \underline{v}_{n+1} > \bar{v} \quad \text{for } 0 < x < a, \ n = 1, 2, 3, \ldots;$$

furthermore, the problem (1.5) and (1.3) has a unique positive solution y, to which the sequence $\{V - \underline{v}_n\}$ converges monotonically upwards.

Case (iii): $b < 0$. To obtain an upper bound for the solution y, we consider the following nonhomogeneous problem:

$$L_0 U = 0, \qquad U(0) = 1, \qquad B(U(a)) = 0, \tag{3.12}$$

whose solution is

$$U(x) = 1 - \frac{1}{b}\left(\frac{x}{a}\right)^{1-b} \quad \text{for } 0 \le x \le a.$$

LEMMA 18. U is an upper bound for the solution y of the problem (1.5) and (1.3).

Proof. From (1.5), (1.3), and (3.12), we have

$$L_0(U - y) = -cx^{p+b}y^q, \qquad (U - y)(0) = 0, \qquad B((U - y)(a)) = 0.$$

It follows from Lemma 6 that $U > y$ for $0 < x < a$.

Let $\bar{u} \equiv U - y$. From (1.5), (1.3), and (3.12), we have

$$L_0\bar{u} = -cx^{p+b}(U - \bar{u})^q, \qquad \bar{u}(0) = 0, \qquad B(\bar{u}(a)) = 0.$$

Let us construct a sequence $\{\bar{u}_n\}$ as follows:

$$\bar{u}_0 \equiv 0 \quad \text{for } 0 \le x \le a;$$

for $n = 0, 1, 2, \ldots,$

$$L_r\bar{u}_{n+1} = -x^{p+b}[c(U - \bar{u}_n)^q + r\bar{u}_n], \qquad \bar{u}_{n+1}(0) = 0, \qquad B(\bar{u}_{n+1}(a)) = 0.$$

We note that $U(x)$ attains its maximum $1 - 1/b$ at $x = a$. A proof similar to that of Theorem 13 establishes the following result, giving upper bounds and existence of a unique solution constructively.

THEOREM 19. Let $r \ge \max\{b^2/a^{2\beta}, cq(1 - 1/b)^{q-1}\}$. For $n = 1, 2, 3, \ldots,$

$$0 < \bar{u}_n < \bar{u}_{n+1} < \bar{u} \quad \text{for } 0 < x < a;$$

furthermore, the problem (1.5) and (1.3) has a unique solution y, to which the sequence $\{U - \bar{u}_n\}$ converges monotonically downwards.

We can also construct another sequence $\{\underline{u}_n\}$ as follows:

$$\underline{u}_0 \equiv U \quad \text{for } 0 \le x \le a;$$

for $n = 0, 1, 2, \ldots,$

$$L_r\underline{u}_{n+1} = -x^{p+b}[c(U - \underline{u}_n)^q + r\underline{u}_n], \qquad \underline{u}_{n+1}(0) = 0, \qquad B(\underline{u}_{n+1}(a)) = 0.$$

The following result gives lower bounds and existence of a unique solution constructively. Its proof is again similar to that of Theorem 13.

THEOREM 20. Let $r \ge \max\{b^2/a^{2\beta}, cq(1 - 1/b)^{q-1}\}$. For $n = 1, 2, 3, \ldots,$

$$U > \underline{u}_n > \underline{u}_{n+1} > \bar{u} \quad \text{for } 0 < x < a;$$

furthermore, the problem (1.5) and (1.3) has a unique positive solution y, to which the sequence $\{U - \underline{u}_n\}$ converges monotonically upwards.

We note that although Theorems 19 and 20 give the same solution y, the positivity of y is a direct consequence of the construction in Theorem 20 only. A similar remark on Theorems 16 and 17 may be made.

4. Isolated neutral atom. Since at a local maximum, $y'' < 0$ and $y' = 0$, it follows that a nonnegative solution of the problem (1.5) and (1.4) cannot attain its local maximum inside the interval $(0, \infty)$. Hence, its maximum is attained at $x = 0$, and y is bounded by 1.

We have the following uniqueness result.

THEOREM 21. There exists at most one nonnegative solution of the problem (1.5) and (1.4).

Proof. Let y_3 and y_4 be two distinct nonnegative solutions of the problem (1.5) and (1.4), and let $\theta \equiv y_3 - y_4$. Then

$$L_0\theta = cqx^{p+b}\eta^{q-1}\theta, \qquad \theta(0) = 0, \quad \lim_{x\to\infty} \theta(x) = 0, \tag{4.1}$$

where η lies between y_3 and y_4. Without loss of generality, suppose $\theta > 0$ somewhere inside the interval $(0, \infty)$. Then, θ attains its positive maximum at some point there. At this point, the left-hand side of (4.1) is negative while its right-hand side is positive. This contradiction proves the theorem.

To obtain a lower bound for y, we consider the problem:

$$L_r Z = 0, \qquad Z(0) = 1, \qquad \lim_{x\to\infty} Z(x) = 0. \tag{4.2}$$

By using the general solution (2.4) of $L_r w = 0$, and $\lim_{x\to\infty} w_1(x) = \infty$, we obtain

$$Z(x) = \frac{2}{\Gamma(\nu)}\left(\frac{|\alpha|}{2}\right)^{\nu} x^{(1-b)/2} K_\nu(|\alpha| x^\beta) > 0.$$

Since

$$L_r(y - Z) = x^{p+b} y(cy^{q-1} - r),$$

it follows from $y \le 1$, $q > 1$, and Lemma 4 that by choosing $r \ge c$, we have $y \ge Z$ for $0 < x < \infty$. This also shows that y is positive.

Now, let $\underline{z} \equiv y - Z$. From (1.5), (1.4), and (4.2), we have

$$L_0\underline{z} = x^{p+b}[c(Z + \underline{z})^q - rZ], \qquad \underline{z}(0) = 0, \qquad \lim_{x\to\infty} \underline{z}(x) = 0.$$

Let us construct a sequence $\{\underline{z}_n\}$ as follows:

$$\underline{z}_0 \equiv 0 \quad \text{for } 0 \le x < \infty;$$

for $n = 0, 1, 2, \ldots,$

$$L_r\underline{z}_{n+1} = x^{p+b}[c(Z + \underline{z}_n)^q - r(Z + \underline{z}_n)], \qquad \underline{z}_{n+1}(0) = 0, \quad \lim_{x\to\infty} \underline{z}_{n+1}(x) = 0.$$

The following result gives lower bounds and existence of a unique positive solution constructively. The procedure of its proof by using Lemma 4 is similar to that of Theorem 13, and hence is omitted here.

THEOREM 22. Let $r \geq cq$. For $n = 1, 2, 3, \ldots$,

$$0 < \underline{z}_n < \underline{z}_{n+1} < \underline{z} \quad \text{for } 0 < x < \infty;$$

furthermore, the problem (1.5) and (1.4) has a unique positive solution y, to which the sequence $\{Z + \underline{z}_n\}$ converges monotonically upwards.

5. Numerical results. The following computations are performed by the Honeywell 68/80 Multics computer system with subroutines from the IMSL Library. We apply the above constructive methods to obtain numerical solutions. We study the problem (1.5) and (1.3) by considering three different cases: (i) $0 < b < 1$, (ii) $b = 0$, and (iii) $b < 0$. Examples 1, 2, and 3 illustrate these cases while Example 4 is for the problem (1.5) and (1.4).

Example 1. Let $a = 2$, $b = 1/2$, $c = 1$, $p = -1/2$, and $q = 3/2$. We have $\nu = 1/3$, and $\beta = 3/4$. We use the subroutine ZBRENT (for computing, to single precision, the zero of a function which changes sign in a given interval) to compute r_1; this gives $r_1 = 0.4084$. By Theorem 14, $y(a) \leq 0.7813$. Thus, M may be taken to be 1.0000. By Theorem 13, we can choose $r = 1.5000$. To obtain $\underline{w}_{n+1}$ from $\underline{w}_n$ for $n \geq 0$, we have from (3.8) the representation formula:

$$\underline{w}_{n+1}(x) = \int_0^a G(x;\xi)\xi^{p+b}\{c[W(\xi) + \underline{w}_n(\xi)]^q - r[W(\xi) + \underline{w}_n(\xi)]\}\, d\xi,$$

where W is given by (3.5). To integrate the above integral, we use subroutines ICSCCU (to perform, to single precision, cubic spline interpolation), ICSEVU (to evaluate, to single precision, a cubic spline), MGAMAD (=DGAMMA to evaluate, to double precision, the gamma function of a double precision argument), MMBSIR (to compute, to double precision, a modified Bessel function of the first kind of nonnegative real order for real positive arguments with exponential scaling option), MMBSKR (to compute, to double precision, a modified Bessel function of the second kind of nonnegative real fractional order for real positive arguments scaled by exp(arg)), and DCADRE (to do numerical integration, to single precision, of a function using cautious adaptive Romberg extrapolation). In this way, we obtain $\underline{w}(x)$ to the desired degree of accuracy. This in turn gives $y(x)$. For the above calculations, we divide the interval $[0, a]$ into ten equal subintervals. The results, to 4 decimal points, are given in Table 1.

TABLE 1

$a = 2,\ b = 1/2,\ c = 1,\ p = -1/2,\ q = 3/2$

x	.2000	.4000	.6000	.8000	1.0000	1.2000	1.4000	1.6000	1.8000	2.0000
$y(x)$	.6685	.5805	.5388	.5229	.5249	.5413	.5704	.6116	.6651	.7314

Example 2. We consider the Thomas–Fermi model (1.1) and (1.3) for the neutral atom with several Bohr radii a. This corresponds to $b = 0$, $c = 1$, $p = -1/2$, and $q = 3/2$. We have $\nu = 2/3$, and $\beta = 3/4$. For each value of a, we use the subroutine ZXMWD to compute $-m_1$. This determines the upper bound $V(x)$. Similar to Example 1, we compute $\bar{v}_{n+1}$ from $\bar{v}_n$ for $n \geq 0$ by using the representation formula for $\bar{v}_{n+1}$ with subroutines ICSCCU, ICSEVU, MGAMAD, MMBSIR, MMBSKR, and DCADRE. In this way, we obtain $\bar{v}(x)$, and hence $y(x)$. To find $y'(0)$ for a given value of a, we use the subroutine DRVTE (for calculating, to double precision, the first, second or third derivative of a user supplied function). To compute the value of a such that $y'(0)$ is equal to a prescribed value, we use, in addition to the subroutines for computing $\bar{v}_{n+1}$ for each value of a, the subroutine ZBRENT.

Luning's existence and uniqueness result for the problem (1.1) and (1.3) requires

$$y'(0) = \gamma / a, \tag{5.1}$$

where γ is a constant such that $\gamma \geq -1$. We also obtained the estimates:

$$a < 6/(5^{2/3}) \quad \text{for } \gamma \geq -1, \tag{5.2}$$

$$a < \left(\frac{16}{15} + \frac{16\gamma}{49}\right)^{-2/3} \quad \text{for } \gamma \geq 0. \tag{5.3}$$

These restrict the range of possible values of a for existence and uniqueness of a solution. Such a restriction is not imposed here nor in the original Thomas–Fermi model.

Using our technique, and rounding the results to 4 significant figures, we find for $a = 6/(5^{2/3})$ that $m_1 = -.5583$, and $V(a) = 0.8544$. By Theorem 16, we may choose $r = 1.500$. We obtain $y'(0) = -1.471$. The numerical solution y, to 4 decimal points, is given in Table 2.

TABLE 2

$a = 6/5^{2/3}$, $b = 0$, $c = 1$, $p = -1/2$, $q = 3/2$

x	$y(x)$	x	$y(x)$
.0000	1.0000	.7332	.6087
.0001	.9999	.8797	.5865
.0002	.9997	1.0262	.5746
.0003	.9996	1.1728	.5719
.0004	.9994	1.3193	.5779
.0005	.9993	1.4658	.5921
.1470	.8542	1.6124	.6143
.2936	.7595	1.7589	.6448
.4401	.6918	1.9054	.6836
.5866	.6430	2.0520	.7312

We find the value of a such that $y'(0) = 0$ to be .8257, compared with $a < .9579$ obtained from (5.3). For $y'(0) = -1$, for example, we obtain $a = 1.193$; from (5.1), $\gamma = -1.193$, for which neither (5.2) nor (5.3) is applicable. The above results show the limitation of Lunings' results, and illustrate that accurate solutions can be obtained by our method. For the above calculations, we divide, for each value of a, the interval $[0, a]$ into 19 subintervals with end-points, x_i $(1 \leq i \leq 20)$, chosen as follows:

$$x_i = 10^{-4}(i-1) \quad \text{for } 1 \leq i \leq 6,$$

$$x_i = 5 \times 10^{-4} + (i-6)(a - 5 \times 10^{-4})/14 \quad \text{for } 7 \leq i \leq 20.$$

We remark that more points are chosen close to $x = 0$ in order to compute $y'(0)$ accurately.

The Thomas–Fermi equation (1.1) with the condition $y(0) = 1$ leads to the formal series solution (cf. Luning),

$$y(x) = 1 + b_2 x + \cdots .$$

If b_2 $(= y'(0)) > -1.588$ (to 4 significant figures), then the series converges to the solution of the problem (1.1) and (1.3) for some prescribed value a. If $b_2 = -1.588$, then the series converges to the solution of the problem (1.1) and (1.4). By dividing the interval $[0, 70]$ into 165 subintervals with end-points x_i given by

$$\begin{aligned} x_i &= 10^{-4}(i-1) && \text{for } 1 \le i \le 6, \\ x_i &= 10^{-1}(i-6) && \text{for } 7 \le i \le 106, \\ x_i &= 10 + (i - 106) && \text{for } 107 \le i \le 166, \end{aligned}$$

our computational method gives for $a = 70$, $y'(0) = -1.582$. Theorem 8 implies that increasing a decreases the value $y(a)$. From $B(y(a)) = 0$, we obtain $y'(a) = y(a)/a$. This gives $\lim_{a\to\infty} y'(a) = 0$, which in turn implies $\lim_{a\to\infty} y(a) = 0$ since the tangent line at $x = a$ must pass through the origin. Thus, it follows that increasing a makes $y'(0)$ approach the value -1.588, and hence, the problem (1.1) and (1.4) may be approximated by the problem (1.1) and (1.3) for sufficiently large a.

Example 3. Let $a = 2$, $b = -1$, $c = 1$, $p = -1/2$, and $q = 3/2$. We then have $\nu = 4/3$, and $\beta = 3/4$. To satisfy Theorem 19, let $r = 2.122$. Similarly, we compute $\bar{u}_{n+1}$ from $\bar{u}_n$ for $n \ge 0$ by its representation formula with subroutines ICSCCU, ICSEVU, MGAMAD, MMBSIR, MMBSKR, and DCADRE. In this way, we obtain $\bar{u}(x)$, and hence $y(x)$. For the above calculations, we divide the interval $[0, a]$ into ten equal subintervals. The results, rounded to 4 decimal points, are given in Table 3.

TABLE 3

$a = 2,\ b = -1,\ c = 1,\ p = -1/2,\ q = 3/2$

x	.2000	.4000	.6000	.8000	1.0000	1.2000	1.4000	1.6000	1.8000	2.0000
$y(x)$	.9308	.8511	.7827	.7296	.6931	.6742	.6738	.6935	.7353	.8020

Example 4. We consider the Thomas–Fermi model (1.1) and (1.4) for an isolated neutral atom. Here, $b = 0$, $c = 1$, $p = -1/2$, and $q = 3/2$. We then have $\nu = 2/3$, and $\beta = 3/4$. By Theorem 22, we may choose $r = 3/2$; this gives $|\alpha| = (8/3)^{1/2}$. As before, $\underline{z}_{n+1}$ can be computed from its representation formula by using subroutines ICSCCU, ICSEVU, MGAMAD, MMBSIR, MMBSKR, and DCADRE. In this way, we obtain $\underline{z}(x)$, and hence $y(x)$. Since $I_\nu(|\alpha|200^\beta) = .2230\times 10^{37}$, and $K_\nu(|\alpha|200^\beta) = .2581 \times 10^{-38}$, a slight increase in the argument puts the computation of I_ν and K_ν beyond the range of the computer. Thus in each iteration, we integrate from 0 to 200, instead of from 0 to ∞. Since the slope y' is more negative near $x = 0$, more points are chosen there. We divide the interval $[0, 200]$ into 141 subintervals with endpoints

x_i given by $x(1) = 0.00000$, $x(2) = 0.00001$, $x(3) = 0.00002$, $x(4) = 0.00003$,

$$x_i = (i-4)/10 \quad \text{for } 5 \le i \le 104,$$
$$x_i = 10 + 5(i-104) \quad \text{for } 105 \le i \le 142.$$

For illustrative purpose, 24 data, rounded to 4 decimal points, are given in Table 4.

TABLE 4

$b = 0,\ c = 1,\ p = -1/2,\ q = 3/2$

x	$y(x)$	x	$y(x)$	x	$y(x)$
.1000	.8817	.9000	.4529	5.0000	.0788
.2000	.7931	1.0000	.4240	6.0000	.0594
.3000	.7206	1.5000	.3148	7.0000	.0461
.4000	.6595	2.0000	.2430	8.0000	.0365
.5000	.6070	2.5000	.1930	9.0000	.0295
.6000	.5612	3.0000	.1566	10.0000	.0242
.7000	.5208	3.5000	.1294	15.0000	.0107
.8000	.4849	4.0000	.1084	20.0000	.0057

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