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A NOTE ON THE THOMAS-FERMI EQUATION

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Abstract. This work is conceived as a theoretical study. In this paper we consider the non-linear differential equation of the second order, which is known in applications as the Thomas-Fermi equation. We deal with setting the conditions under which this equation exhibits singularity in $(0, \infty)$. In the available literature, the authors investigate the singularity of the above equation at point 0, using numerical solution methods. The investigated equation has a wide application in quantum mechanics. The Thomas-Fermi equation represents models of atomic ions with a finite charge cloud and an overall positive charge. The boundary of the charge cloud is defined by the condition $y(x) = 0$, where $y(x)$ represents the charge density at a given point x. We illustrate the existence of singular solutions numerically with two examples. In addition, to its role in quantum mechanics, the equation also has potential applications in biochemistry. For example, if the atomic ions, e.g. sodium and chlorine ions penetrate the bacterium, they can cause the death of the bacterium.

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1. Introduction

The purpose of this paper is to establish the conditions under which the Thomas--Fermi equation

$$\frac{d^2 y(x)}{dx^2} = \frac{1}{\sqrt{x}} y^{\frac{2}{3}}, \quad x \geq 0, \tag{1}$$

has the singular solution in $(0, \infty)$. This equation arises in the modeling of certain phenomena in the atomic structure of matter [1-3]. The Thomas-Fermi equation makes it possible to analyze the electron distribution within an atom, as well as the charge densities of atoms containing large numbers of electrons. The charge density at each point x is represented by $y(x)$. In recent years, a wide range of approximate solutions has been derived for the Thomas-Fermi equation [3-6]. There exists hundreds of publications on this subject. Some authors use the variational approach to the Thomas-Fermi equation [7, 8]. Authors in [9, 10] consider the application of the Thomas-Fermi equation to the calculation of statistical potential of atomic ions. Some authors [11-15] numerically solve the Thomas-Fermi equation with the boundary conditions: $y(0) = 1, y(\infty) = 0$. Equations of the same type as the Thomas-Fermi equation, also known as Emden-Fowler equations, have been recently studied in discrete form [16, 17]. However, there seems to be a lack of publications in which the Thomas-Fermi equation has a singular solution in $(0, \infty)$.

Although the Thomas-Fermi equation is widely applied in quantum mechanics, its models also hold potential for biochemistry. For example, they can be used to describe the behaviour of atomic ions, such as sodium and chlorine, in bacterial systems. When these ions infiltrate a bacterium, they may cause its destruction, highlighting the possible biological relevance of the Thomas-Fermi equation [18].

2. Singular solution of the equation (1)

In this section, we present the conditions under which the equation (1) has singularity. We will call a solution singular if $y(x) = 0$ for some $x > 0$.

Lemma 1. *Suppose that* $y(x),\ x > 0$ *is a positive solution of equation (1) and*

$$-y'(x_1) > \frac{1}{\sqrt{x_1}} y^{1,5}(x_1),\ \ x_1 \geq 0. \tag{2}$$

Then there exists $x_2 > x_1$ *such that* $y'(x_2) = 0$.

PROOF. From (2) and (1), it follows that $y'(x_1) < 0$ and $y'(x) < 0,\ x \geq x_1$ is increasing, since $y''(x) > 0,\ x \geq x_1$. Assume that $y'(x) \to 0$, as $x \to \infty$. Then $y'(x) < 0, x \geq x_1$, and we have

$$\left(\frac{1}{\sqrt{x}} y^{1,5}(x)\right)' = \frac{1}{2\sqrt{x}} \sqrt{y(x)} \left(-\frac{1}{x} y(x) + 3y'(x)\right) < 0,\ \ x \geq x_1. \tag{3}$$

So the function

$$\frac{1}{\sqrt{x}} y^{1.5}(x),\ \ x \geq x_1$$

has a decreasing character. With regard to (2), we get

$$-y'(x) > \frac{1}{\sqrt{x}} y^{1.5}(x),\ \ x_1 \leq x \leq x_2.$$

Then we have

$$-y'(x) > y''(x),$$

$$1 > -\frac{y''(x)}{y'(x)}, \quad x_1 \leq x \leq x_2.$$

Integrating, we obtain

$$\int_{x_1}^{x_2} dx > -\int_{x_1}^{x_2} \frac{y''(x)}{y'(x)} dx,$$

$$x_2 - x_1 > -\ln|y'(x_2)| + \ln|y'(x_1)| = \ln\left|\frac{y'(x_1)}{y'(x_2)}\right|,$$

$$|y'(x_2)|e^{x_2 - x_1} > |y'(x_1)|, \quad x_1 \leq x_2.$$

Since $y'(x) \to 0$, as $x \to \infty$, and with regard to condition (2), we take $x_1 < x_2$, such that

$$|y'(x_2)|e^{x_2 - x_1} < \varepsilon$$

where

$$0 < \varepsilon \leq |y'(x_1)| \leq |y'(x_2)| - \frac{1}{\sqrt{x_1}} y^{1.5}(x_1).$$

Then we have

$$\varepsilon > |y'(x_2)|e^{x_2 - x_1} > |y'(x_1)|, \quad x_1 < x_2.$$

$$|y'(x_1)| - \frac{1}{\sqrt{x_1}} y^{1.5}(x_1) \geq \varepsilon > |y'(x_1)|,$$

$$|y'(x_1)| - \frac{1}{\sqrt{x_1}} y^{1.5}(x_1) > |y'(x_1)|,$$

$$-\frac{1}{\sqrt{x_1}} y^{1.5}(x_1) > 0,$$

which is a contradiction.

Then $y'(x)$ is not going to 0, as $x \to \infty$. If $y'(x) \to K < 0$, then $y'(x) \leq K$, $x \geq x_1$, and integrating, we get

$$\int_{x_1}^{x} y'(s) ds \leq \int_{x_1}^{x} K \, ds,$$

$$y(x) - y(x_1) \leq K(x - x_1).$$

Then $y(x) \to -\infty$, as $x \to \infty$. So, there exists $x_2 > x_1$ such that $y'(x_2) = 0$.

Theorem 1. *Suppose that* $y(x)$, $x > 0$, *is a solution of Eq. (1), inequality (2) holds and*

$$0 < y^{1.5}(x_1) \le \sqrt{x_1},\ x_1 > 0.$$

Then $y(x)$, $x > 0$, is a singular solution of Equation (1) on interval $(0, \infty)$.

PROOF. Assume that $y(x)$, $x > 0$ is a positive solution of Eq. (1). According to Lemma 1, there exists $x_2 > x_1$ such that $y'(x_2) = 0$.

The Mean Value Theorem yields

$$y'(x_2) - y'(x) = (x_2 - x)y''(\beta),\ \ \beta \in (x, x_2),\ \ x > 0$$
$$-y'(x) = (x_2 - x)\frac{1}{\sqrt{\beta}}y^{1.5}(\beta),\ \ \beta \in (x, x_2). \tag{4}$$

Since the function

$$\frac{1}{\sqrt{x}}y^{1.5}(x),\ \ x > x_1$$

has decreasing character, then by virtue of (4), we obtain

$$-y'(x) \le (x_2 - x)\frac{1}{\sqrt{(x)}}y^{1.5}\big((x)\big),\ \ x_1 \le x \le x_2.$$

With regard to (1), we have

$$-y'(x) \le (x_2 - x)y''(x),\ \ x_1 \le x \le x_2,$$

$$\frac{1}{x_2 - x} \le -\frac{y''(x)}{y'(x)}.$$

Integrating, we get

$$\int_{x_1}^{x_2} \frac{1}{x_2 - x}\,dx \le -\int_{x_1}^{x_2} \frac{y''(x)}{y'(x)}\,dx\,,$$

$$-\lim_{x \to x_2} \ln(x_2 - x) + \ln(x_2 - x_1) \le -\lim_{x \to x_2} \ln|y'(x)| + \ln|y'(x_1)|.$$

Since

$$\lim_{x \to x_2} \ln(x_2 - x) = -\infty,\ \ \lim_{x \to x_2} \ln|y'(x)| = -\infty,$$

$$\ln(x_2 - x_1) \le \ln|y'(x_1)|,$$

$$x_2 - x_1 \le -y'(x_1).$$

With regard to (4), we obtain

$$-y'(x_1) = (x_2 - x_1)\frac{1}{\sqrt{\beta}} y^{1.5}(\beta), \ \ \beta \in (x_1, x_2),$$

$$-y'(x_1) = (x_2 - x_1)\frac{1}{\sqrt{x_1}} y^{1.5}(x_1).$$

Then we get

$$x_2 - x_1 \le -y'(x_1) < (x_2 - x_1)\frac{1}{\sqrt{x_1}} y^{1.5}(x_1),$$

$$\sqrt{x_1} < y^{1.5}(x_1), \ \ x_1 > 0,$$

which contradicts that

$$0 < y^{1.5}(x_1) \le \sqrt{x_1}, \ \ x_1 > 0.$$

Example 1. Consider that $y(0.2) = 0.5$, $y'(0.2) = -0.9$, $x_1 = 0.2$. Then we have $y^{1.5}(0.2) = 0.353553$, $\sqrt{0.2} = 0.447214$, $\frac{1}{\sqrt{0.2}} y^{1.5}(0.2) = 0.790568$.

Thus $-y'(0.2) > \frac{1}{\sqrt{0.2}} y^{1.5}(0.2)$ and $y^{1.5}(0.2) < \sqrt{0.2}$. Then the solution $y(x)$ of equation (1) is singular in the interval $(0, \infty)$.

Example 2. Consider that $y(0.5) = 0.6$, $y'(0.5) = -0.7$, $x_1 = 0.5$. Then we have $y^{1.5}(0.5) = 0.464758$, $\sqrt{0.5} = 0.707107$, $\frac{1}{\sqrt{0.5}} y^{1.5}(0.5) = 0.657267$.

Thus $-y'(0.5) > \frac{1}{\sqrt{0.5}} y^{1.5}(0.5)$ and $0 < y^{1.5}(0.5) < \sqrt{0.5}$. Then the solution $y(x)$ of equation (1) is singular in the interval $(0, \infty)$.

3. Conclusions

In this contribution, we focus exclusively on the theoretical analysis of the solution to the Thomas-Fermi differential equation and on the investigation of its singularity. The aim of the article is to provide and supplement information on singular solutions of the Thomas-Fermi equation. The paper establishes conditions for the existence of a singular solution of the Thomas-Fermi equation on the interval $(0, \infty)$. Analytical procedures are used to achieve the goal. The solutions of the equation have considerable potential in the investigation of certain phenomena in the atomic structure of matter and also in biochemistry.

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