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ON A GENERALIZATION OF THE THOMAS-FERMI EQUATION

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Dedicated to Academician O. Borůvka on his 80th birthday anniversary

The Thomas-Fermi equation is used in physical research for atomic calculations. It is closely connected with three sets of boundary conditions, corresponding to three different physical situations:

- 1. x(0) = 1, x(a) = 0 (the ionized atom),
- 2. x(0) = 1, $\lim_{t \to \infty} x(t) = 0$ (the isolated neutral atom),
- 3. x(0) = 1, -x(b) + bx'(b) = 0 (the neutral atom with Bohr radius b) ([3, p. 515]).

Thanks to its meaning, the Thomas-Fermi equation has attracted the attention of many mathematicians, among them let us mention Hille [2], Lunning [3], Marić [4].

In the paper the mentioned boundary value problems are studied in a more general setting and the existence as well as the uniqueness of a solution to such generalized problems are established under various conditions. The extension of some results by Opial [5, pp. 228—231], Bebernes and Jackson [1], is attained not only for working under Carathéodory conditions instead of continuity, but for a more general formulation of boundary conditions.

In what follows, the function $f: G = [0, \infty) \times [0, \infty) \rightarrow R$ will be considered, on which some of the following conditions will be imposed as needed:

- (A₁) f satisfies Carathéodory conditions, i.e. $f(., x_0)$ is measurable in $[0, \infty)$ for each fixed $x_0 \in [0, \infty)$, for all $t_0 \in [0, \infty)$ $f(t_0, .)$ is continuous in $[0, \infty)$ and for each compact set $[a, b] \times [c, d] \subset G$ there exists a function $m \in L([a, b])$ such that $|f(t, x)| \le m(t)$ $((t, x) \in [a, b] \times [c, d])$,
- $(A_2) f(t,0) \le 0 (0 \le t < \infty),$
- (A₃) there exists an $h \ge 0$ such that $f(t, x) \ge 0$ $(0 \le t < \infty, h \le x < \infty)$,
- (A'₃) there exists an h > 0 and a k > 0 such that $f(t, x) \ge k$ $(0 \le t < \infty, h \le x < \infty)$,
- (A_3'') $f(t,x) \ge 0$ $(0 \le t < \infty, 0 \le x < \infty)$

- (A_4) f(t, .) is nondecreasing in $[0, \infty)$ for each $t \in [0, \infty)$,
- (A'_4) f(t, .) is increasing in $[0, \infty)$ for any $t \in [0, \infty)$,
- (A₅) there exists a $c \ge h$ such that $\int_0^\infty f(s, c) ds = \infty$,
- (A'₅) for any c > 0 $\int_0^\infty f(s, c) ds = \infty$,
- (A₆) for any $0 \le a_1 < b_1 \lim_{k \to \infty} \int_{a_1}^{b_1} (s a_1) f[s, h + k(s a_1)] ds = \infty$,
- (A_6') for any $0 \le a_1 < b_1$ and any l < 0

$$\lim_{k \to \infty} \left(lk + \int_{a_1}^{b_1} (s - a_1) f[s, h + k(s - a_1)] ds \right) = \infty.$$

Since the function $f_0(t, x) = t^{-1/2}x^{3/2}$ $(0 < t < \infty, 0 \le x < \infty)$ with $f_0(0, x) = x$ $(0 \le x < \infty)$ satisfies all listed assumptions except (A'₃), the differential equation

$$(1) x'' = f(t, x)$$

under these conditions represents a generalization of the Thomas-Fermi equation.

With respect to (A_1) , by a solution of (1) on an interval i any function x such that x' is locally absolutely continuous on i and x satisfies (1) on i a.e. is understood.

Consider the boundary conditions

(2)
$$a_0x(a) - b_0x'(a) = A$$
$$a_1x(b) + b_1x'(b) = B$$

where the real numbers a, b, A, B, a_i, b_i (i = 0, 1) are such that

(3)
$$0 \le a < b, a_i, b_i \ge 0, a_i + b_i > 0 \quad (i = 0, 1), A, B \ge 0.$$

We shall call a function $\alpha \ge 0$ with absolutely continuous derivative on [a, b] a lower solution of (1), (2) when

$$\alpha''(t) \ge f[t, \alpha(t)]$$
 a.e. in $[a, b]$,
 $a_0\alpha(a) - b_0\alpha'(a) \le A$
 $a_1\alpha(b) + b_1\alpha'(b) \le B$

An upper solution $\beta \ge 0$ of (1), (2) is provided with absolutely continuous derivative on [a, b] and satisfies

$$\beta''(t) \le f[t, \beta(t)]$$
 a.e. in $[a, b]$,
 $a_0\beta(a) - b_0\beta'(a) \ge A$
 $a_1\beta(b) + b_1\beta'(b) \ge B$

The existence result will be based on the following lemma which is an easy consequence of Theorem 8, [7, p. 50].

Lemma 1. Assume that f satisfies assumption (A_1) , a, b, a_i , b_i (i = 0, 1) fulfil (3) and there exists a lower solution α and an upper solution β of (1), (2) with $\alpha(t) \leq \beta(t)$ ($\alpha \leq t \leq b$). Then there exists a solution x of (1), (2) which satisfies

(4)
$$\alpha(t) \leq x(t) \leq \beta(t) \quad (a \leq t \leq b)$$

Proof. Since α , β satisfy the first three conditions from the mentioned Theorem 8, we have to find the functions φ , ψ which fulfil the conditions 4.—6. from that theorem. Let $H = \max \beta(t)$ ($a \le t \le b$) and let $m_1 \in L([a, b])$ be such that

$$|f(t,x)| \le m_1(t)$$
 $((t,x) \in [a,b] \times [0,H])$. Put $\psi = \max \left(\max_{\alpha \le t \le b} |\alpha'(t)|, \max_{\alpha \le t \le b} |\beta'(t)|, \right)$

$$\int_a^b m_1(s) \, \mathrm{d}s + 2H/(b-a), \ \varphi = -\psi. \text{ Then}$$

 $4. \varphi \leq \psi$.

5. $\varphi \leq \alpha'(t)$, $\beta'(t) \leq \psi$ $(a \leq t \leq b)$.

6. Let x be a solution of (1) satisfying (4). Then there exists a $c \in (a, b)$ such that $|x'(c)| = |x(b) - x(a)|/(b-a) \le 2H/(b-a)$ and from $x'(t) = x'(c) + \int_{c}^{t} f[s, x(s)] ds$ we get that $|x'(t)| \le 2H/(b-a) + \int_{a}^{b} m_1(s) ds \le \psi$. Hence

$$\varphi \leq x'(t) \leq \psi$$

for all $t \in [a, b]$.

By Theorem 8, [7, p. 50], all assumptions of which are satisfied, there exists a solution x of (1), (2) which satisfies (4) and (5).

 (A_2) together with $A, B \ge 0$ imply that the function $\alpha(t) = 0$ $(a \le t \le b)$ is a lower solution of (1), (2). By (A_3) , we have that each linear function $\beta(t) = kt + q$ with $\beta(t) \ge h$ $(a \le t \le b)$ satisfies $\beta''(t) \le f[t, \beta(t)]$ in [a, b]. Thus β will be an upper solution of (1), (2) if it satisfies the boundary inequalities required for such a solution. According to the form of boundary conditions (2) we have to consider the following cases.

If a_0 , $a_1 > 0$, then

$$\beta(t) = H_1 \quad (a \le t \le b)$$

where $H_1 = \max (h, A/a_0, B/a_1)$ is an upper solution of (1), (2). In case $a_0 = 0$, $a_1 > 0$

$$\beta(t) = -\frac{A}{b_0}t + q$$

where $q = \max \left(h + \frac{A}{b_0} b, \frac{1}{a_1} \left(B + b_1 \frac{A}{b_0} + a_1 \frac{A}{b_0} b \right) \right)$ is an upper solution of (1), (2). When $a_0 > 0$, $a_1 = 0$,

$$\beta(t) = \frac{B}{b_1}t + q$$

with

$$q = \max \left(h - \frac{B}{b_1} a, \frac{1}{a_0} \left(A + b_0 \frac{B}{b_1} - a_0 \frac{B}{b_1} a \right) \right)$$

is an upper solution of (1), (2).

Finally, if $a_0 = a_1 = 0$ and A = B = 0, then

$$\beta(t) = h$$

is an upper solution of (1), (2).

The results can be summarized in

Theorem 1. If f satisfies (A_1) — (A_3) , then for any a, b, A, B, a_i , b_i (i = 0, 1) satisfying (3) and such that

if
$$a_0 = a_1 = 0$$
, then $A = B = 0$

there exists a solution x of the BVP (1), (2) which satisfies

$$0 \le x(t) \le \beta(t) \quad (a \le t \le b)$$

with β determined by one of the equalities (6)—(9) according to the values of a_0 , a_1 .

The case $a_0 = a_1 = 0$ in full generality can be dealt with by using a quadratic function in the role of an upper solution of (1), (2). This requires a stronger assumption than (A_3) . The obtained result is given in

Theorem 2. Let f satisfy assumptions (A_1) , (A_2) and (A'_3) . Then for any a, b, A, B, a_i , b_i (i = 0, 1) satisfying (3) and such that $a_0 = a_1 = 0$,

$$(10) k(b-a) \ge \frac{A}{b_0} + \frac{B}{b_1}$$

there exists a solution x of the BVP (1), (2) which satisfies

$$0 \le x(t) \le \beta(t) \quad (a \le t \le b)$$

where

$$\beta(t) = \frac{k}{2} (t - c)^2 + h \quad (a \le t \le b)$$

and c is a real number fulfilling

$$(11) a + \frac{A}{kb_0} \le c \le b - \frac{B}{kb_1}$$

Proof. First we remark that (10) implies that a c satisfying (11) does exist. Further with respect to (A_3') , from $\beta(t) \ge h$ $(a \le t \le b)$ we get $\beta''(t) \le f[t, \beta(t)]$ in [a, b]. In view of (11), $\beta'(a) = k$ $(a-c) \le -A/b_0$ and $\beta'(b) = k(b-c) \ge B/b_1$.

Thus β is an upper solution of (1), (2) and the statement of Theorem 2 follows from Lemma 1.

Remark. The condition (10) represents a restriction either on k (k has to be sufficiently great) or on b-a ([a,b] should be sufficiently long). In the case of the Thomas-Fermi equation for a given interval [a,b] and given $A, B, b_0, b_1 \ge 0$ we can take h sufficiently great so that k satisfy (10). Hence any BVP (1), (2) has a solution for this equation.

In order to prove uniqueness of the solution of (1), (2) we need assumptions (A_4) or (A'_4) .

Theorem 3. If f satisfies (A_1) , (A_4) , and (A'_4) if $a_0 = a_1 = 0$, then for any a, b, A, B, a_i , b_i (i = 0, 1) satisfying (3) there exists at most one solution of the BVP (1), (2).

Proof. Let there exist two different solutions x_1 , x_2 of (1), (2). Denote $u = x_1 - x_2$. Properly choosing the indices, we may suppose that there exists a point $s \in (a, b)$ at which u(s) > 0. Let $i \subset [a, b]$ be the maximal interval containing s in which u(t) > 0. By (A_4) , u' is nondecreasing in the closure of i. According to the form of i, the following cases may arise.

- 1. $i = (t_1, t_2)$. Then $u(t_1) = u(t_2) = 0$, $u'(t_1) \ge 0$, $u'(t_2) \le 0$. Since u' is nondecreasing in $[t_1, t_2]$, u'(t) = 0 in $[t_1, t_2]$ and $u(t) = u(t_1) = 0$ in (t_1, t_2) which opposes the fact that u(t) > 0 in i.
- 2. $i = [t_1, t_2)$. Then $t_1 = a$, $u(t_2) = 0$, $u'(t_2) \le 0$ and the following subcases have to be considered.
- a) $b_0 = 0$. By (3), $a_0 > 0$ and hence, (2) implies that u(a) = 0. This is in contradiction with $t_1 \in i$.
- b) $a_0 = 0$. Now we have u'(a) = 0 and since u' is nondecreasing in $[t_1, t_2]$, $u'(t_2) \le 0$, the identity u'(t) = 0 in $[a, t_2]$ is true. Thus $u(t) = u(t_2) = 0$ is valid for all $t \in [a, t_2)$ which again gives a contradiction.
- c) $a_0 > 0$, $b_0 > 0$. From (2) u'(a) > 0 follows which together with monotonicity of u' in $[t_1, t_2]$ opposes the fact that $u'(t_2) \le 0$.
- 3. $i = (t_1, t_2]$. Then $t_2 = b$, $u(t_1) = 0$, $u'(t_1) \ge 0$ and we come to contradiction by similar considerations as in the case 2.
 - a) When $b_1 = 0$, we get that u(b) = 0 and this contradicts the fact that $t_2 \in i$.
- b) $a_1 = 0$ implies u'(b) = 0 and this involves $u'(t) \equiv 0$ in $[t_1, b]$. Therefore $u(t) \equiv u(t_1) = 0$ in $[t_1, t_2]$ which leads to contradiction.
- c) $a_1>0$, $b_1>0$. (2) implies that u'(b)<0 and therefore $u'(t_1)\ge 0$ cannot happen.
- 4. $i = [t_1, t_2] = [a, b]$. u' is nondecreasing in [a, b] and we have to check the following subcases.
- a) $b_0 = 0$ ($b_1 = 0$). This subcase cannot happen, since $b_0 = 0$ ($b_1 = 0$) implies that u(a) = 0 (u(b) = 0).

In the remaining subcases $b_0 > 0$, $b_1 > 0$ will be supposed.

- b) $a_0 = 0$, $a_1 = 0$. Then we have u'(a) = u'(b) = 0 and hence, $u'(t) \equiv 0$ in [a, b]. This implies that $x_1(t) = x_2(t) + c$ in [a, b] with a c > 0 and further, $f[t, x_2(t)] = f[t, x_2(t) + c]$ a.e. in [a, b] which is, in view of (A_4) , impossible.
- c) $a_0 = 0$, $a_1 > 0$. The boundary conditions (2) give that u'(a) = 0, u'(b) < 0 and this contradicts the fact that u' is nondecreasing.
- d) $a_0 > 0$, $a_1 = 0$. In this subcase u'(a) > 0, u'(b) = 0 which opposes the monotonicity of u'.
- e) $a_0 > 0$, $a_1 > 0$. Then (2) implies that u'(a) > 0, u'(b) < 0 which cannot happen.

We have shown that the existence of two different solutions of (1), (2) leads to contradiction which proves Theorem 3.

Remarks. 1. From the proof of Theorem 3 we see that this theorem remains to be true when the strict monotonicity of f is required only on a subinterval of (a, b).

2. Since all three theorems hold for the Thomas-Fermi equation, in case of this equation any BVP (1), (2) has a unique solution.

Consider the boundary conditions in $[a, \infty)$

(12)
$$a_0x(a) - b_0x'(a) = A$$

$$\sup_{a \le t < \infty} |x(t)| < \infty$$

where $a \ge 0$, a_0 , $b_0 \ge 0$, $a_0 + b_0 > 0$, $A \ge 0$.

Theorem 4. If f satisfies (A_1) — (A_3) and $a_0 > 0$, then there exists a solution x of (1), (12) (in $[a, \infty)$) which satisfies

$$0 \le x(t) \le H_2 \quad (a \le t < \infty)$$

with $H_2 = \max\left(h, \frac{A}{a_0}\right)$.

If f satisfies (A_1) , (A_2) , (A'_3) and $a_0 = 0$, then there exists a solution x of (1), (12) which satisfies

$$0 \leq x(t) \leq H_3 \quad (a \leq t < \infty)$$

where $H_3 = h + \frac{A^2}{h_0^2 k}$.

Proof. Consider the sequence of boundary conditions

(2_n)
$$a_0x(a) - b_0x'(a) = A$$

 $x(a+n) = 0 \quad (n=1, 2, ...)$

Since f satisfies (A_1) — (A_3) , by Theorem 1 for each natural n there exists a solution x_n of (1), (2_n) satisfying the inequalities

$$(13) 0 \leq x_n(t) \leq H_2 (a \leq t \leq a+n) \text{when } a_0 > 0,$$

$$0 \le x_n(t) \le -\frac{A}{b_0}(t-a-n) + h$$
 $(a \le t \le a+n)$ if $a_0 = 0$

In the latter case the estimation from above can be improved. When $0 \le x_n(t) \le h$ for all $t \in [a, a+n]$, we have

$$(14) 0 \leq x_n(t) \leq H_3 (a \leq t \leq a+n)$$

Suppose now that there exists a point t_0 , $a \le t_0 < a + n$, at which $x_n(t_0) > h$. In view of (A_3') , $x_n'(t_0) \ge 0$ would imply that $x_n(t) > h$ for all t, $t_0 \le t \le a + n$. This contradicts $x_n(a+n) = 0$. Hence there exists only one (maximal) interval $[a, t_1]$, $t_1 < a + n$, in which $x_n(t) \ge h$ and $x_n'(t) < 0$. Since $x_n''(t) \ge k$ a.e. in $[a, t_1]$ and $x_n'(a) = -\frac{A}{b_0}$, we have

$$0 > x'_n(t) \ge -\frac{A}{h_0} + k(t-a) \quad (a \le t \le t_1)$$

from where $t_1 - a < \frac{A}{kb_0}$, and further

$$x_n(t) \ge x_n(a) - \frac{A}{b_0}(t-a) + \frac{k}{2}(t-a)^2 \quad (a \le t \le t_1)$$

Clearly $x_n(t_1) = h$ and thus, $x_n(a) \le h + \frac{A}{b_0}(t_1 - a) < h + \frac{A^2}{kb_0^2}$. As x_n is decreasing in $[a, t_1]$ and $0 \le x_n(t) \le h$ in $[t_1, a + n]$, (14) is true also in this case.

Fix a natural number n_0 and consider the sequence $\{x_n\}_{n=n_0}^{\infty}$ in $[a, a+n_0]$. By (13) and (14), respectively, this sequence is uniformly bounded in the mentioned interval and thus, (A_1) implies that there is an $m_2 \in L$ ($[a, a+n_0]$) such that $|f[t, x_n(t)]| \leq m_2(t)$ ($t \in [a, a+n_0]$, $n \geq n_0$). Then $|x'_n(t_2) - x'_n(t_1)| \leq \int_{t_1}^{t_2} m_2(s) \, ds$ ($a \leq t_1 < t_2 \leq a+n_0$, $n \geq n_0$) and hence, $\{x'_n\}_{n=n_0}^{\infty}$ is equicontinuous in $[a, a+n_0]$ and, as there is a c_n , $a < c_n < a+n_0$, with $|x'_n(c_n)| = |x_n(a+n_0) - x_n(a)|/n_0 \leq H_4/n_0$, where $H_4 = \max(H_2, H_3)$, $\{x'_n\}_{n=n_0}^{\infty}$ is uniformly bounded in $[a, a+n_0]$, too. Therefore $\{x_n\}_{n=n_0}^{\infty}$ is equicontinuous in this interval and there exists a subsequence $\{x_{n_k}\}$ of $\{x_n\}$ which together with $\{x'_{n_k}\}$ uniformly converges in $[a, a+n_0]$. In the same way we get that there exists a subsequence $\{x_{n_k}\}$ of $\{x_{n_k}\}$ such that both sequences $\{x_{n_{k_0}}\}$, $\{x'_{n_{k_0}}\}$ are uniformly convergent in $[a, a+n_0+1]$. Therefore the diagonalization process can be applied which yields a subsequence $\{x_m\}$ of $\{x_n\}$ that locally uniformly converges to a function x on $[a, \infty)$ and $\{x'_m\}$ to x' on the same interval. Clearly x satisfies (12) as well as the inequalities (13) and (14), respectively. Since x_m satisfy in $[a, a+n_0]$ the equation $x_m(t) = x_m(a) + x'_m(a)$

 $(t-a) + \int_a^t (t-s)f[s, x_m(s)] ds$, by the limit process we get that x satisfies (1) in $[a, a+n_0]$ and hence in the whole interval $[a, \infty)$. The proof of Theorem 4 is complete.

Remark. Theorem 4 extends and, in a certain sense, strenghtens Theorems II and III by Opial in [5, pp. 229—230].

A uniqueness result is given by

Theorem 5. If f satisfies (A_1) , (A_4) , and (A'_4) if $a_0 = 0$, then for any $a \ge 0$, $a_0 \ge 0$, $a_0 + b_0 > 0$, $A \ge 0$ there exists at most one solution of (1), (12).

Proof. Suppose that there are two different solutions x_1 , x_2 in $[a, \infty)$ of (1), (12). Denote $u = x_1 - x_2$. The following cases may happen.

1. $u(t) \neq 0$ in $[a, \infty)$, say u(t) > 0. If $a_0 > 0$, then $b_0 > 0$ and u'(a) > 0. By (A_4) , we get $u''(t) \ge 0$ a.e. in $[a, \infty)$ and hence u' is nondecreasing in that interval. Therefore $u'(t) \ge u'(a) > 0$ in $[a, \infty)$ and $u(t) \ge u(a) + u'(a)$ (t-a) tends to ∞ which contradicts the boundedness of x_1, x_2 . If $a_0 = 0$, then u'(a) = 0, but u' is increasing. Hence for a $t_1 > a$, $u'(t) > u'(t_1) > 0$ $(t_1 < t < \infty)$ and again we come to contradiction.

2. If there is a $t_2 > a$ such that $u(t_2) = 0$, then by Theorem 3, u(t) = 0 in $[a, t_2]$ and hence we may suppose that there is a $t_3 \ge a$ at which $u(t_3) = 0$ and for $t > t_3$ $u(t) \ne 0$, say u(t) > 0. Then proceeding as in the foregoing case we come to contradiction. This contradiction proves Theorem 5.

Remark. Theorem 5 extends the result of Theorem IV by Opial in [5, p. 230]. Both Theorems 4 and 5 bring a result symmetric to that given by Bebernes and Jackson in Theorem 3.1, [1, p. 39]. Of course they have assumed continuity of f and f(t, 0) = 0 in $[0, \infty)$ and they considered a special boundary condition $(b_0 = 0)$. A Mambriani's result given in the monograph by Sansone [6, p. 377] also follows from Theorems 4 and 5.

In the case $a_0 = 0$ Theorem 4 cannot be applied to the Thomas-Fermi equation. However the following theorem is of use.

Theorem 6. If f satisfies (A_1) — (A_5) (i.e. (A_1) , (A_2) , (A_3) , (A_4) , (A_5)), then for any $a \ge 0$, $a_0 = 0$, $b_0 > 0$, $A \ge 0$ there exists a solution x of (1), (12) such that

$$0 \le x(t) \le H_4$$

where
$$H_4 = c + \frac{A}{b_0}(t_3 - a)$$
 and t_3 is such that $\int_a^{t_3} f(s, c) ds = \frac{A}{b_0}$.

Proof. First we remark that (A_5) guarantees the existence of t_3 with the above mentioned property. By Theorems 1 and 3 there exists a unique solution x_n of (1), (2_n) (n=1, 2, ...). Now we proceed similarly as in the proof of Theorem 4, case $a_0=0$, with the only exception how the boundedness from above of the sequence $\{x_n\}$ is shown. Again for each natural n there may exist at most one maximal

interval $[a, t_1]$ in which $x_n(t) \ge h$ and $x'_n(t) < 0$. Suppose that there is a $t_2 \le t_1$ such that $x_n(t_2) = c$. Since x_n is convex in $[a, t_2]$, we have

$$x_n(t) \le c + \frac{A}{b_0} (t_2 - t) \quad (a \le t \le t_2)$$

and as

$$0 > x'_n(t_2) = -\frac{A}{b_0} + \int_a^{t_2} f[s, x_n(s)] \, ds \ge -\frac{A}{b_0} + \int_a^{t_2} f(s, c) \, ds$$

and $\int_a^t f(s,c) ds$ is a nondecreasing function of $t, t_2 < t_3$. Therefore $0 \le x_n(t) \le H_4$ in $[a, t_2]$ as well as in [a, a+n]. When $0 \le x_n(t) < c$ in $[a, t_1]$, we have the same result. Hence H_4 is an upper bound for all x_n as well as for x in their interval of definition. The proof of the theorem is completed.

The behaviour of bounded solutions of (1) in $[a, \infty)$ is described by

Theorem 7. Let f satisfy the assumptions (A_1) , (A_3) , (A_4) and (A'_5) . Then for any $a \ge 0$ each bounded solution x of (1) in $[a, \infty)$ is nonincreasing, convex and

$$\lim_{t\to\infty} x(t) = \lim_{t\to\infty} x'(t) = 0$$

Moreover, there exists at most one solution of the BVP (1), (12) for any $a \ge 0$, $a_0 \ge 0$, $a_0 + b_0 > 0$, $A \ge 0$.

Proof. Suppose x is a solution of (1) in $[a, \infty)$. Then by (A_{β}) , x is convex and there exists $\lim_{t\to\infty} x'(t)$ (finite or infinite). When x is bounded, $\lim_{t\to\infty} x'(t) = 0$ necessarily must hold and thus, $x'(t) \le 0$ ($a \le t < \infty$). Therefore x is nonincreasing and $\lim_{t\to\infty} x(t) = c \ge 0$. If c > 0, then on basis of the inequality $x'(t) - x'(a) = \int_a^t f[s, x(s)] ds \ge \int_a^t f(s, c) ds$ and by (A_5') , we get that $\lim_{t\to\infty} x'(t) = \infty$ which contradicts the above proved equality $\lim_{t\to\infty} x'(t) = 0$.

As to the last statement, with respect to Theorem 5, it suffices to consider the case $a_0=0$. Looking through the proof of that theorem and keeping the notations from that proof we see that two cases have to be investigated. 1. $u(t)=x_1(t)-x_2(t)>0$ in $[a,\infty)$. Then u'(a)=0 and u' is nondecreasing. Since $\lim_{t\to\infty} u'(t)=\lim_{t\to\infty} [x_1'(t)-x_2'(t)]=0$, u'(t)=0 in $[a,\infty)$ and by $\lim_{t\to\infty} u(t)=\lim_{t\to\infty} [x_1(t)-x_2(t)]=0$, we have u(t)=0 in $[a,\infty)$ what is a contradiction. 2. $u(t_3)=0$, u(t)>0 in (t_3,∞) , then u' is nondecreasing and since $\lim_{t\to\infty} u'(t)=0$, $u'(t)\leq 0$ in (t_3,∞) . Therefore u is nonincreasing in $[t_3,\infty)$. By $u(t_3)=0$,

 $\lim_{t\to\infty} u(t) = 0$, we get that u(t) = 0 in $[t_3, \infty)$ what gives a contradiction. Thus the last statement of the theorem has been proved.

In the next section the BVP (1),

(15)
$$a_0x(a) - b_0x'(a) = A - a_1x(b) + b_1x'(b) = B$$

will be considered where $0 \le a < b$, a_0 , $b_0 \ge 0$, $a_0 + b_0 > 0$, $A \ge 0$, a_1 , $b_1 > 0$, and B are arbitrary numbers.

Suppose that f satisfies assumptions (A_1) — (A_4) . Then by Theorems 1 and 3, for any $C \ge 0$ there exists a unique solution x(., C) of the BVP (1),

(16)
$$a_0x(a) - b_0x'(a) = A$$

 $x(b) = C$

Denote x(., C) as x. Consider the composite function

$$F[x(t), x'(t)] = a_0 x(t) - b_0 x'(t) +$$

$$+ [-a_1 x(t) + b_1 x'(t) - [a_0 x(t) - b_0 x'(t)]](t - a)/(b - a) \quad (a \le t \le b)$$

Clearly

(17)
$$F[x(a), x'(a)] = a_0 x(a) - b_0 x'(a) = A$$
$$F[x(b), x'(b)] = -a_1 x(b) + b_1 x'(b)$$

Since

(18)
$$[F[x(t), x'(t)]]' = a_0 x'(t) - b_0 f[t, x(t)] + \frac{1}{b-a} [(-a_0 - a_1)x(t) + (b_0 + b_1)x'(t)] +$$

$$+\frac{t-a}{b-a}[(-a_0-a_1)x'(t)+(b_0+b_1)f[t,x(t)]]$$
 a.e. in $[a,b]$

and

$$-\frac{a_0 + a_1}{b - a} \int_a^t (s - a) x'(s) \, ds =$$

$$= -\frac{a_0 + a_1}{b - a} (t - a) x(t) + \frac{a_0 + a_1}{b - a} \int_a^t x(s) \, ds$$

by integration of (18) from a to t we get

$$F[x(t), x'(t)] = F[x(a), x'(a)] +$$

$$+ \left(a_0 + \frac{b_0 + b_1}{b - a}\right) [x(t) - x(a)] - \frac{a_0 + a_1}{b - a} (t - a)x(t) +$$

$$+\frac{b_0+b_1}{b-a}\int_a^t (s-a)f[s,x(s)] ds - b_0\int_a^t f[s,x(s)] ds \quad (a \le t \le b)$$

and hence

(19)
$$F[x(b), x'(b)] = A + \left(\frac{b_0 + b_1}{b - a} - a_1\right) x(b) - \left(a_0 + \frac{b_0 + b_1}{b - a}\right) x(a) + \frac{b_0 + b_1}{b - a} \int_a^b (s - a) f[s, x(s)] ds - b_0 \int_a^b f[s, x(s)] ds$$

We shall show that F[x(b), x'(b)] is a continuous function of C. When $0 \le C_2 < C_1$, then by Theorem 3, $u(t) = x(t, C_1) - x(t, C_2) \ge 0$ for all $t \in [a, b]$ and by (A_4) , u' is nondecreasing. Denote $\{C_n\}$ a decreasing sequence converging to C (an increasing sequence can be dealt with in a similar way). Then $x_n = x(., C_n)$ is a nonincreasing sequence in [a, b] bounded from below by x = x(., C) in [a, b]. Hence there exists $\lim_{n \to \infty} x_n(t) = y(t)$ ($a \le t \le b$). The functions x_n are solutions of (1) which attain the values $x_n(a)$ and $x_n(b)$, respectively, at the points a and b, respectively, and therefore, they can be represented as the solutions of the integral equation

(20)
$$x_n(t) = w_n(t) + \int_a^b G(t, s) f[s, x_n(s)] \, \mathrm{d}s \quad (a \le t \le b)$$

where $w_n'' = 0$ in [a, b], $w_n(a) = x_n(a)$, $w_n(b) = x_n(b)$ and G is the Green function of z'' = 0, z(a) = z(b) = 0. The limit process can be applied and we get that y satisfies $y(t) = w(t) + \int_a^b G(t, s) \ f[s, y(s)] \ ds$, where $w(t) = y(a) + \frac{y(b) - y(a)}{b - a} \ (t - a)$, $(a \le t \le b)$. Hence y is the solution of (1) which satisfies $y(a) = \lim_{n \to \infty} x_n(a)$, y(b) = x(b). Now two cases have to be considered. If y(a) = x(a), then the uniqueness of two-point BVP for (1) implies that y(t) = x(t) in [a, b], and by (19) we have that $\lim_{n \to \infty} F[x_n(b), x_n'(b)] = F[x(b), x_n'(b)]$. When y(a) > x(a), then by Theorem 3, $y(t) \ge x(t)$ in [a, b]. Therefore $y'(b) \le x'(b)$ and since u' = y' - x' is nondecreasing in [a, b], $u'(t) \le 0$ in [a, b]. On the other hand, from (20) we get that $\lim_{n \to \infty} x_n'(a) = y'(a)$ and with respect to the first condition in (16), $a_0 y(a) - b_0 y'(a) = A$. However, y(a) > x(a), and thus y'(a) > x'(a). This contradicts the inequality $u'(a) \le 0$ obtained above. Thus y(a) > x(a) cannot happen and the continuous dependence of F[x(b), x'(b)] on C is proved.

Suppose now that $b_0 = 0$. Then, in view of (16), (19) can be written in the form

(21)
$$F[x(b), x'(b)] = -\frac{Ab_1}{(b-a)a_0} + \left(\frac{b_1}{b-a} - a_1\right)C + \frac{b_1}{b-a} \int_a^b (s-a)f[s, x(s)] ds$$

The properties of F[x(b), x'(b)] depend on the sign of $\frac{b_1}{b-a}-a_1$. If $\frac{b_1}{b-a}-a_1>0$, then by (21) and (A₄), this function is increasing in $[0, \infty)$ and $\lim_{C\to\infty} F[x(b), x'(b)] = \infty$. Hence F[x(b), x'(b)] as a function of C maps $[0, \infty)$ on an interval $[B_0, \infty)$. With respect to (17), the existence of the solution of (1), (15) is equivalent to the existence of the solution of (1), (16) for which F[x(b), x'(b)] = B and this is possible if and only if $B \in [B_0, \infty)$. As to $B_0, B_0 = b_1 x'(b, 0) \le 0$.

The results can be summarized in

Theorem 8. Suppose that f satisfies assumptions (A_1) — (A_4) , $b_0 = 0$, $\frac{b_1}{b-a} - a_1 > 0$. Then for each $A \ge 0$ there exists a $B_0 \le 0$ such that for each $B \in [B_0, \infty)$ there exists a unique solution of (1), (15) while for $B < B_0$ there is no solution of that BVP.

Consider now the case $b_0 = 0$,

$$\frac{b_1}{b-a} - a_1 = 0$$

Then, with respect to (A₄), from (21) we get that

(23)
$$F[x(b), x'(b)] = \frac{-b_1}{b-a} \frac{A}{a_0} + \frac{b_1}{b-a} \int_a^b (s-a)f[s, x(s)] ds$$

and F[x(b), x'(b)] is a nondecreasing function of C. Assume that besides (A_1) — (A_4) , (A_6) is true. Suppose further, that for each $C \ge 0$ we have

$$(24) -a_1 x(b) + b_1 x'(b) < B$$

which asserts that there is no solution of the BVP (1), (15) for a $B \ge 0$. Let C > h. (22), (24) imply that $x'(b) < \frac{1}{b-a} \left(\frac{B(b-a)}{b_1} + x(b) \right)$. The right-hand side of this inequality represents the direction of the segment of the straight-line

$$y_{c}(t) = -\frac{B(b-a)}{b_{1}} + \frac{C + \frac{B(b-a)}{b_{1}}}{b-a}(t-a) \quad (a \le t \le b)$$

which goes through the points $\left(a, -\frac{B(b-a)}{b_1}\right)$, (b, x(b)). Hence $x(t) > y_C(t)$ is valid, first in an interval $(b-\delta, b)$, and then, by (A_3) , in $[a^*, b)$, where $y_C(a^*) = h$. Thus $\frac{b_1}{b-a} \int_a^b (s-a) f[s, x(s)] ds \ge \frac{b_1}{b-a} \int_a^{a_1^*} (s-a) f[s, x(s, h)] ds + \frac{b_1}{b-a} \int_{a_1^*}^b (s-a) f[s, x(s, C)] ds \ge D + \frac{b_1}{b-a} \int_{a_1^*}^b (s-a^*) f[s, y_C(s)] ds$ where $D = \frac{b_1}{b-a} \int_a^{a_1^*} (s-a) f[s, x(s, h)] ds$, C > h, and $y_C(a^*) = h$, therefore $a^* = a + \frac{1}{k} \left(h + \frac{B(b-a)}{b_1}\right)$, $k = \frac{C + \frac{B(b-a)}{b_1}}{b-a}$, $y_C(s) = h + k(s-a^*)$, $(a^*) \le s \le b$.

When $C \to \infty$, then k also tends to infinity and a_1^* goes to a. Nevertheless, for all $k \ge k_0$ we have $\frac{b_1}{b-a} \int_{a_1^*(k)}^b (s-a_1^*(k)) \ f[s,h+k(s-a_1^*(k))] \ ds \ge \frac{b_1}{b-a} \int_{a_1^*(k_0)}^b (s-a_1^*(k_0)) \ f[s,h+k(s-a_1^*(k_0))] \ ds$ and the last expression tends to ∞ as $k \to \infty$, in view of (A₆). This guarantees that F[x(b),x'(b)] given by (23), attains an arbitrarily large value of B. Since this expression is a nondecreasing continuous function of C, the last statement is in contradiction with (24). Thus F[x(b),x'(b)] attains all nonnegative values of B. Its value for C=0 is B_0 that is considered in the last theorem. Thus we have proved

Theorem 9. Let f satisfy assumptions (A_1) — (A_4) , (A_6) and let $b_0 = 0$, $\frac{b_1}{b-a} - a_1 = 0$. Then for each $A \ge 0$ there is a $B_0 \le 0$ such that for each $B \in [B_0, \infty)$ there exists at least one solution of (1), (15) while for $B < B_0$ there is no solution of that BVP.

Remark. Theorem 9 guarantees the existence of a solution of the Thomas-Fermi equation satisfying the boundary conditions which characterize the neutral atom with any Bohr radius b. In [3, p. 516] the existence of such a solution has been proved only for some values of b. Thus Theorem 9 generalizes and extends Theorem 1 from that paper.

The last case $\frac{b_1}{b-a} - a_1 < 0$ can be dealt with in a similar way.

Theorem 10. Assume that f satisfies assumptions (A_1) — (A_4) , (A_6) . Let $b_0 = 0$, $\frac{b_1}{b-a} - a_1 < 0$, $A \ge 0$. Denote $B_0 = b_1 x'(b, 0)$. Then for each $B \in [B_0, \infty)$ there exists at least one solution of (1), (15).

Proof. Again we have to show that F[x(b), x'(b)] as a function of C maps $[0, \infty)$ on $[B_0, \infty)$ or a greater interval. This function is now represented by (21), from where we see that it need not be monotonous since the second and the third

term show an opposite monotonicity. Still it is continuous. Let $B \in (B_0, \infty)$ and suppose that (24) holds for each $C \ge 0$. Using the same notations as in the proof of the foregoing theorem we come to the inequality

(25)
$$F[x(b), x'(b)] \ge -\frac{b_1}{b-a} \frac{A}{a_0} + \frac{b_1}{b-a} - a_1 C + D + \frac{b_1}{b-a} \int_{a_1}^{b} (s - a_1^*) f[s, y_C(s)] ds$$
Since $C = k(b-a) - \frac{B(b-a)}{b_1}$, and putting
$$E = -\frac{b_1}{b-a} \frac{A}{a_0} + D - \left(\frac{b_1}{b-a} - a_1\right) \frac{B(b-a)}{b_1}$$

$$I = (b_1 - a_1(b-a))(b-a)/b_1$$

we can write (25) in the form

$$F[x(b), x'(b)] \ge E + \frac{b_1}{b-a} \left[lk + \int_{a_1^*}^b (s - a_1^*) f[s, h + k(s - a_1^*)] \, ds \right]$$

Applying (A₆) we get, similarly as in the proof of Theorem 9, that

$$\lim_{C \to \infty} \left[lk + \int_{a_1^*}^b (s - a_1^*) f[s, h + k(s - a_1^*)] \, ds = \infty \right]$$

This stands in contradiction with (24). Hence F[x(b), x'(b)] attains all values B greater or equal to B_0 and Theorem 10 is thus proved.

The study of the case $b_0 > 0$ will start with the following

Lemma 2. Let $a_0 \ge 0$, $b_0 > 0$, $0 \le a < b$, $a_1 > 0$, $b_1 > 0$ be arbitrary numbers. Then the function

(26)
$$w(t) = w(a) + \left[\frac{a_0}{b_0} w(a) - \frac{A}{b_0} \right] (t - a) \quad (a \le t \le b)$$

satisfies (15) and $w(t) \ge 0$ in [a, b] if either

(27)
$$-a_1 + \frac{a_0}{b_0} [b_1 - a_1(b - a)] = 0, \quad B = -A \frac{a_1}{a_0}$$

and

$$w(a) \ge \frac{A(b-a)}{b_0 + a_0(b-a)}$$

or if

(28)
$$-a_1 + \frac{a_0}{b_0} [b_1 - a_1(b - a)] > 0 \quad \left(-a_1 + \frac{a_0}{b_0} [b_1 - a_1(b - a)] < 0 \right)$$

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$$B \ge B_0 = \frac{1}{b_0} \left\{ \frac{A(b-a)}{b_0 + a_0(b-a)} \left[-a_1b_0 + a_0(b_1 - a_1(b-a)) \right] - A[b_1 - a_1(b-a)] \right\}$$

$$(B \le B_0)$$

and

$$w(a) = \frac{Bb_0 + A[b_1 - a_1(b-a)]}{-a_1b_0 + a_0[b_1 - a_1(b-a)]}$$

Proof. First we see that (26) satisfies the first condition in (15). The second condition is fulfilled by this function iff

(29)
$$\left\{-a_{1} + \frac{a_{0}}{b_{0}} [b_{1} - a_{1}(b - a)]\right\} w(a) - \frac{A}{b_{0}} [b_{1} - a_{1}(b - a)] = B$$
Further $w(b) = w(a) \left[1 + \frac{a_{0}}{b_{0}} (b - a)\right] - \frac{A}{b_{0}} (b - a)$, and hence, $w(b) \ge 0$ iff
$$(30) \qquad w(a) \ge \frac{A(b - a)}{b_{0} + a_{0}(b - a)}$$

Since $\frac{A(b-a)}{b_0+a_0(b-a)} \ge 0$, (30) implies that $w(t) \ge 0$ for all $t \in [a, b]$.

Three cases may arise. If (27) is fulfilled, then $a_0 > 0$, $b_1 - a_1(b - a) = \frac{a_1b_0}{a_0}$ and (29) holds.

If $-a_1 + \frac{a_0}{b_0}[b_1 - a_1(b - a)] > 0$, then (29) follows from $w(a) = \frac{Bb_0 + A[b_1 - a_1(b - a)]}{-a_1b_0 + a_0[b_1 - a_1(b - a)]}$ and (30) is satisfied when $B \ge B_0$ where B_0 is given by (28).

The case $-a_1 + \frac{a_0}{b_0} [b_1 - a_1(b - a)] < 0$ can be dealt with in a similar way.

Now we can prove

Theorem 11. Let f satisfy assumptions (A_1) , (A_2) , (A_3') , (A_4) , let $a_0 \ge 0$, $b_0 > 0$, $0 \le a < b$, $a_1 > 0$, $b_1 > 0$, $A \ge 0$ and let either (27) or (28) be fulfilled. Then there exists a solution of (1), (15).

Proof. As (27) or (28) is assumed, by Lemma 2 there exists a linear function w in the form (26) which satisfies (15) and $w(t) \ge 0$ in [a, b]. Theorem 1 supplies the existence of a solution x_1 of (1) which satisfies $x_1(a) = w(a)$, $x_1(b) = w(b)$. (A₃') implies that x_1 is a convex function and hence, $x_1'(a) \le w'(a) = w'(b) \le x_1'(b)$. Thus

$$(F[x_1(a), x_1'(a)] =) a_0 x_1(a) - b_0 x_1'(a) = A_1 \ge A$$

 $(F[x_1(b), x_1'(b)] =) -a_1 x_1(b) + b_1 x_1'(b) = B_1 \ge B$

For the solution x_2 of (1) which is determined by the conditions $x_2(a) = 0$, $x_2(b) = w(b)$, we have

$$F[x_2(a), x_2'(a)] = A_2 \le 0$$

 $F[x_2(b), x_2'(b)] = B_2$

and by (A_4) either $x_1(t) = x_2(t)$ for all $t \in [a, b]$ or $x_2(t) \le x_1(t)$ in [a, b]. In the first case we get $A_1 = A_2 = A = 0$, $B_1 = B_2 \ge B$. The second case is more general and it will be investigated thoroughly. Then x_2 is a solution of (1), (15) with $A_2 \le 0$, $B_2 \ge B$. Here also negative values of A are admitted in (15).

Consider now the system of solutions x_3 of (1) which satisfy the boundary conditions

$$x_3(a) = D$$
 $(0 \le D \le w(a)), x_3(b) = w(b)$

In view of Theorem 3, $F[x_3(a), x_3'(a)]$ is a function of D which will be shown to be increasing and continuous in $[0, \infty)$. Suppose $x_{3,i}$ (i = 1, 2) are two solutions of (1) with

$$x_{3,i}(a) = D_i$$
, $D_1 > D_2 \ge 0$, $x_{3,i}(b) = w(b)$ $(i = 1, 2)$

Then $u(t) = x_{3,1}(t) - x_{3,2}(t) \ge 0$ in [a, b], u(b) = 0, hence $u'(b) \le 0$. By (A_4) , u' is nondecreasing in [a, b], therefore $u'(t) \le u'(b) \le 0$ in that interval. This implies that u is a nonincreasing function and

(31)
$$u(a) \ge u(t) \ge u(b) = 0 \quad (a \le t \le b)$$

At the same time u(a) > 0, $u'(a) \le 0$ imply that

$$F(x_{3,1}(a), x'_{3,1}(a)) > F[x_{3,2}(a), x'_{3,2}(a)]$$

which proves that $F[x_3(a), x_3(a)]$ is increasing in $D(x_3(b))$ being fixed).

Now we shall prove continuity of $F[x_3(a), x_3'(a)]$. (31) implies when $\{D_n\}$ is a decreasing sequence such that $\lim_{n\to\infty} D_n = D \ge 0$, and $\{x_{3,n}\}$ is the sequence of solutions of (1) satisfying

$$x_{3,n}(a) = D_n, \quad x_{3,n}(b) = w(b)$$

then $x_{3,n}(a) - x_3(a) = D_n - D \ge x_{3,n}(t) - x_3(t) \ge 0$ $(a \le t \le b)$ and hence $\lim_{n \to \infty} x_{3,n}(t) = x_3(t)$ in [a, b]. $x_{3,n}$ can be written in the form

$$x_{3,n}(t) = w_{3,n}(t) + \int_a^b G(t,s)f[s,x_{3,n}(s)] ds$$

where $w_{3,n}'' = 0$, $w_{3,n}(a) = x_{3,n}(a)$, $w_{3,n}(b) = x_{3,n}(b)$ and G is the Green function of x'' = 0, x(a) = x(b) = 0. By differentiating we come to

$$x'_{3,n}(t) = w'_{3,n}(t) + \int_a^b \frac{\partial G(t,s)}{\partial t} f[s, x_{3,n}(s)] ds \quad (a \le t \le b)$$

and

$$\lim_{n \to \infty} x'_{3,n}(t) = w'_3(t) + \int_a^b \frac{\partial G(t,s)}{\partial t} f[s, x_3(s)] ds = x'_3(t) \quad (a \le t \le b)$$

Therefore $\lim_{n\to\infty} F[x_{3,n}(a), x'_{3,n}(a)] = F[x_3(a), x'_3(a)]$ which shows the continuity of $F[x_3(a), x'_3(a)]$ in D.

For D=0 $F[x_2(a), x_2'(a)]=A_2 \le 0$ and for D=w(a) $F[x_1(a), x_1'(a)]=A_1 \ge A$. Hence there is a unique D_4 , $0 \le D_4 \le w(a)$, such that for the solution x_4 of (1) with $x_4(a)=D_4$, $x_4(b)=w(b)$ the expression $F[x_4(a), x_4'(a)]=A$. As $x_4(t) \le x_1(t)$ in [a,b], $x_4(b)=x_1(b)$, we have $x_4'(b) \ge x_1'(b)$ and thus, $F[x_4(b), x_4'(b)]=B_4 \ge B_1 \ge B$. Now we apply the continuity of F[x(b), x'(b)] in C(F[x(a), x'(a)]) being fixed as it was shown above. If C=0, then $F[x(b), x'(b)] \le 0$. Therefore there is a point C_5 , $0 \le C_5 \le w(b)$ such that the solution x_5 of (1) which is determined by $F[x_5(a), x_5'(a)]=A$, $x_5(b)=C_5$ satisfies $F[x_5(b), x_5'(b)]=B$ and thus x_5 is a solution of (1), (15). The proof of Theorem 11 is complete.

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SÚHRN

O ZOVŠEOBECNENÍ THOMASOVEJ-FERMIHO ROVNICE

V. Šeda, Bratislava

V práci sa dokazuje existencia a jednoznačnosť riešenia troch druhov okrajových úloh pre zovšeobecnenú Thomasovu-Fermiho rovnicu. Rozšírené a zovšeobecnené sú niektoré výsledky Opiala, Berbernesa a Jacksona, a to používaním Carathéodoryho podmienok a všeobecnejšou formuláciou okrajových podmienok.

РЕЗЮМЕ

ОБ ОБОБЩЕНИИ УРАВНЕНИЯ ТОМАСА-ФЕРМИ

В. Шеда

В работе доказывается существование и единственность решения трех видов краевых задач для обобщенного дифференциального уравнения Томаса-Ферми. Здесь распространены и обобщены некоторые результаты Опяла, Бебернеса и Джэксона, благодаря использованию условий Каратеодори и более общей формулировке краевый условий.