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Abstract

Full Text

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On a Boundary-Value Problem for the Thomas-Fermi and Thomas-Fermi-Dirac Equations

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Nonnegative solutions of the boundary-value problem are considered:

$$\varphi''(x) = f(x, \varphi(x))\psi(x); \tag{1}$$

$$\varphi(0) = y_0, \qquad R\varphi'(R) - \varphi(R) = -q, \tag{2}$$

where $y_0 > 0,\ q < y_0,\ R > 0$. It is assumed that the functions $f(x, y)$ and $\psi(x)$ satisfy the conditions: 1) $f(x, y)$ is defined and continuous for $x \geq 0,\ y \geq 0$; 2) $f(x, y)$ is an increasing function of y in the domain $x \geq 0,\ y \geq 0$; 3) $\psi(x)$ is continuous for $x > 0$, positive for $x > 0$, and integrable on every interval $[0, X]$, where $X > 0$. Let, in addition, either conditions 4)–6) be fulfilled: 4) $f(x, 0) > 0$ for $x > 0$; 5) $f(x, y)$ satisfies a Lipschitz condition with respect to y in the domain $Q \geq y \geq a > 0,\ P \geq x \geq 0$, for arbitrary positive P, Q, a; 6)

$$\int_0^{+\infty} \psi(x) f(x, 0)\, dx = +\infty;$$

or conditions 4′–6′: 4′ $f(x, 0) \equiv 0$ for $x \geq 0$; 5′ $f(x, y)$ satisfies a Lipschitz condition with respect to y in the domain $Q \geq y \geq 0,\ P \geq x \geq 0$, for arbitrary $P > 0,\ Q > 0$;

$$6') \quad \int_0^{+\infty} \psi(x)\, dx = +\infty.$$

Problems of this type occur in the statistical theory of the atom for the Thomas-Fermi and Thomas-Fermi-Dirac equations ([1]).

Problem (1), (2) for $q = 0$ and under conditions 1)–3), 4′–6′ was considered in the note ([2]). Under assumptions 1)–6) and for $y_0 > q \geq 0$ ([3]) it was proved:

Theorem 1. *There exists an $\bar{x}(q)$ such that, for all R satisfying the inequalities*

$$0 < R \leq \bar{x}(q), \tag{3}$$

and only for them, problem (1), (2) has a solution, and it is unique for each R.

Here results are obtained for the case $q < 0$.

Theorem 2. *Under conditions 1)–3),* $4'$*–*$6'$*, and* $q < 0$*, for every* $R > 0$ *there exists a unique solution of problem (1), (2).*

Theorem 3. *Under conditions 1)–6) and* $q < 0$*, there exists an* $\bar{x}(q)$ *such that, for every* R *satisfying the inequalities* $0 < R < \bar{x}(q)$*, problem (1), (2) has a unique solution. For* $R \geq \bar{x}(q)$*, all solutions of problem (1), (2) are obtained as solutions of equation (1) under the conditions*

$$\varphi(0) = y_0, \qquad \varphi(\xi) = 0, \qquad \varphi'(\xi) = 0, \tag{4}$$

where $\xi = \bar{x}(0) < \bar{x}(q)$.

If, in addition to conditions 1)–6), the following condition is fulfilled: 7) $f(x, y)$ *has a continuous derivative* $\partial f/\partial y$ *for* $\delta \geq y > 0$*, for some* $\delta > 0$*, such that* $\partial f/\partial y = O(y^{-\mu})$*, where* $\mu < 1$*, for small* y*, or condition* $5'$*, then problem (1), (4) has a unique solution, and for* $x \geq \xi$ *(uniqueness for* $0 \leq x \leq \xi$

follows from the maximum conditions), and the solution of problem (1), (2) exists for those R satisfying (3), and only for them.

To prove Theorems 1-3, one considers the problem equivalent to the given one: to find $y(x)$ and C such that the equation

$$y''(x) = f(x, y(x) + Cx)\psi(x) \tag{5}$$

and the conditions

$$y(0) = y_0, \tag{6}$$

$$y(R) = q, \qquad y'(R) = 0, \qquad y(x) \geq -Cx \quad (0 \leq x \leq R). \tag{7}$$

are satisfied.

Obviously, $\varphi(x) = y(x) + Cx$, $\varphi'(R) = C$. Under conditions 1)-6) it is proved that there exists an interval of values of C, $(\overline{C}, +\infty)$, such that for every $C \in [\overline{C}, +\infty)$ there exists a solution $y(x)$ of equation (5) satisfying the initial condition (6) and, at some point $x = \overline{x}(q, C)$, the conditions

$$y(\overline{x}) = q, \qquad y'(\overline{x}) = 0, \tag{8}$$

with $y(x) > -Cx$ for $C > \overline{C}$, $\overline{x} \geq x \geq 0$. For fixed q, the function $\overline{x} = \overline{x}(q, C)$ depends continuously on C and decreases monotonically as C increases;

moreover, for every $\eta > 0$ there is a sufficiently large C such that $\overline{x}(q, C) \le \eta$. Denote $\overline{x}(q) = \overline{x}(q, \overline{C})$, and let $Y(x)$ be the corresponding solution of (5), (6), (8), where $C = \overline{C}$. In the case $q > 0$ we have $\overline{x} = q/|\overline{C}|$, $\overline{C} < 0$, $Y(x) > -\overline{C}x$ for $0 \le x < \overline{x}$. In the case $q < 0$, $y = Y(x)$ is tangent to the straight line $y = -\overline{C}x$ at the point $x = \xi = \overline{x}(0)$, $\overline{C} > 0$. The uniqueness of the solution of problem (1), (4) under the additional condition 7) for $f(x, y)$ can be proved with the aid of the corresponding integral equation and inequalities of Chaplygin type [5]. For the Thomas-Fermi-Dirac equation $y'' = (y^{1/2} + \beta x^{1/2})^3 x^{-1/2}$, $\beta > 0$, condition 7) is fulfilled and the solution exists only for $R \le \overline{x}$.

No two integral curves of problem (1), (2) intersect for $x > 0$. Under conditions 1)-6) and fixed $q < 0$, all integral curves of problem (1), (2) for $R < \overline{x}$ are bounded below by the curve $\varphi = \Phi(x)$, the greatest solution of problem (1), (4) for $x \ge 0$, with

$$\overline{x}\,\Phi'(\overline{x}) - \Phi(\overline{x}) = -q.$$

If $\varphi = \varphi(x)$ is the least solution of (1), (4), then there exists an x_0 such that

$$x_0\varphi'(x_0) - \varphi(x_0) = -q.$$

For $R > x_0$, problem (1), (2) has no solution. From the continuity and monotonicity of the function $D(x) = x\varphi'(x) - \varphi(x)$ it follows that any solution $\varphi(x)$ of problem (1), (2) for $R = R_1$, $q = q_1 < y_0$, is the analytic continuation of the solution for each $q \in (q_1, y_0)$ and some $R = R_q$. If $q_1 < q_2 < y_0$, then $\overline{x}(q_1) > \overline{x}(q_2)$; in particular, if $q_1 > 0$, $q_2 < 0$, then $\overline{x}(q_1) < \overline{x}(0) < \overline{x}(q_2)$. Under conditions 1)-3), 4′)-6′), the domain of admissible values of C (i.e., values for which there exist $y(x) \ge -Cx$, tangent to the straight line $y = q$ and satisfying condition (6)) is the interval $(0, +\infty)$, and the solution exists for every $R > 0$ ($q < 0$).

The desired solution (5), (6), (7) satisfies the equation

$$y(x) = q + \int_x^R (s - x)\psi(s) f(s, y(s) + Cs)\, ds, \qquad 0 \le x \le R. \tag{9}$$

Conversely, $y(x)$ and C satisfying (9), (6) with $y(x) \ge -Cx$ satisfy (5), (6), (7). Let $0 < R < \bar{x}$. Consider the case $q < 0$ (the case $q \ge 0$ was considered in (3)). Set

$$y^{(0)}(x) = \begin{cases} q, & x \ge \dfrac{|q|}{C}, \\ -Cx, & x < \dfrac{|q|}{C}; \end{cases} \qquad y^{(k)}(x) = \begin{cases} Y_k(x), & Y_k(x) \ge -Cx, \\ -Cx, & Y_k(x) < -Cx, \end{cases} \tag{10}$$

where

$$Y_k(x) = q + \int_x^R (s-x)\psi(s) f(s, y^{(k-1)}(s) + Cs)\, ds, \qquad k = 1, 2, \ldots$$

Theorem 4. *If there exists a solution of equation (9), $y(x) > -Cx$ for $0 \leq x \leq R$, for some C, then the sequence (10) converges uniformly to the solution.*

Theorem 5. *If for some $C = C_1$ there exists a solution $y_1(x)$ of equation (9), with $y_1(x) > -C_1 x$ for $0 \leq x \leq R$, then there exists a $C_2 < C_1$ such that for all $C_2 \leq C \leq C_1$ there exists a solution of equation (9), and it depends continuously on the parameter C.*

Let $C \in (C^{(1)}, C^{(2)})$ ($C^{(2)}$ can be found using (10), (6), $C^{(1)} \geq |q|/R$).

Set, for example, $C^{(3)} = \dfrac{C^{(1)} + C^{(2)}}{2}$, and find $y^{(k)}(x, C^{(3)})$. If there exist k_1 and x_1 such that $y^{(k_1)}(x, C^{(3)}) > -C^{(3)}x$ for all $x_1 \leq x \leq R$ and $y^{(k_1)}(x_1, C^{(3)}) > y_0$, then $C < C^{(3)}$, $C \in (C^{(1)}, C^{(3)})$. Otherwise $C \in [C^{(3)}, C^{(2)}]$. Putting $C^{(4)} = \dfrac{C^{(1)} + C^{(3)}}{2}$ or $C^{(4)} = \dfrac{C^{(2)} + C^{(3)}}{2}$ in the latter case, and continuing this process, we obtain a sequence of intervals nested in one another and contracting to the point $C = C(R)$. Starting from some $C^{(n)}$, all solutions of (9) corresponding to the left endpoints of these intervals converge to the desired one according to Theorem 5. We shall now find ξ, $\varphi(x)$, $\Phi(x)$, $\bar{x}$, $\bar{C}$. Put

$$\varphi^{(0)}(x, \xi) = 0, \qquad \varphi^{(k)}(x, \xi) = \int_x^\xi (s-x)\psi(s) f(s, \varphi^{(k-1)}(s, \xi))\, ds \quad (k = 1, 2, \ldots). \tag{11}$$

If there exists a solution $\varphi(x, \xi)$ of the integral equation

$$\varphi(x, \xi) = \int_x^\xi (s-x)\psi(s) f(s, \varphi(s, \xi))\, ds, \qquad x \geq 0, \tag{12}$$

for some ξ, then the sequence (11) converges to the solution $\varphi(x, \xi)$. With the aid of (11) and the condition $y(0) = y_0$, as well as the inequality $\varphi(x) \leq y_0(1 - x/\xi)$, $0 \leq x \leq \xi$, one can find an interval (ξ_1, ξ_2) such that $\xi \in (\xi_1, \xi_2)$. Next, proceeding in the same way as in the determination of $C = C(R)$, we find ξ and then $\varphi(x)$ for $x \geq 0$, using (11)*. To determine $\Phi(x)$ for $x \geq \xi$ ($\Phi(x) = \varphi(x)$ for $0 \leq x \leq \xi$) and $\bar{x}$, put

$$\Phi_0(x) = u(x), \qquad \Phi^{(k)}(x) = \int_\xi^x (x-s)\psi(s) f(s, \Phi^{(k-1)}(s))\, ds, \tag{13}$$

where

$$u(x) = \frac{1}{2} A_n (x - \xi)^2, \qquad A_n = \max_{\substack{\xi \le x \le R_1 \\ 0 \le y \le y_0}} \{\psi(x) f(x, y)\}.$$

From the inequalities

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* If equation (12) has more than one solution, then, in order to find $\varphi(x)$ for $0 \le x \le \xi$, we obtain a two-point problem $(\varphi(0) = y_0,\ \varphi(\xi) = 0)$.

it follows from Chaplygin' s theorem ([5]) that any solution of (1), (4) is smaller than $u(x)$ inside the rectangle $\xi \le x \le R_1,\ 0 \le y \le n y_0$. Then the sequence (13) converges to $\Phi(x)$, the greatest solution of problem (1), (4) for $x \ge \xi$. One can choose n and R_1 so that, for some $x = \bar{x} < R_1$, the equality

$$\int_\xi^{\bar{x}} s\psi(s) f(s, \Phi(s))\, ds = |q|, \quad \text{where } \Phi(x) = \lim_{k \to \infty} \Phi^{(k)}(x),$$

will hold, i.e. $\Phi(x)$ satisfies the condition $\bar{x}\Phi'(\bar{x}) - \Phi(\bar{x}) = -q$. In this case

$$\bar{C} = \Phi'(\bar{x}) = \int_\xi^{\bar{x}} \psi(s) f(s, \Phi(s))\, ds.$$

If

$$\int_\xi^{x_0} \psi(s) f(s, \varphi(s))\, ds = |q|,$$

where $\varphi(x)$ is the least solution of (1), (4) for $x \ge \xi$, then for $R > x_0$ problem (1), (2) has no solution.

For the Thomas-Fermi-Dirac equation in the case $q = 0$, an example was considered in the note ([4]).

Remark. For $q \ge y_0$, problem (1), (2) has no solution.

Theorem 6. *Under conditions 1)–3), 4′)–6′) and $y_0 > q > 0$, there exists such a finite interval $(0, \bar{x}(q))$ that for all $R \in (0, \bar{x}(q)]$, and only for them, there exists a solution of problem (1), (2), and it is unique for each R.*

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Note: Figure translations are in progress. See original paper for figures.