On a Neumann Boundary Value Problem for Painlevé II in Two Ion Electro-Diffusion

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Abstract

A two-point Neumann boundary value problem for a two ion electro-diffusion model reducible to the Painlevé II equation is investigated. The problem is unconventional in that the model equation involves yet-to-be determined boundary values of the solution. In prior work by Thompson, the existence of a solution was established subject to an inequality on the physical parameters. Here, a two-dimensional shooting method is used to show that this restriction may be removed. A practical algorithm for the solution of the boundary value problem is presented in an appendix.

1 Introduction

In [10], a two-point boundary value problem was investigated which arises in the study of two ions of the same valency migrating across a liquid junction such as a membrane. The relevant model equations are derived in [1, 2] and , in a more general multi-ion context, in [7]. Their underlying Painlevé structure has recently been analyzed in [3].

Elimination of the ionic concentrations in the two-ion problem leads to a nonlinear equation for the unknown y, proportional to the electric field E, namely [10]

$$y''(x) = f(x, y(x); y(0), y(1)), \quad x \in (0, 1) \tag{1.1}$$

where

$$f(x, y; y(0), y(1)) := y\left[\lambda - \frac{\left(y(0)^2 - y^2\right)}{2} + Ax\right] - AD, \tag{1.2}$$

with

$$A = l\lambda + \frac{\left(y(0)^2 - y(1)^2\right)}{2}, \tag{1.3}$$

and the liquid junction occupies the region $0 \le x \le 1$. The quantities $l > 0, \lambda > 0$ and D with $-1 < D < 1$ are parameters as described in [10]. As noted in [10], if y is a solution of (1.1) for the parameters l, λ, D then $-y$ is a solution for $l, \lambda, -D$. It is also easy to see that, when $D = 0$, the only solution is $y(x) \equiv 0$. Hence, it may be assumed, without

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loss of generality, that $D > 0$. Electrical neutrality in the reservoirs imposes the Neumann boundary conditions

$$y'(0) = y'(1) = 0. \tag{1.4}$$

The boundary value problem determined by (1.1) $-$ (1.4) is unconventional in that the nonlinear model equation (1.1) involves the solution-dependent quantities $y(0)$ and $y(1)$. Accordingly, traditional existence theory and numerical methods are not appropriate to treat this problem.

Thompson in [10] used degree theory and the well-established method of upper and lower solutions (see e.g. [4]) to prove the existence of a positive solution to the boundary value problem (1.1) $-$ (1.4) when $D > 0$ and subject to the constraint

$$\lambda \geq 2l \left[1 - \frac{1}{(1+l)^2}\right] D^2. \tag{1.5}$$

Here, our object is to establish that this restriction may be removed. The method adopted involves the reduction of the original problem to an equivalent one amenable to a two-dimensional shooting method, which is an extension of the well-known one-dimensional shooting method. The latter has recently been applied successfully by the second author [5, 6] to study a variety of boundary value problems.

2 A Painlevé II Reduction

The two ion model equation (1.1) adopts the form

$$y'' = y\left(\zeta + \frac{y^2}{2} + \mu x\right) + \nu \tag{2.1}$$

and, on introduction of the scaling and translation

$$y = \xi U, \quad x = \eta X + \delta \tag{2.2}$$

with

$$\xi\eta = \pm 2, \quad \delta = -\zeta/\mu, \quad \eta = \mu^{-1/3} \tag{2.3}$$

reduction is obtained to the canonical Painlevé II equation

$$\frac{d^2U}{dX^2} = 2U^3 + XU + \bar{\alpha} \tag{2.4}$$

where the parameter $\bar{\alpha}$ is given by

$$\bar{\alpha} = \nu\eta^2 = -\mu^{1/3} D \tag{2.5}$$

Here,

$$\mu = l\lambda + \frac{y_0^2 - y_1^2}{2} = l\lambda + 2\mu^{1/3}\left(U_0^2 - U_1^2\right) \tag{2.6}$$

with the notation $y\,|_{x=0} = y_0\,,\ y\,|_{x=1} = y_1\,,\ U\,|_{x=0} = U_0\,,\ U\,|_{x=1} = U_1\,.$ Thus, (2.6) provides a cubic equation for the Painlevé parameter $\bar{\alpha}$ in terms of the physical parameters l, λ, D and the boundary terms $U_0 = U\,\big|_{X=-\delta/\eta}\,,\ U_1 = U\,\big|_{X=(1-\delta)/\eta}\,.$ In general, the study of the existence properties for the original boundary value problem under the above Painlevé II reduction is not tractable in view of the complicated nature of the dependence of $\bar{\alpha}$ on the boundary terms and the transition $x = 0 \to X = -\delta/\eta$, $x = 1 \to X = (1-\delta)/\eta$. However, it is noted that if $\delta = 1$, $\eta = -1$ so that $\zeta = 1$, $\mu = -1$ then $x = 0 \to X = 1$, $x = 1 \to X = 0$ and $\bar{\alpha} = D$ under the canonical reduction. Thus, a Neumann problem for the conventional Painlevé II equation where $\bar{\alpha}$ is independent of the boundary conditions is obtained. Existence results for the Painlevé II equation under Dirichlet and periodic-type boundary conditions have been investigated in [8], while the application of boundary value problems has been undertaken in [9]. Here, however, in view of the intractable nature of the Neumann boundary value problem $(1.1) - (1.4)$ under the above reduction, an alternative formulation is adopted which allows a novel application of an exact shooting method.

3 An Equivalent Problem. Two Dimensional Shooting. A Result in Differential Inequalities

The scaled quantity

$$z(x) = \frac{y(x)}{y(0)} \tag{3.1}$$

is introduced so that (1.1) yields

$$z''(x) = g(x, z(x), \gamma, z(1)), \quad x \in (0,1), \tag{3.2}$$

where

$$g(x, z, \gamma, z_1) = z(x)\left\{\lambda - \frac{\gamma^2}{2}(1 - z(x)^2) + \left[l\lambda + \frac{\gamma^2}{2}(1 - z_1^2)\right]x\right\} - \frac{[l\lambda + \frac{\gamma^2}{2}(1 - z_1^2)]D}{\gamma} \tag{3.3}$$

with $\gamma = y_0 = y(0) > 0$, $z_1 = z(1)$. If we set

$$\alpha = \frac{l\lambda + \frac{\gamma^2}{2}(1 - z_1^2)}{\gamma} \tag{3.4}$$

then the model equation adopts the compact form

$$z''(x) = \left[\lambda - \frac{\gamma^2}{2}(1 - z(x)^2) + \gamma\alpha x\right] z(x) - \alpha D \tag{3.5}$$

where, if α is specified, then l can be recovered via

$$l = \frac{\gamma\alpha - \frac{\gamma^2}{2}(1 - z_1^2)}{2} \tag{3.6}$$

and z now satisfies the boundary conditions

$$z(0) = 1, \quad z'(0) = 0, \tag{3.7}$$

and

$$z'(1) = 0. \tag{3.8}$$

The following observation turns out to be useful in the sequel:

Lemma 1 *Let $x_0 < x_1$ be two points in $[0, 1]$ such that $z(x_0) \leq z(x_1)$. Then $z''(x_0) < z''(x_1)$.*

Proof. This is a consequence of the fact that the righthand side of (3.5) is an increasing function of z for fixed x and a strictly increasing function of x for fixed z. ∎

In the original problem, given the physical parameters $\lambda, l > 0$ and D, we seek a function $y(x)$ that satisfies (1.1) $-$ (1.4). This is equivalent to finding a suitable $\gamma > 0$ and a function $z(x)$ that satisfies (3.5), (3.7), and (3.8). As it stands, the latter problem is as difficult as the original one since the differential equation (3.5) contains the undetermined parameter γ as well as the parameter α dependent on the yet-to-be-determined value z_1. Here, the problem is modified by not specifying a value for the constant l at the outset, but rather, by starting with two given constants $\alpha > 0$ and $\gamma \geq 0$. Note that we allow γ to be 0 for convenience, even though $\gamma > 0$ in the boundary value problem (3.1) $-$ (3.3). Here, we proceed without the requirement that the boundary condition (3.8) hold 'a priori'. Accordingly, instead of a boundary value problem, we are concerned with an initial value problem, namely, (3.5) $-$ (3.7). Suppose that a positive solution $z(x)$ exists (it must be unique) on the whole interval $[0, 1]$. We can then compute the pair of values $z'(1)$ and l (recovered using (3.6)). This defines a continuous operator $T(\alpha, \gamma) = (z'(1), l)$ from $\mathbb{R}^2 \to \mathbb{R}^2$. The original boundary value problem will have a solution if and only if the operator equation $T(\alpha, \gamma) = (0, l)$, with $\alpha > 0$ and $\gamma > 0$, where l now equals the value prescribed in the original problem. We term this technique the two-dimensional shooting method.

It is known that a solution of the initial value problem always exists in a neighborhood of the origin, but there may not be a positive solution defined on the whole of $[0, 1]$. Firstly, the solution may become zero at some point in $(0, 1]$ and then becomes negative beyond that. Secondly, due to the existence of the term z^2 on the right hand side of the equation (3.5), the solution may blow up at some point in $(0, 1]$ and then $z'(1)$ is not defined. In the next section, it is shown how the operator T can be modified to take care of such adverse circumstances.

In what follows, we describe the topological degree result to be used in proving our main result.

Let Ω be an open subset of the plane $\mathbb{R}^2$ with boundary $\partial\Omega$ a simple curve (see Figure 1). T is a continuous mapping from $\overline{\Omega} = \Omega \cup \partial\Omega$ to $\mathbb{R}^2$. Let $(c, d) \in \mathbb{R}^2$ be a point not in the image of $\partial\Omega$. Denote by A a variable point on the boundary $\partial\Omega$. As A traverses the

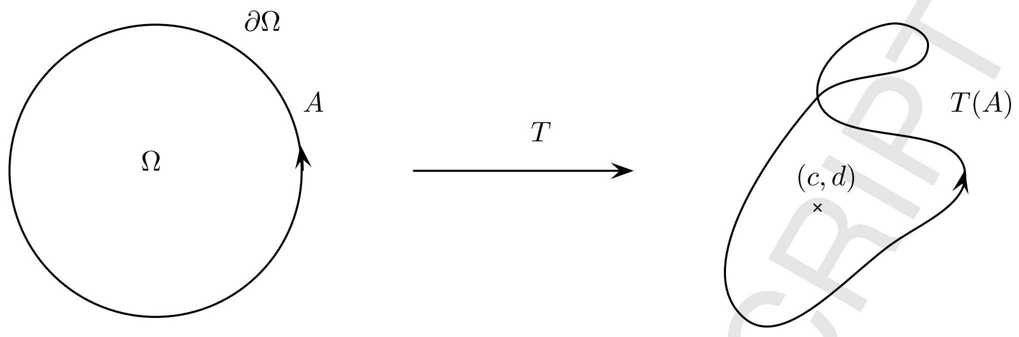

Figure 1:

boundary (in a chosen, e.g. counterclockwise, direction), its image $T(A)$ traces out a closed curve that does not pass through the point (c, d). As in complex analysis, we can define the winding number of this curve with respect to (c, d), by measuring the total change of the argument (as a multiple of 2π) of the vector joining (c, d) and the variable point $T(A)$. For two-dimensional space, this number is equivalent to the topological degree of the mapping T at (c, d).

It is useful to recall that if T is homotopic to another mapping T_1 and the point (c, d) is not on the combined image of $\partial\Omega$ under the homotopy, then the degree of T with respect to (c, d) and that of T_1 are the same.

An important result in degree theory states:

> *If the degree of a continuous mapping T with respect to a point (c, d) is non-zero, then the equation $T(\alpha, \gamma) = (c, d)$ has a solution $(\alpha, \gamma) \in \Omega$.*

To apply this result to our problem, we set $(c, d) = (0, l)$ and proceed to find a suitable region Ω such that the winding number of $T(\partial\Omega)$ with respect to $(0, l)$ is non-zero. In the next section, it will be shown that if we choose two large enough numbers α^* and γ^*, then the interior of the rectangle with vertices $P = (\lambda/D, 0)$, $Q = (\alpha^*, 0)$, $R = (\alpha^*, \gamma^*)$, and $S = (\lambda/D, \gamma*)$ will serve as our Ω.

We now state a simple result in the theory of differential inequalities that will be useful in the next section.

Lemma 2 *Suppose $Z(x)$ and $U(x)$ are functions defined on an interval $[0, x_1]$ and that they satisfy*

$$Z''(x) \geq F(x, Z(x)), \tag{3.9}$$

$$U''(x) = F(x, U(x)), \tag{3.10}$$

where the continuous function $F(x, Z)$ is increasing in Z for each fixed $x \in [0, x_1]$. If in addition, it is assumed that,

$$Z(0) \geq U(0), \quad Z'(0) \geq U'(0). \tag{3.11}$$

then

$$Z(x) \geq U(x), \quad Z'(x) \geq U'(x), \quad \forall x \in [0, x_1]. \tag{3.12}$$

Proof. This can be found in any standard monograph on differential inequalities, (e.g. [7] or [4]). It is included here for reference purposes.

The result is first established under the stronger assumption that the inequalities in (3.9) and (3.11) are strict, with the stronger conclusion that $Z(x) > U(x)$ for all $x \in [0, x_1]$. Suppose that the conclusion is false. Then there is a point $\xi \in (0, x_1]$ at which $Z(\xi) = U(\xi)$, while $Z(x) > U(x)$ for all $x < \xi$. Then we must have

$$Z'(\xi) \leq U'(\xi). \tag{3.13}$$

On the other hand, since F is an increasing function of Z,

$$Z''(x) > F(x, Z(x)) \geq F(x, U(x)) = U''(x) \tag{3.14}$$

for all $x < \xi$. This together with the second inequality in (3.11) implies that $Z'(\xi) > U'(\xi)$, in contradiction to (3.13). This completes the proof for the special case. The conclusion for the general situation then follows by a continuity argument. ∎

4 The Main Result

The central result is as follows:

Theorem 1 *Given any $\lambda, l > 0$ and $D \in (0, 1]$, the boundary value problem (1.1) − (1.4) has a positive solution.*

The above will be established by a series of Lemmas. As indicated earlier, (3.5) is to be first solved subject to the initial conditions (3.7) ignoring the boundary condition (3.8). We seek to extend the solution to a maximum interval of definition (being a subset of $[0, 1]$) with the requirement that the solution remains positive and bounded (by a suitably chosen number, say 2). Three possibilities exist:

(E1) The solution does not attain the value $z = 2$ and eventually bends down to intersect the x-axis. Let $\sigma_0 \leq 1$ be the first point when $z(\sigma_0) = 0$.

(E2) The solution eventually increases to attain the value $z = 2$. Let $\sigma_1 \leq 1$ be the first point when $z(\sigma_1) = 2$.

(E3) The solution satisfies $0 < z(x) < 2$ for all $x \in [0, 1]$.

We define the "endpoint" of the solution z as the point $(\sigma_0, 0)$, $(\sigma_1, 2)$ or $(1, z(1))$, and denote by σ the value σ_0, σ_1, or 1, respectively, according to one of the three possibilities listed above. Once the endpoint of the solution is determined, we define

$$\delta = z'(\sigma) \tag{4.1}$$

and, with (3.6) in mind, set

$$L = \frac{\gamma\alpha - \frac{\gamma^2}{2}(1 - z(\sigma)^2)}{\lambda}. \tag{4.2}$$

As we vary the parameters λ, α, and γ in the equation, the endpoint changes accordingly. In general, the dependence of the endpoint on these parameters need not be continuous. Such a situation can occur, for example, when a solution $z(x)$ is non-negative and tangential to the x-axis at $\sigma_0 < 1$, but otherwise can be extended to the entire interval $[0, 1]$. By varying the parameters slightly, it may be possible to elevate the graph of the solution so that it no longer touches the x-axis. In this way, the endpoint jumps discontinuously from the point $(\sigma_0, 0)$ to a point lying on the vertical line $x = 1$. Lemma 1 shows that this cannot happen with our present equation (3.5).

Lemma 3 *For the possibilities (E1), (E2), z satisfies:*

1. $z'(\sigma_0) < 0$.
2. $z'(\sigma_1) > 0$.

As a consequence, the endpoint, the derivative $z'(\sigma)$ at the endpoint, and the value L are all continuous functions of the parameters λ, α and γ.

Proof. For the case (E1), we know that $z'(\sigma_0) \leq 0$, so that it is only necessary to show that $z'(\sigma_0) \neq 0$. Suppose that this is false. Then $z(\sigma_0)$ is a local minimum (when considered in the left neighbourhood of σ_0), implying that $z''(\sigma_0) \geq 0$. But from (3.2), we have $z''(\sigma_0) = -\alpha < 0$, a contradiction.

For the case (E2), let $x_0 \in [0, \sigma_1]$ be where $z(x)$ attains its minimum. Clearly, x_0 cannot be σ_1. So $x_0 < \sigma_1$. At x_0, $z'(x_0) = 0$ and $z''(x_0) \geq 0$. In $[x_0, \sigma_1]$, $z(x)$ is increasing. By Lemma 1, $z''(x) > z''(x_0) \geq 0$ for all $x \in (x_0, \sigma_1]$ and the desired conclusion follows.

Next, let us indicate how the continuous dependence of the endpoint on α and γ may be established. For the case (E3), this is just the classical result of continuous dependence of a solution on parameters. For the case (E1), $z(\sigma_0) = 0$ and $z'(\sigma_0) < 0$. The solution can then be continued to a small neighborhood of $x = \sigma_0$, with $z(x) < 0$ for $x > \sigma_0$. Let us take two points $\xi_1 < \sigma_0 < \xi_2$, both of them are very close to σ_0. Then $z(\xi_1) > 0$ and $\zeta(\xi_2) < 0$. If we vary λ, α, and/or γ very slightly, it can be ensured that $\bar{z}(\xi_1)$ is still > 0

and $\bar{z}(\xi_2)$ is still < 0. Here, $\bar{z}$ denotes the solution of the initial value problem using the new parameters. By the Intermediate Value Theorem, $\bar{z}$ has a zero in $[\xi_1, \xi_2]$ and thus it is very close to the original zero σ_0 of z. The case (E2) can be handled in a similar manner. ∎

We can now define the continuous operator $T : \mathbb{R}^2 \to \mathbb{R}^2$ by

$$T(\alpha, \gamma) := (\delta, L) = (z'(\sigma), L). \tag{4.3}$$

For the purpose of visualization, we describe the image space as the two-dimensional plane spanned by the δ and L axes (see Figure 2). Note again that, although in the reduction of the original boundary value problem to the new initial value problem, only $\gamma > 0$ is allowed, the new problem can, however, be studied with $\gamma \in (-\infty, \infty)$. Hence, T can be defined even for $\gamma \leq 0$.

If $z'(\sigma) = 0$, then by Lemma 3, we must have case (E3) and $\sigma = 1$. If, furthermore, $L = l$, then (4.2) coincides with (3.6) and z is a solution of the original boundary value problem. Therefore, the validity of Theorem 1 is equivalent to the claim that the operator equation

$$T(\alpha, \gamma) = (0, l) \tag{4.4}$$

has a solution with $\alpha > 0$ and $\gamma > 0$. In what follows, this claim is proved using the topological degree method described in Section 3. We start by establishing:

Lemma 4 *For cases (E2) or (E3), z cannot have more than one local minimum in $[0, 1]$. Assume that $\alpha D \geq \lambda$ and z has a local minimum in $[0, 1)$. Then $\delta > 0$ and $L \geq 0$.*

Proof. If z has a local minimum at a point x_0, then $z''(x) > 0$ for $x > x_0$. Hence, $\delta > 0$ and z cannot have another local minimum beyond x_0. For case (E2), $z(\sigma) = 2$ and from (4.2), we see that $L \geq 0$. If we have case (E3), then $\sigma = 1$. If $z(1) \geq 1$, then (4.2) again gives $L \geq 0$. Now suppose that $z(1) < 1$. On return to the original form of (3.2) and (3.3) and substitution of $x = 1$, we obtain

$$z''(1) = z(1)(\lambda + L\lambda) - \alpha D. \tag{4.5}$$

Since $z''(1) > 0$, it follows that

$$z(1)(\lambda + L\lambda) > \alpha D, \tag{4.6}$$

whence

$$L\lambda > \frac{\alpha D}{z(1)} - \lambda \geq \alpha D - \lambda \geq 0, \tag{4.7}$$

so that, $L \geq 0$. ∎

We now choose any number

$$\alpha^* > \frac{\lambda + l\lambda}{D}, \tag{4.8}$$

and another sufficiently large number γ^*, the value of which will be specified later in Lemma 9. Let $PQRS$ be the rectangle with vertices $P = (\lambda/D, 0)$, $Q = (\alpha^*, 0)$, $R = (\alpha^*, \gamma^*)$, and $S = (\lambda/D, \gamma*)$. Below, we study the image of each the sides of this rectangle under the operator T.

Lemma 5 *$T(A) = (\delta, 0)$, with $\delta < 0$ for every point $A = (\alpha, 0)$ on the line PQ. In particular, the point P is mapped to $P' = (0, 0)$ and $P'Q'$, the image of PQ, is a line segment contained in the negative part of the δ-axis (see Figure 2).*

Proof. When $\gamma = 0$, the differential equation (3.5) reduces to $z''(x) = \lambda z - \alpha D$ while $L = 0$. The assertions of the Lemma are readily verified. In particular, for the point P, $\alpha = \lambda/D$ and $z(x) = 1$ is the solution of the initial value problem. It follows that $T(P) = (0, 0)$. It is seen that when α increases from P to Q, the corresponding value $z'(\sigma)$ decreases and is negative. Accordingly $T(A)$ lies on the negative part of the δ-axis. ∎

The next Lemma shows that if $z(x)$ satisfies also the boundary condition (3.8) at $x = 1$, then z must be a decreasing function and the only critical points are $x = 0$ and $x = 1$. Note that by Lemma 3, (3.8) implies that we are in case (E3).

Lemma 6 *Suppose $\gamma \geq 0$. If the positive function $z(x)$ also satisfies (3.8), then $z'(x) \leq 0$ for all $x \in [0, 1]$, $z''(0) \leq 0$, and $z''(1) \geq 0$.*

Proof. If $\gamma = 0$, then z can only satisfy (3.8) in the trivial case when $\alpha = \lambda/D$ and $z \equiv 1$. Hence, we may assume that $\gamma > 0$. By Lemma 4, $z(x)$ cannot have a local minimum in [0,1), for otherwise $\delta > 0$, contradicting (3.8). Hence, $x = 1$ is the only local minimum. As a consequence, $z(x)$ is a decreasing function in $[0, 1]$. The conclusions $z''(0) \leq 0$ and $z''(1) \geq 0$ follow from the fact that $x = 0$ is a maximal critical point and $z = 1$ is a minimal critical point. ∎

Lemma 7 *Let A be a point on the line QR and $T(A) = (\delta, L)$. If $\delta = 0$, then $L > l$.*

Proof. Since $A = (\alpha, \gamma)$ lies on QR, $\alpha = \alpha^*$. If $\delta = 0$, then we have case (E3) and the endpoint must be $(1, z(1))$. From Lemma 6, $z''(1) \geq 0$, $z(1) \leq 1$. Adopting the same arguments in the proof of Lemma 4, it is seen that at $x = 1$,

$$z''(1) = z(1)(\lambda + L\lambda) - \alpha^* D, \tag{4.9}$$

whence

$$L\lambda \geq \frac{\alpha^* D}{z(1)} - \lambda > \alpha^* D - \lambda > l\lambda, \tag{4.10}$$

from the definition of α^* (3.4), and so $L > l$. ∎

Let us interpret the conclusion of this Lemma geometrically (see Figure 2). The image of the line QR under T is a curve $Q'R'$ in the (δ, L) plane. Below, it will be shown that, once γ^* has been suitably chosen, the image point R' lies in the first quadrant of the plane, $\delta > 0$, $L > 0$. The curve will, therefore, intersect the positive δ-axis at one or more points, but all of them must lie above the point $(0, l)$. In Figure 2, one such curve $Q'R'$ is depicted. Note that the curves $P'Q'$, $Q'R'$, $R'S'$, and $S'P'$ in Figure 2 do not represent actual curves computed from a numerical solution of the initial value problem. Rather, these curves are drawn only to satisfy the assertions of the various Lemmas, but otherwise arbitrarily.

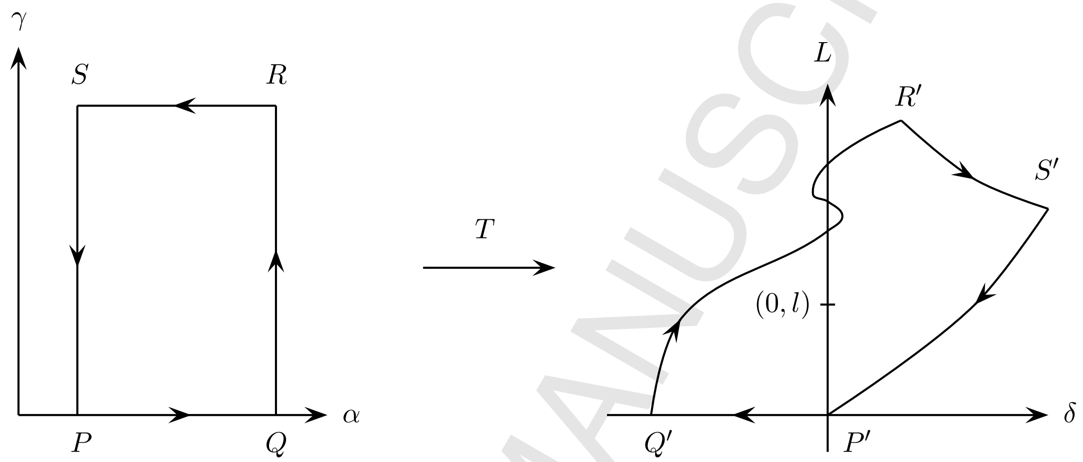

Figure 2:

Next we consider the line SP.

Lemma 8 *The image, $S'P' = T(SP)$, of the line SP lies in the first quadrant. Furthermore, except for the point P', no other points of the curve $S'P'$ lie on the L-axis.*

Proof. On the line SP, $\alpha = \lambda/D$ and $z(x)$ satisfies the differential inequality

$$z''(x) \geq \left\{\lambda - \frac{\gamma^2}{2}(1 - z(x)^2)\right\} z(x) - \lambda \tag{4.11}$$

Using Lemma 2, it is readily seen that $z(x) \geq W(x) \equiv 1$. Hence, $x = 0$ is a local minimum and the desired conclusion follows from Lemma 4. ∎

The next Lemma deals with the remaining side RS of the rectangle.

Lemma 9 *Provided that γ^* is chosen large enough, the image of RS is contained in the first quadrant of the (δ, L) plane.*

Proof. According to Lemma 4, it only remains to show that z has a local minimum at some $x_0 < 1$, or equivalently that, $z'(x_0) = 0$.

By Lemma 8, we already know that S' is in the first quadrant. So it may be assumed that the point A on RS under consideration is different from S. In other words, we can assume $\alpha > \lambda/D$. This implies that z is initially decreasing near $x = 0$. If $z(\xi) = 1$ for some $\xi > 0$, then z must have a local minimum in $(0, \xi)$ and we are done. Hence, we may assume that $z(x) \leq 1$ or all $x \in [0, 1]$. We will show below that this cannot happen if γ^* is sufficiently large.

Let us suppose the contrary, and that we do have $z(x) \leq 1$ for all x. For points on RS, $\gamma = \gamma^*$, and then

$$\frac{\gamma^{*2}}{2}(1 - z(x)^2)z \leq \gamma^{*2}(1 - z(x)) \tag{4.12}$$

and z satisfies the differential inequality

$$\begin{aligned} z''(x) &\geq -\gamma^{*2}(1 - z(x)) + (\lambda + \gamma^*\alpha x)z(x) - \alpha D \\ &\geq -\gamma^{*2}(1 - z(x)) + (\lambda + \gamma^*\alpha x)z(x) - \alpha. \end{aligned} \tag{4.13}$$

The fact $D \leq 1$ is used above to obtain the second inequality and is the key to why Theorem 1 cannot hold for all $D \in (0, \infty)$.

We show below that if γ^* is chosen large enough, then $z(x)$ will remain close to 1 for all x. In particular, we make the assumption (to be justified later) that

$$z(x) \geq m := \frac{2\alpha^* + \lambda}{2(\alpha^* + \lambda)}. \tag{4.14}$$

Then it follows from (4.13) that

$$z''(x) \geq -\gamma^{*2}(1 - z(x)) + (\lambda + \gamma^*\alpha x)m - \alpha. \tag{4.15}$$

Let $W(x)$ solves the initial value problem

$$W''(x) = -\gamma^{*2}(1 - W(x)) + (\lambda + \gamma^*\alpha x)m - \alpha, \tag{4.16}$$

$$W(0) = 1, \quad W'(0) = 0. \tag{4.17}$$

Then, by Lemma 2, $z(x) \geq W(x)$ and $z'(x) \geq W'(x)$. If we can show that $W(x) \geq m$, then (4.14) will be verified, and if it can be shown that $W(1) \geq 1$, then $z(1) \geq 1$ and the desired contradiction follows.

In fact, $W(x)$ can be explicitly computed to give

$$W(x) = 1 + C_1 e^{\gamma^* x} + C_2 e^{-\gamma^* x} - R(x) \tag{4.18}$$

where C_1 and C_2 are constants and $R(x)$ is a linear function of x given in turn by

$$\begin{aligned} C_1 &= \frac{(\lambda+\alpha)m-\alpha}{2\gamma^{*2}} \\ &= \frac{\lambda(2\alpha^*+\lambda-\alpha)}{4\gamma^{*2}(\alpha^*+\lambda)}, \end{aligned} \tag{4.19}$$

$$C_2 = \frac{(\lambda-\alpha)m-\alpha}{2\gamma^{*2}}, \tag{4.20}$$

$$R(x) = \frac{1}{\gamma^*}\left[\alpha m x + \frac{\lambda m-\alpha}{\gamma^*}\right]. \tag{4.21}$$

With the appearance of γ^* in the denominators, $|C_2|$ and $|R(x)|$ can be made arbitrarily small by choosing γ^* large enough. Hence, the last two terms in the right-hand side of (4.18) can be made as small as necessary. On the other hand, because $\alpha < \alpha^*$,

$$C_1 \geq \frac{\lambda}{4\gamma^{*2}} > 0. \tag{4.22}$$

Hence the term $C_1 e^{\gamma^* x}$ on the right-hand side of (4.18) is positive. We can therefore make $W(x) > m$ for all x by choosing γ^* large enough and (4.14) is justified.

At $x = 1$, the term $C_1 e^{\gamma^* x}$ is greater than $\dfrac{\lambda e^{\gamma^*}}{4\gamma^{*2}}$ which $\to \infty$ as $\gamma^* \to \infty$. Hence $W(1) \to \infty$ as $\gamma^* \to \infty$, contradicting our assumption that $z(x) \leq 1$ for all $x \in [0,1]$. This complete the proof of the Lemma. ∎

Combination of Lemmas 5, 7, 9, and 8, provides adequate knowledge about the image of the boundary of the rectangle $PQRS$ to allow us to conclude that the winding number of the closed curve $P'Q'R'S'P'$ with respect to the point $(0,l)$ is -1. This fact can be rigorously justified using homotopic deformation of the image of the boundary of $PQRS$ under T. We omit the details. Hence, the operator equation (4.4) has a solution (α,γ) in the interior of the rectangle $PQRS$, which is equivalent to the existence of a solution to the original boundary value problem. The proof of our main result is thus complete.

Remark: By more carefully tracking the parameter D in the calculations, one can actually show that Lemma 9 holds for values of D slightly larger than 1. More precisely, we can prove that Lemma 9, and hence also Theorem 1, remains valid when $D \leq \sqrt{(l+1)^2+1} - l$. We are not going to pursue in that direction, but leave the details to the readers.

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Appendix I

A Numerical Algorithm

No numerical treatment of the two-ion boundary value problem (1.1) $-$ (1.4) has been undertaken in the literature and our topological existence proof does not lead directly to a practical algorithm. Preliminary numerical studies of the problem (with $D = 1$) are presented below. The algorithm is implemented in MATLAB.

The procedure adopted was as follows:

1. Create a global variable `gamma` (corresponding to γ). Define a function (using a MATLAB script file, the so-called `.m` file) `delta(a)` that takes the input value `a` (corresponding to α), solves the initial value problem (3.5) and (3.7), with $\alpha =$ `a` and $\gamma =$ `gamma`, and returns the value of $\delta = z'(\sigma)$.
2. Use a nonlinear equation solver, such as `fzero` or `bisection` (which uses the bisection method and is available in the public domain) to solve the equation `delta(a) = 0`. The pair of values `(gamma, a)` will then be associated with a solution $z(x)$ of the boundary value problem (3.5), (3.7), and (3.8).
3. For each pair (`gamma, a`), compute the value `L` using the formula (4.2).
4. Considering `L` as the image of `gamma` under a nonlinear function, we can once again use an equation solver to find a suitable `gamma` so that `L =` l.
5. Scale z by `gamma` (and D if necessary) to recover the solution y of the original boundary value problem (1.1) $-$ (1.4).

In Step 2, we mention that `gamma` needs to be a global variable. This is because in MATLAB, parameters that appear in a differential equation cannot be passed directly as function arguments to the script file that defines the differential equation. Either we have to modify the script file every time a parameter value is changed or we let the script file access the value of a variable parameter via a global variable. In fact, we also need to create a global variable `alpha` for the parameter α used in the differential equation.

In Step 2, we make use of a convenient feature of the MATLAB ode solvers, such as `ode45`, namely, one can specify a set of *events* to instruct the solver to stop when one of the events becomes true. In our situation, the events arise when $z(x)$ becomes 0 and when $z(x)$ becomes 2. This directs the solver to stop right at the endpoint. What would happen if the *events* feature is not invoked? In the case of (E1), $z(x)$ becomes negative but the solver will not detect that and still return the value $z'(1)$, which will not be what we want. In the case of (E2), there is a possibility that the solution blows up at a point before reaching $x = 1$ and the solver will become broken. What can be done if an ode solver does not have this *events* feature? An alternative is to modify the differential equation by "truncating" the nonlinear function f. For example, one can redefine $f = -\alpha$ when $z \leq 0$, and replace the power z^2 by $(\min(z, 2))^2$.

In Step 3, the existence of an `a` that solves `delta(a) = 0` for any given `gamma` can be readily proved using a one-dimensional shooting method. One can even show that `a` depends continuously on `gamma`. In practice, the equation solver, however, can become unstable and fail to converge when γ is very large. Extra precaution has to be taken to check for the exit status to make sure that the solver succeeds. The solver requires the input of either an initial guess or an initial bounding interval, a good choice of these can help with the convergence. The error tolerance of the ode solver and the equation solver may also need to be fine-tuned to ensure greater accuracy. In our experiments, for example, with $\lambda = 1$ and `gamma` > 50, the computed `a` and `L` start to become unreliable. An asymptotic analysis is suggested here.

Numerical results indicate that the dependence of `a` on `gamma` is always monotone and so the corresponding mapping is one-to-one, and the inverse mapping exists and is continuous. However, we are not able to confirm this theoretically and would like to raise this as a conjecture, as follows:

Conjecture *For each given $\gamma > 0$, there exists one and only one α such that the associated $z(x)$ of the initial value problem (3.5) and (3.7) also satisfies the boundary condition (3.8). The mapping from γ to α is continuous. The value L derived from α is also a monotone function of γ. This last statement is equivalent to the assertion that the original boundary value problem has a unique solution.*

If this conjecture is true, then in Step 5, we can assert that `L` is a continuous function of `gamma` and the existence of a suitable `gamma` that gives `L =` l is guaranteed. This amounts to an alternative proof of our main result Theorem 1 without resort to topological degree theory.

Figures 3 and 4 depict the numerical result of one of our experiments, with $\lambda = 1$. Figure 3 shows the graph of `a` as a function of `gamma`, which is monotone and `a` $\to \infty$ as `gamma` $\to \infty$. Figure 4 shows the graph of `L` as a function of `gamma`, which again appears to be monotone. Note also that `L` $\to 0$ as `gamma` $\to 0$ and `L` $\to \infty$ as `gamma` $\to \infty$. Hence, `L` traverses every possible value of l.

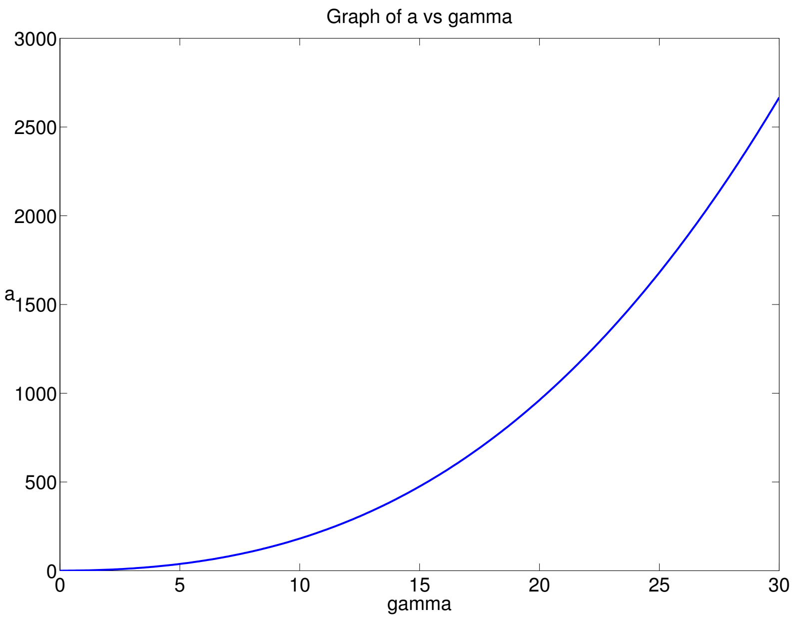

Figure 3.

γ	α	L	γ	α	L
0	1.000000	0.0000			
1	1.677795	1.4797	16	34.697209	301.0864
2	2.800175	3.8542	17	37.871820	356.6989
3	4.238718	7.0153	18	41.158186	418.6787
4	5.857366	11.1617	19	44.554830	487.3320
5	7.599814	16.7386	20	48.060433	562.9621
6	9.455765	24.2675	21	51.673750	645.8692
7	11.428326	34.2531	22	55.393610	736.3500
8	13.523144	47.1657	23	59.218899	834.6981
9	15.742717	63.4256	24	63.148613	941.2052
10	18.087400	83.4176	25	67.181818	1056.1613
11	20.556212	107.5023	26	71.317598	1179.8524
12	23.147429	136.0246	27	75.555081	1312.5623
13	25.858967	169.3175	28	79.893436	1454.5766
14	28.689080	207.7120	29	84.331872	1606.1723
15	31.635753	251.5289	30	88.869631	1767.6262

Table 1.

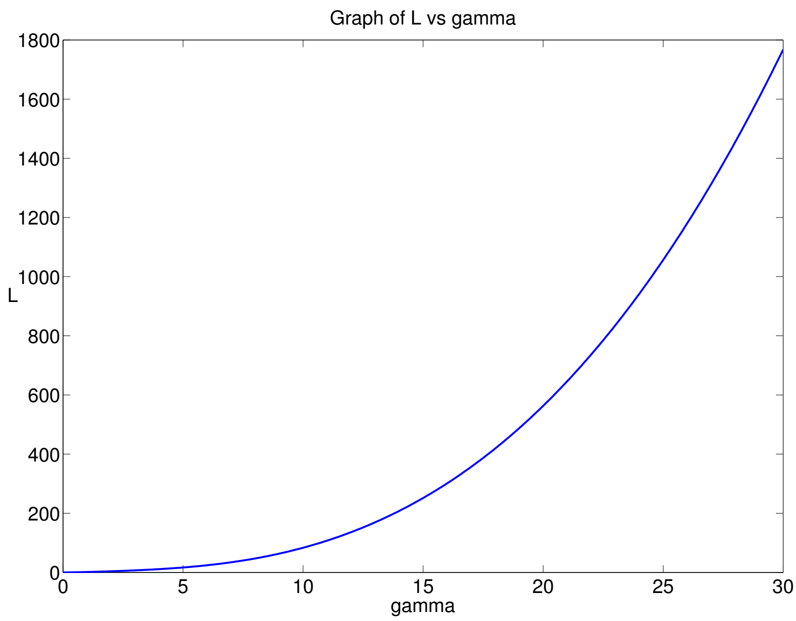

Figure 4.

Appendix II

Numerical Results for $D > 1$

We can apply the same algorithm to the problem when the parameter D takes a value greater than 1. Figures 5 and 6 depict the results for $D = 2$ corresponding to those of Figures 3 and 4, respectively. We have kept $\lambda = 1$. Note that `a` still depends on `gamma` continuously and monotonically. However, Figure 6 shows that `L` is no longer monotone in `gamma`. There exist a maximum value $L^* = M(l)$ that `L` can reach. In other words, there will be no solution to the boundary value problem if $l > L^*$. This is equivalent to saying that a Thompson-type condition has to be imposed to ensure the existence of a solution. Another implication of the shape of the curve is that, in general, for some given values of l there can be two different solutions. It would be interesting if all these observations can be verified rigorously.

One may be curious to find out why the same proof for Theorem 1 would not work for $D > 1$. Which argument breaks down? In fact, all the Lemmas in Section 3 except Lemma 9 still hold. It is, however, interesting to note that even though Lemma 7 is theoretically valid, for α^* sufficiently large, it holds in a void context. The conclusion of the Lemma is a conditional assertion: *If* the image curve $Q'R'$ intersects the δ-axis, then at the intersection point, $L > 0$. The truth is that for $D > 1$ the curve $Q'R'$ may not intersect the δ-axis at all.

For Lemma 9, a differential inequality for $z(x)$ similar to (4.15) and the corresponding differential equation (4.16) for W still hold, except that there is now a factor 2 in the first term of the righthand sides. The extra factor 2 lends more weight for the negative first term which tends to bend the graph of W downwards, so that the conclusions $W(x) > m$ and $W(1) > 1$ cannot be established. This is manifested in the fact that in the explicit expression (4.18), the constant C_1 is no longer positive.

If we try to construct a geometric visualization analogous to Figure 2 for $D > 1$. We will see that the curve $Q'R'$ will be contained in the fourth quadrant and so it will not cross the δ-axis. Instead, the curve $R'S'$ is going to intersect the δ-axis. But since $R'S'$ is not subjected to Lemma 7, the intersection point can be below the point $(0, l)$. In this way, the topological degree of the T about $(0, l)$ will be zero and the operator equation $T(\alpha, \gamma) = (0, l)$ may is not guaranteed to have a solution.

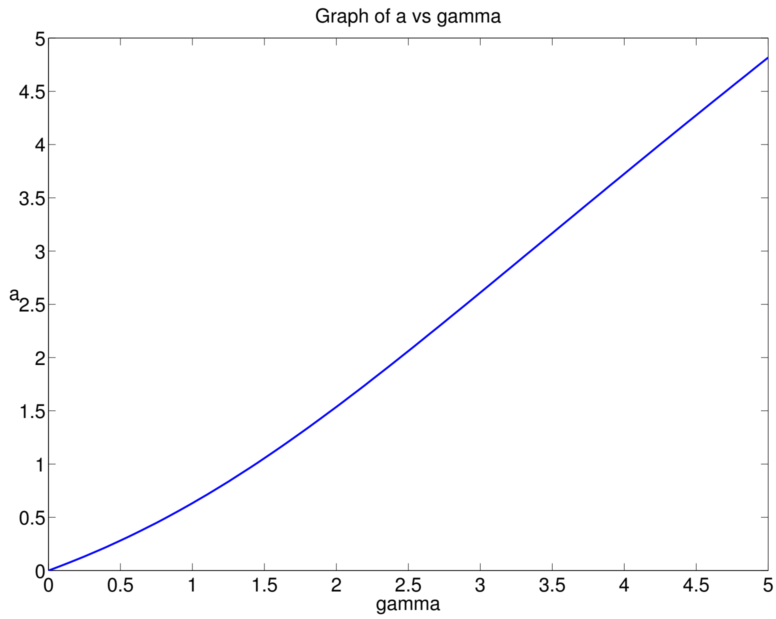

Figure 5.

γ	α	L	γ	α	L
0.0	0.50000000	0.00000000	2.6	0.83442709	0.92754486
0.2	0.52401700	0.10417835	2.8	0.85305764	0.89139118
0.4	0.54967282	0.21474765	3.0	0.86997720	0.83651922
0.6	0.57663579	0.32840002	3.2	0.88523042	0.76389767
0.8	0.60451674	0.44151195	3.4	0.89888922	0.67469821
1.0	0.63289484	0.55036737	3.6	0.91104568	0.57022646
1.2	0.66134453	0.65137562	3.8	0.92180564	0.45186035
1.4	0.68945964	0.74125805	4.0	0.93128306	0.32099735
1.6	0.71687256	0.81718776	4.2	0.93959513	0.17901140
1.8	0.74326732	0.87687753	4.4	0.94685842	0.02721954
2.0	0.76838679	0.91861941	4.6	0.95318583	-0.13314215
2.2	0.79203501	0.94128393	4.8	0.95868432	-0.30093427
2.4	0.81407552	0.94428861	5.0	0.96345348	-0.47512266

Table 2.

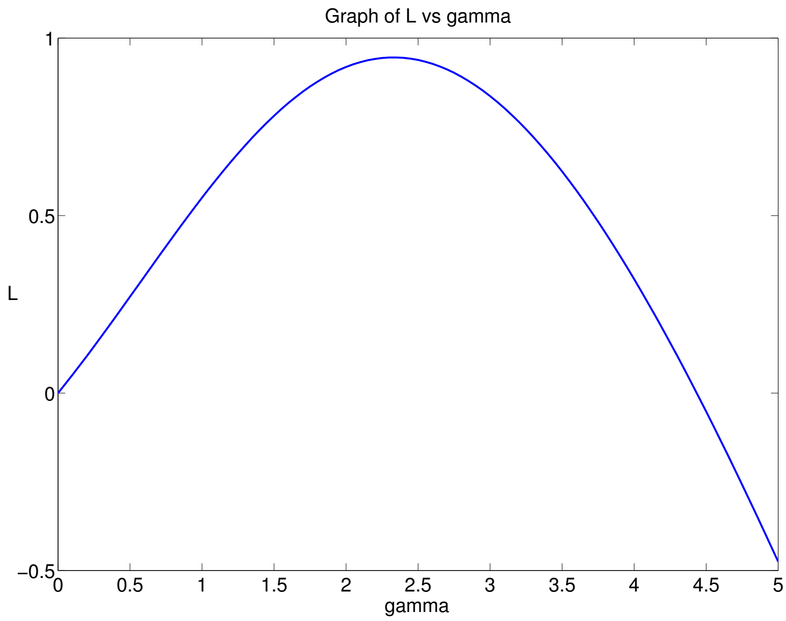

Figure 6.