A CONSTRUCTIVE METHOD FOR THE THOMAS-FERMI EQUATION*

BY

C. Y. CHAN (*University of Southwestern Louisiana*)

AND

S. W. DU (*Miami University*)

1. Introduction. In working on potentials and charge densities in atoms, Thomas [3] and Fermi [1] independently studied the nonlinear second-order differential equation

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

For an ionized atom, the boundary conditions are given by

$$y(0) = 1, \quad y(a) = 0. \quad (1.2)$$

The problem (1.1) and (1.2) was studied by Mooney [2] using monotone methods with both the Picard and Newton algorithms.

Mooney showed that a solution y of the problem (1.1) and (1.2) satisfies the inequalities

$$0 < y \leq 1 - x/a \quad \text{for } 0 < x < a,$$

and by letting

$$u = 1 - x/a - y,$$

it follows that

$$0 \leq u < 1 - x/a \quad \text{for } 0 < x < a,$$

and the problem (1.1) and (1.2) becomes

$$u'' = -x^{-1/2}(1 - x/a - u)^{3/2}, \quad u(0) = 0 = u(a). \quad (1.3)$$

In particular, the Picard scheme $\{u_n\}$, $n = 0, 1, 2, \dots$, defined by

$$\begin{aligned} Lu_{n+1} &= -x^{-1/2}(1 - x/a - u_n)^{3/2} - \frac{3}{2}x^{-1/2}u_n, \\ u_{n+1}(0) &= 0 = u_{n+1}(a), \end{aligned} \quad (1.4)$$

where

$$Lu = u'' - \frac{3}{2}x^{-1/2}u,$$

---

* Received November 19, 1984.

converges monotonically upwards if $u_0 \equiv 0$, and monotonically downwards if $u_0 = 1 - x/a$ to the unique solution of the problem (1.3). With $u_0 \equiv 0$, u_1 constructed by (1.4) gives a lower bound for the problem (1.3). By letting $u_1 = 1 - x/a - H$, it follows that

$$\begin{aligned} LH &= x^{-1/2}(1 - x/a)^{3/2} - \frac{3}{2}x^{-1/2}(1 - x/a), \\ H(0) &= 1, \quad H(a) = 0, \end{aligned} \quad (1.5)$$

and hence u_1 generates an upper bound H for the problem (1.1) and (1.2). Similarly, with $u_0 = 1 - x/a$, u_1 constructed by (1.4) corresponds to $h = 1 - x/a - u_1$ given by

$$Lh = 0, \quad h(0) = 1, \quad h(a) = 0, \quad (1.6)$$

which generates a lower bound for the problem (1.1) and (1.2). Mooney claimed that there were no known analytic solutions for both problems (1.5) and (1.6) (cf. problems (6.1) and (6.3) of his paper). If this were true, there would be no analytic solution for each subsequent iterate.

In this paper, we show that problems (1.5) and (1.6) have analytic solutions, through the use of the modified Bessel functions. These imply that each of their subsequent iterates constructed by (1.4) has an analytic solution. Without establishing the actual rate of convergence, Mooney showed that the rate of convergence of the Newton scheme to the solution of the problem (1.3) was faster than that of the Picard scheme with $u_0 \equiv 0$. Here, we show that starting at any point in the interval $[0, a]$, an interval of the same length can be chosen such that the Picard scheme generates linear convergence, although the partial derivative of the right-hand side of (1.1) with respect to y is unbounded at $x = 0$; we also establish an existence result. Because of the nonlinearity $y^{3/2}$ in (1.1) and the boundary condition $y(a) = 0$, such an interval cannot be determined for the Newton scheme to generate quadratic convergence.

2. Ionized atom. Let us consider the nonhomogeneous problem

$$Lw = f(x), \quad 0 < x < a, \quad (2.1)$$

$$w(0) = 0 = w(a). \quad (2.2)$$

To use modified Bessel functions to solve this problem, we note that the left-hand side of (2.1) may be written as

$$w'' + x^{-2}(\alpha^2 \beta^2 x^{2\beta} + 1/4 - \nu^2 \beta^2)w$$

with

$$\alpha = \pm(8/3)^{1/2}i, \quad \beta = 3/4, \quad \nu = 2/3.$$

Thus, the complementary solution w_c of (2.1) is given by

$$w_c(x) = x^{1/2} [k_1 J_\nu(\alpha x^\beta) + k_2 J_{-\nu}(\alpha x^\beta)], \quad (2.3)$$

where J_λ denotes the Bessel function of order λ , and k_1 and k_2 are arbitrary constants. Since the modified Bessel function I_ν is given by

$$I_\nu(\mu) = [\exp(-i\pi\nu/2)] J_\nu(i\mu),$$

we may rewrite (2.3) as

$$w_c(x) = c_1 B_1(x) + c_2 B_2(x), \quad (2.4)$$

where

$$B_1(x) = x^{1/2} I_{2/3}(|\alpha|x^\beta), \quad B_2(x) = x^{1/2} I_{-2/3}(|\alpha|x^\beta),$$

and c_1 and c_2 are arbitrary constants. Explicitly,

$$B_1(x) = \left(\frac{2}{3}\right)^{1/3} x \sum_{n=0}^{\infty} \frac{(|\alpha|x^\beta/2)^{2n}}{(n!)\Gamma(n+5/3)} > 0 \quad \text{for } x > 0,$$

$$B_2(x) = \left(\frac{2}{3}\right)^{-1/3} \sum_{n=0}^{\infty} \frac{(|\alpha|x^\beta/2)^{2n}}{(n!)\Gamma(n+1/3)} > 0 \quad \text{for } x \geq 0,$$

where Γ denotes the gamma function. A solution of $Lw = 0$ satisfying $w(0) = 0$ is given by $B_1(x)$, while that satisfying $w(a) = 0$ is given by

$$B_1(x) - (B_1(a)/B_2(a))B_2(x).$$

A direct computation shows that their Wronskian is

$$3^{3/2}B_1(a)/(4\pi B_2(a))$$

using the fact (cf. Watson [4, p. 77]) that the Wronskian of $I_{2/3}(z)$ and $I_{-2/3}(z)$ is $-\sqrt{3}/(\pi z)$. Thus, Green's function $G(x; \xi)$ corresponding to the problem (2.1) and (2.2) is given by

$$G(x; \xi) = \begin{cases} \frac{4\pi B_1(x)}{3^{3/2}} \left[\frac{B_2(a)}{B_1(a)} B_1(\xi) - B_2(\xi) \right] & \text{for } 0 \leq x \leq \xi, \\ \frac{4\pi B_1(\xi)}{3^{3/2}} \left[\frac{B_2(a)}{B_1(a)} B_1(x) - B_2(x) \right] & \text{for } \xi \leq x \leq a. \end{cases}$$

The solution w is given by

$$w(x) = \int_0^a G(x; \xi) f(\xi) d\xi. \quad (2.5)$$

With

$$f(x) = -x^{-1/2}(1 - x/a)^{3/2},$$

(2.5) gives u_1 when u_0 is taken to be identically zero. This in turn solves (1.5):

$$H(x) = 1 - \frac{x}{a} + \int_0^a G(x; \xi) \xi^{-1/2}(1 - \xi/a)^{3/2} d\xi. \quad (2.6)$$

Thus, we have the following theorem.

THEOREM 1. The solution of the problem (1.5) is given by (2.6).

To solve (1.6), we note that it follows from (2.4) that the general solution of $Lh = 0$ is given by

$$h(x) = c_1 B_1(x) + c_2 B_2(x),$$

where the constants c_1 and c_2 are determined by $h(0) = 1$, and $h(a) = 0$. Therefore,

$$h(x) = \left(\frac{2}{3}\right)^{1/3} \Gamma\left(\frac{1}{3}\right) [B_2(x) - (B_2(a)/B_1(a))B_1(x)], \quad (2.7)$$

and we have the following result.

THEOREM 2. The solution of the problem (1.6) is given by (2.7).

The construction of the sequence $\{u_n\}$ by (1.4) with $u_0 \equiv 0$ is equivalent to constructing the sequence $\{Y_n\}$:

$$Y_0 = 1 - x/a, \quad 0 \leq x \leq a,$$

and for $n = 0, 1, 2, \dots$,

$$LY_{n+1} = x^{-1/2}Y_n(Y_n^{1/2} - \tfrac{3}{2}),$$

$$Y_{n+1}(0) = 1, \quad Y_{n+1}(a) = 0.$$

To show that these generate linear convergence and to obtain an existence result, let us consider Green's function $G_r(x; \xi)$ corresponding to $v'' = 0$ for $0 \leq r < x < a$:

$$G_r(x; \xi) = \begin{cases} \frac{(x-r)(\xi-a)}{a-r} & \text{for } r \leq x \leq \xi, \\ \frac{(\xi-r)(x-a)}{a-r} & \text{for } \xi \leq x \leq a, \end{cases}$$

which is negative for $r < x < a$. Since $\{Y_n\}$ is a monotonically decreasing sequence (cf. Mooney), we have, after dropping out the nonpositive terms,

$$Y_n - Y_{n+1} \leq -\frac{3}{2} \int_0^a G_0(x; \xi) \xi^{-1/2} [Y_{n-1}(\xi) - Y_n(\xi)] d\xi.$$

Let

$$\rho_i = \max_{0 \leq x \leq \sigma} (Y_i - Y_{i+1}),$$

where σ is a constant to be determined later on. A direct computation gives

$$\rho_n \leq \left\{ \max_{0 \leq x \leq \sigma} [2x(a^{1/2} - x^{1/2})] \right\} \rho_{n-1}.$$

Let us choose the interval $0 \leq x \leq \sigma$ such that the quantity inside the braces is less than one. This can be achieved, for example, by choosing $\sigma = 1/(6\sqrt{a})$. The sequence $\{Y_n\}$ converges linearly and uniformly to a solution of the problem (1.1) and (1.2) for $0 \leq x \leq \sigma$. Since the problem has at most one solution (cf. Mooney), we have existence of a unique solution Y for $0 \leq x \leq \sigma$.

To prove global existence, we start with $x = \sigma - \tau$, where τ is an arbitrarily chosen positive constant such that $\sigma - \tau > 0$. We then construct $\{y_n\}$ as follows:

$$y_0 = \frac{a-x}{a-(\sigma-\tau)} Y(\sigma-\tau) \quad \text{for } \sigma-\tau < a, \sigma-\tau \leq x,$$

and for $n = 0, 1, 2, \dots$,

$$Ly_{n+1} = x^{-1/2}y_n(y_n^{1/2} - \tfrac{3}{2}), \tag{2.8}$$

$$y_{n+1}(\sigma-\tau) = Y(\sigma-\tau), \quad y_{n+1}(a) = 0.$$

As before, we obtain

$$y_n - y_{n+1} \leq -\frac{3}{2} \int_{\sigma-\tau}^a G_{\sigma-\tau}(x; \xi) \xi^{-1/2} [y_{n-1}(\xi) - y_n(\xi)] d\xi.$$

Since

$$\begin{aligned} -\frac{3}{2} \int_r^a G_r(x; \xi) \xi^{-1/2} d\xi &= \frac{2}{a-r} \left[-(a-r)x^{3/2} + (a-x)r^{3/2} + (x-r)a^{3/2} \right] \\ &< \frac{2(x-r)(a^{3/2} - r^{3/2})}{a-r} \quad \text{for } x \geq r \\ &< 6(x-r)a^{1/2}, \end{aligned}$$

we have

$$\max(y_n - y_{n+1}) < \left\{ \max[6(x - \sigma + \tau)a^{1/2}] \right\} [\max(y_{n-1} - y_n)],$$

where the maximum is taken over the interval $\sigma - \tau \leq x \leq \eta$; obviously, η can be chosen to be $2\sigma - \tau$, for example, with $\sigma = 1/(6\sqrt{a})$. We then have a unique solution for $0 \leq x \leq 2\sigma - \tau$. Proceeding in this way, we obtain existence of a unique solution for $0 \leq x \leq a$.

We state the above result in the following theorem.

THEOREM 3. The problem (1.1) and (1.2) has a unique solution y for which there exists an interval of length σ such that the sequence $\{y_n\}$ constructed by

$$y_0 = \frac{a-x}{a-r} y(r), \quad 0 \leq r < a, \quad r \leq x,$$

$$y(0) = 1,$$

converges linearly and uniformly for $r \leq x \leq r + \sigma$, where y_{n+1} is given by (2.8) subject to $y_{n+1}(r) = y(r)$, $y_{n+1}(a) = 0$ for $n = 0, 1, 2, \dots$.

We remark that starting with $r = 0$, $y(r)$ is known successively on each subinterval $r \leq x \leq r + \sigma$.

REFERENCES

- [1] E. Fermi, *Un metodo statistico per la determinazione di alcune Proprietà dell'atome*, Rend. Accad. Naz. del Lincei, Cl. Sci. Fis., Mat. e Nat. **6**, 602-607 (1927)
- [2] J. W. Mooney, *Monotone methods for the Thomas-Fermi equation*, Quart. Appl. Math. **36**, 305-314 (1978)
- [3] L. H. Thomas, *The calculation of atomic fields*, Proc. Cambridge Philos. Soc. **23**, 542-548 (1927)
- [4] G. N. Watson, *A treatise on the theory of Bessel functions*, 2nd ed., Cambridge University Press, London, p. 77 (1958)