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An Upper and Lower Solution Approach for a Generalized Thomas–Fermi Theory of Neutral Atoms

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This paper presents an upper and lower solution theory for boundary value problems modelled from the Thomas–Fermi equation subject to a boundary condition corresponding to the neutral atom with Bohr radius.

Key words: Boundary value problem, upper and lower solution, Thomas–Fermi theory, existence

1 INTRODUCTION

In 1927, L. H. Thomas and E. Fermi independently derived a boundary value problem for determining the electrical potential in an atom. There analysis leads to the nonlinear second order differential equation

$$y'' = t^{-1/2}y^{3/2}.$$

The boundary conditions in investigating

(a) the neutral atom with Bohr radius a are given by

$$y(0) = 1, \quad ay'(a) = y(a);$$

(b) the ionized atom are given by

$$y(0) = 1, \quad y(a) = 0;$$

(c) the isolated neutral atom are given by

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

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Almost all the papers in the literature (see [1,4,5,7] and the references therein) discuss boundary condition (b) or (c). Only a handful of papers [2,6] have discussed the boundary condition (a). This paper discusses boundary condition (a) and we present an upper and lower solution theory for such problems. In fact our theory applies to the more general equation (considered in [2])

$$y'' + \frac{b}{t}y = f(t,y), \quad 0 \le b < 1,$$

and we discuss this also in Section 2.

2 EXISTENCE

Motivated by the Thomas–Fermi problem in Section 1 we begin by discussing the two point boundary value problem

$$\begin{cases} y'' = qf(t,y), & 0 < t < a \\ y(0) = a_0 \\ ky'(a) = y(a), & k \ge a \end{cases} \tag{2.1}$$

where $a > 0$ is fixed. By an upper solution β to (2.1) we mean a function $\beta \in C^1[0,a] \cap C^2(0,a)$ with

$$\begin{cases} \beta''(t) \le q(t)f(t,\beta(t)), & 0 < t < a \\ \beta(0) \ge a_0 \\ k\beta'(a) \ge \beta(a) \end{cases} \tag{2.2}$$

and by a lower solution α to (2.1) we mean a function $\alpha \in C^1[0,a] \cap C^2(0,a)$ with

$$\begin{cases} \alpha''(t) \ge q(t)f(t,\alpha(t)), & 0 < t < a \\ \alpha(0) \le a_0 \\ k\alpha'(a) \le \alpha(a) \end{cases} \tag{2.3}$$

In our first existence result we will assume the following conditions are satisfied:

$$q \in C(0,a) \cap L^1[0,a] \text{ with } q > 0 \text{ on } (0,a) \tag{2.4}$$

$$f\colon [0,a] \times \mathbf{R} \to \mathbf{R} \text{ is continuous} \tag{2.5}$$

and

$$\begin{cases} \text{there exists } \alpha, \beta \text{ respectively lower and upper} \\ \text{solutions of (2.1) with } \alpha(t) \le \beta(t) \text{ for } t \in [0,a]. \end{cases} \tag{2.6}$$

THEOREM 2.1 *Suppose* (2.4)–(2.6) *hold. Then* (2.1) *has a solution* $y \in C^1[0,a] \cap C^2(0,a)$ *with* $\alpha(t) \le y(t) \le \beta(t)$ *for* $t \in [0,a]$.

Proof To show (2.1) has a solution we consider the boundary value problem

$$\begin{cases} y'' - y = f^*(t, y), & 0 < t < a \\ y(0) = a_0 \\ ky'(a) = y(a) \end{cases} \tag{2.7}$$

where

$$f^*(t, y) = \begin{cases} q(t)[f(t, \beta(t)) + r(y - \beta(t))] - \beta(t), & y > \beta(t) \\ q(t)f(t, y) - y, & \alpha(t) \le y \le \beta(t) \\ q(t)[f(t, \alpha(t)) + r(y - \alpha(t))] - \alpha(t), & y < \alpha(t) \end{cases}$$

and $r: \mathbf{R} \to [-1, 1]$ is the radial retraction defined by

$$r(x) = \begin{cases} x, & |x| \le 1 \\ \dfrac{x}{|x|}, & |x| > 1. \end{cases}$$

Solving (2.9) is equivalent to finding a fixed point of the operator N where $N: C[0, a] \to C[0, a]$ is given by (here $y \in C[0, 1]$)

$$Ny(t) = Ae^t + (a_o - A)e^{-t} - \frac{1}{2}e^{-t}\int_0^t e^s f^*(s, y(s))\,ds + \frac{1}{2}e^t\int_0^t e^{-s} f^*(s, y(s))\,ds$$

where

$$A = \frac{a_o(1 + k)e^{-a} - (1/2)(k + 1)e^{-a}\int_0^a e^s f^*(s, y(s))\,ds}{(1 + k)e^{-a} + (k - 1)e^a} - \frac{(1/2)(k - 1)e^a\int_0^a e^{-s} f^*(s, y(s))\,ds}{(1 + k)e^{-a} + (k - 1)e^a}.$$

Remark 2.1 Note $(1 + k)e^{-a} \neq (1 - k)e^a$. To see this notes if $(1 + k)e^{-a} = (1 - k)e^a$ then with $u(t) = e^t - e^{-t}$ we have $u'' - u = 0$, $u(0) = 0$ and $ku'(a) = u(a)$, so $u \equiv 0$, a contradiction.

A standard argument [7] guarantees that $N: C[0, a] \to C[0, a]$ is continuous and compact. Schauder's fixed point theorem guarantees that N has a fixed point y. Thus y is a solution of (2.7).

To finish the proof it remains to show $\alpha(t) \le y(t) \le \beta(t)$ for $t \in [0, a]$. Once this is shown then y is a solution of (2.1) and we are finished. First we show $y(t) \le \beta(t)$ for $t \in [0, a]$. If this is not true then $y - \beta$ attains a positive absolute maximum somewhere on $[0, a]$, say at t_0. Note $t_0 \neq 0$ since $\beta(0) \ge a_0 = y(0)$. Consider first the case $t_0 \in (0, a)$. Then $(y - \beta)'(t_0) = 0$ and $(y - \beta)''(t_0) \le 0$. Also since $y(t_0) > \beta(t_0)$ we have

$$\begin{aligned} (y - \beta)''(t_0) &= f^*(t_0, y(t_0)) + y(t_0) - \beta''(t_0) \ge f^*(t_0, y(t_0)) + y(t_0) - q(t_0)f(t_0, \beta(t_0)) \\ &= \{q(t_0)[f(t_0, \beta(t_0)) + r(y(t_0) - \beta(t_0))] - \beta(t_0)\} + y(t_0) + q(t_0)f(t_0, \beta(t_0)) \\ &= q(t_0)r(y(t_0) - \beta(t_0)) + (y(t_0) - \beta(t_0)) > 0, \end{aligned}$$

a contradiction. Thus $t_0 \notin (0, a)$. It remains to discuss the case $t_0 = a$. Assume $t_0 = a$. Then $(y - \beta)'(a) \geq 0$. Also since $y(0) - \beta(0) \leq 0$ there exists δ, $0 \leq \delta < a$ with $y(t) - \beta(t) > 0$ for $t \in (\delta, a)$ and $y(\delta) - \beta(\delta) = 0$. In addition for $t \in (\delta, a)$ we have

$$\begin{aligned}(y - \beta)''(t) &= f^*(t, y(t)) + y(t) - \beta''(t) \geq f^*(t, y(t)) + y(t) - q(t)f(t, \beta(t)) \\ &= q(t)r(y(t) - \beta(t)) + (y(t) - \beta(t)) > 0.\end{aligned}$$

Consequently $y - \beta$ is convex on (δ, a) and so we have [3 pp. 134],

$$y'(a) - \beta'(a) \geq \frac{[y(a) - \beta(a)] - [y(\delta) - \beta(\delta)]}{a - \delta} = \frac{y(a) - \beta(a)}{a - \delta}. \tag{2.8}$$

We break the proof into two cases, namely $k > a$ and $k = a$.

Case (A) $k > a$.
Then $ky'(a) = y(a)$ and $k\beta'(a) \geq \beta(a)$ together with (2.8) implies

$$\frac{1}{k}[y(a) - \beta(a)] \geq y'(a) - \beta'(a) \geq \frac{y(a) - \beta(a)}{a - \delta} \geq \frac{y(a) - \beta(a)}{a},$$

so $k \leq a$, a contradiction.

Case (B) $k = a$.
We break the argument into two subcases, namely $\delta > 0$ and $\delta = 0$.

Subcase (i) $\delta > 0$.
Then $ay'(a) = y(a)$ and $a\beta'(a) \geq \beta(a)$ together with (2.8) implies

$$\frac{1}{a}[y(a) - \beta(a)] \geq y'(a) - \beta'(a) \geq \frac{y(a) - \beta(a)}{a - \delta} > \frac{y(a) - \beta(a)}{a},$$

a contradiction.

Remark 2.2 If $\beta(0) > a_0$ then $\delta > 0$.

Subcase (ii) $\delta = 0$.
Then $y(0) - \beta(0) = 0$, $y(t) - \beta(t) > 0$ for $t \in (0, a]$ and $(y - \beta)''(t) > 0$ for $t \in (0, a)$. Thus for $t \in (0, a)$ we have by the mean value theorem that

$$(y - \beta)'(a) - (y - \beta)'(t) > 0,$$

and so since $a\beta'(a) \geq \beta(a)$ we have

$$(y - \beta)'(t) < (y - \beta)'(a) \leq \frac{y(a) - \beta(a)}{a} \quad \text{for } t \in (0, a).$$

That is

$$(y-\beta)'(t) < \frac{y(a)-\beta(a)}{a} \quad \text{for } t \in (0,a),$$

so the mean value theorem implies

$$(y-\beta)(a) - (y-\beta)(0) < \frac{y(a)-\beta(a)}{a}a.$$

This together with $y(0) - \beta(0) = 0$ yields

$$y(a) - \beta(a) < y(a) - \beta(a).$$

a contradiction.

Remark 2.3 Notice the argument in subcase (ii) can also be applied to subcase (i).

Thus in both cases we have a contradiction, so $t_0 \neq a$. As a result $t_0 \notin [0,a]$. This implies $y(t) \leq \beta(t)$ for $t \in [0,a]$. A similar argument shows $\alpha(t) \leq y(t)$ for $t \in [0,a]$. As a result

$$y'' - y = qf(t,y) - y \quad \text{for } t \in (0,a),$$

and we are finished. ■

Remark 2.4 (i) In Theorem 2.1, (2.5) could be replaced by the less restrictive condition

$$f^*: [0,a] \times \mathbf{R} \to \mathbf{R} \text{ is continuous.} \tag{2.9}$$

(ii) There is also an analogue of Theorem 2.1 (we leave the details to the reader) for the more general problem

$$\begin{cases} y'' = qf(t,y), & 0 < t < a \\ y(0) = a_0 \\ ky'(a) - y(a) = b_0, & k \geq a. \end{cases}$$

Example 2.1 (Bohr radius Thomas–Fermi equation.)

Consider the boundary value problem

$$\begin{cases} y'' = t^{-1/2}y^{3/2}, & 0 < t < a \\ y(0) = 1 \\ ay'(a) = y(a), \end{cases} \tag{2.10}$$

with $a^3 \geq 9/4$.

To show (2.11) has a solution we will apply Theorem 2.1 to the boundary value problem

$$\begin{cases} y'' = t^{-1/2}|y|^{3/2}, & 0 < t < a \\ y(0) = 1 \\ ay'(a) = y(a), \end{cases} \tag{2.11}$$

with $k = a$, $a_0 = 1$, $q(t) = t^{-1/2}$ and $f(t, y) = |y|^{3/2}$. Clearly (2.4) and (2.5) hold. Now let $\alpha = 0$. We claim α is a lower solution of (2.11). To see this notice

$$\alpha(0) = 0 \leq 1, \quad a\alpha'(a) = 0 = \alpha(a) \quad \text{and} \quad \alpha'' - qf(t, \alpha) = 0 \quad \text{for } t \in (0, a).$$

Next we show

$$\beta(t) = \frac{4}{3}t^{3/2} + \frac{2}{3}a^{3/2}$$

is an upper solution of (2.11). Notice

$$\beta(0) = \frac{2}{3}a^{3/2} \geq \frac{2}{3}\frac{3}{2} = 1 \quad \text{since } a^3 \geq \frac{9}{4},$$

and since $\beta'(t) = 2t^{1/2}$ we have

$$a\beta'(a) = 2a^{3/2} \text{ and } \beta(a) = \frac{4}{3}a^{3/2} + \frac{2}{3}a^{3/2} = 2a^{3/2}, \text{ so } a\beta'(a) = \beta(a).$$

Finally since $\beta''(t) = t^{-1/2}$ we have

$$\beta'' - qf(t, \beta) = t^{-1/2} - t^{-1/2}[\beta(t)]^{3/2} = t^{-1/2}(1 - [\beta(t)]^{3/2}) \leq 0$$

for $t \in (0, a)$, since $\beta(t) \geq \frac{2}{3}a^{3/2} \geq 1$ for $t \in (0, a)$. Thus β is an upper solution of (2.11) so (2.6) holds. Theorem 2.1 guarantees that there exists a solution $y \in C^1[0, a] \cap C^2(0, a)$ to (2.11) with

$$0 \leq y(t) \leq \frac{4}{3}t^{3/2} + \frac{2}{3}a^{3/2} \quad \text{for } t \in [0, a].$$

Now since $y(t) \geq 0$ for $t \in [0, a]$ we have that y is a solution of (2.10).

It is also possible to extend the ideas in this section to other boundary value problems. To show what is possible we consider the boundary value problem (motivated partly from [2])

$$\begin{cases} \frac{1}{p}(py')' = qf(t, y), \quad 0 < t < a \\ y(0) = a_0 \\ \int_0^a (\mathrm{d}s/p(s)) [\lim_{t \to a^-} p(t)y'(t)] = y(a). \end{cases} \tag{2.12}$$

By an upper solution β to (2.12) we mean a function $\beta \in C[0, a] \cap C^2(0, a)$, $p\beta' \in AC[0, a]$ with

$$\begin{cases} \frac{1}{p}(p\beta')'(t) \leq q(t)f(t, \beta(t)), \quad 0 < t < a \\ \beta(0) \geq a_0 \\ \int_0^a (\mathrm{d}s/p(s))[\lim_{t \to a^-} p(t)\beta'(t)] \geq \beta(a), \end{cases} \tag{2.13}$$

and by a lower solution α to (2.12) we mean a function $\alpha \in C[0,a] \cap C^2(0,a)$, $p\alpha' \in AC[0,a]$ with

$$\begin{cases} \frac{1}{p}(p\alpha')'(t) \geq q(t)f(t,\alpha(t)), & 0 < t < a \\ \alpha(0) \leq a_0 \\ \int_0^a (\mathrm{d}s/p(s))[\lim_{t\to a^-} p(t)\alpha'(t)] \leq \alpha(a). \end{cases} \tag{2.14}$$

For our existence result, (2.5) is assumed and also we will suppose the following conditions are satisfied:

$$p \in C[0,a] \cap C^1(0,a) \text{ with } p > 0 \text{ on } (0,a) \tag{2.15}$$

$$q \in C(0,a), \quad q > 0 \text{ on } (0,a) \text{ and } \int_0^a p(s)q(s)\,\mathrm{d}s < \infty \tag{2.16}$$

and

$$\begin{cases} \text{there exists } \alpha, \beta \text{ respectively lower and upper} \\ \text{solutions of (2.12) with } \alpha(t) \leq \beta(t) \text{ for } t \in [0,a]. \end{cases} \tag{2.17}$$

THEOREM 2.2 *Suppose* (2.5), (2.15)–(2.17) *hold. Then* (2.12) *has a solution* $y \in C[0,a] \cap C^2(0,a)$, $py' \in AC[0,a]$ *with* $\alpha(t) \leq y(t) \leq \beta(t)$ *for* $t \in [0,a]$.

Proof To show (2.12) has a solution we consider the boundary value problem

$$\begin{cases} \frac{1}{p}(py')' - y = f^*(t,y), & 0 < t < a \\ y(0) = a_0 \\ \int_0^a (\mathrm{d}s/p(s))[\lim_{t\to a^-} p(t)y'(t)] = y(a) \end{cases} \tag{2.18}$$

where f^* is as in Theorem 2.1. A slight modification of the argument in Theorem 2.1 (see [7, Chapter 3]) guarantees that (2.18) has a solution y.

We now show $y(t) \leq \beta(t)$ for $t \in [0,a]$. If this is not true then $y - \beta$ attains a positive absolute maximum somewhere on $[0,a]$, say at t_0. Note $t_0 \neq 0$. Consider first the case $t_0 \in (0,a)$. Then $(y-\beta)'(t_0) = 0$ and $(p(y-\beta)')'(t_0) \leq 0$. Also since $y(t_0) > \beta(t_0)$ we have

$$\begin{aligned}(p(y-\beta)')'(t_0) &= p(t_0)[f^*(t_0,y(t_0)) + y(t_0)] - (p\beta')'(t_0) \\ &\geq p(t_0)[f^*(t_0,y(t_0)) + y(t_0)] - p(t_0)q(t_0)f(t_0,\beta(t_0)) \\ &= p(t_0)q(t_0)r(y(t_0) - \beta(t_0)) + p(t_0)(y(t_0) - \beta(t_0)) > 0,\end{aligned}$$

a contradiction. Thus $t_0 \notin (0,a)$. It remains to discuss the case $t_0 = a$. Assume $t_0 = a$. Now since $y(0) - \beta(0) \leq 0$ there exists $\delta, 0 \leq \delta < a$ with $y(t) - \beta(t) > 0$ for $t \in (\delta,a)$ and $y(\delta) - \beta(\delta) = 0$. In addition for $t \in (\delta,a)$ we have

$$\begin{aligned}(p(y-\beta)')'(t) &= p(t)[f^*(t,y(t)) + y(t)] - (p\beta')'(t) \\ &= p(t)q(t)r(y(t) - \beta(t)) + p(t)(y(t) - \beta(t)) > 0.\end{aligned}$$

Thus for $t \in (\delta, a)$ we have from the mean value theorem that

$$p(y-\beta)'(a) - p(y-\beta)'(t) > 0,$$

and so since

$$\int_0^a \frac{ds}{p(s)} [\lim_{t\to a^-} p(t)y'(t)] = y(a) \quad \text{and} \quad \int_0^a \frac{ds}{p(s)} [\lim_{t\to a^-} p(t)\beta'(t)] \geq \beta(a),$$

we have

$$p(y-\beta)'(t) < p(y-\beta)'(a) \leq \frac{y(a)-\beta(a)}{\int_0^a (ds/p(s))} \quad \text{for } t \in (\delta, a).$$

That is

$$(y-\beta)'(t) < \frac{1}{p(t)} \frac{y(a)-\beta(a)}{\int_0^a (ds/p(s))} \quad \text{for } t \in (\delta, a),$$

so we have

$$(y-\beta)(a) - (y-\beta)(\delta) < \frac{y(a)-\beta(a)}{\int_0^a (ds/p(s))} \int_\delta^a \frac{ds}{p(t)} \leq y(a) - \beta(a).$$

This together with $y(\delta) - \beta(\delta) = 0$ yields

$$y(a) - \beta(a) < y(a) - \beta(a),$$

a contradiction. Thus $t_0 \neq a$. As a result $t_0 \notin [0, a]$. This implies $y(t) \leq \beta(t)$ for $t \in [0, a]$. A similar argument shows $\alpha(t) \leq y(t)$ for $t \in [0, a]$, and we are finished. ■

Remark 2.5 In Theorem 2.2, (2.5) can be replaced by (2.9).

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