SELF-SIMILAR SOLUTIONS FOR INFILTRATION OF DOPANT INTO SEMICONDUCTORS

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1. Introduction

The study of diffusion of dopant in semiconductors leads to a pair of nonlinear diffusion equations which is coupled in the highest order term. Following the model developed by Zahari & Tuck [ZT] and Hearne [H] to describe the jumping of impurity atoms and host atoms between neighbouring lattice planes in a crystal, one arrives at the set of equations

$$\frac{\partial c}{\partial t} = \frac{D_c}{v^*}\frac{\partial}{\partial x}\Big(v\frac{\partial c}{\partial x} - c\frac{\partial v}{\partial x}\Big) \tag{1.1}$$

$$\frac{\partial h}{\partial t} = \frac{D_h}{v^*}\frac{\partial}{\partial x}\Big(v\frac{\partial h}{\partial x} - h\frac{\partial v}{\partial x}\Big) \tag{1.2}$$

$$c + h + v = L \tag{1.3}$$

in which c, h and v denote the densities of respectively the impurity atom s, the host atoms and the vacancies in the lettice and L the density of the lattice sites. The coefficients D_c and D_h are the diffusivities of the impurity and host atoms and v^* is the equilibrium concentration of the vacancies. The variables t and x denote time and distance in the direction perpendicular to the lattice planes.

Because L is a constant, (1.3) can be used in (1.2) to eliminate h. In view of (1.1) we eventually find the diffusion equation for v

$$\frac{\partial v}{\partial t} + \Big(1 - \frac{D_h}{D_c}\Big)\frac{\partial c}{\partial t} = D_v\frac{\partial^2 v}{\partial x^2}, \tag{1.4}$$

where $D_v = D_h L/v^*$ is the vacancy diffusivity. In many practical situations $D_h \ll D_c$ so that the coefficient of $\partial c/\partial t$ can be taken to be positive. For a more detailed derivation of these equations we refer to a recent review by King [K].

In this paper we discuss the infiltration of impurities into a semi-infinite slab of semiconductor in which initially there are no impurities ($c = 0$) and the concentration of the vacancies is everywhere equal to its equilibrium value v^*. Thus, we have

$$c(x,0) = 0 \quad \text{and} \quad v(x,0) = v^* \qquad \text{for } \; x > 0. \tag{1.5}$$

Then, at $t = 0$, the face of the semiconductor ($x = 0$) is exposed to the impurities at a concentration c^*, but the level of the vacancies is kept at the equilibrium value. This yields the boundary conditions

$$c(0,t) = c^* \quad \text{and} \quad v(0,t) = v^* \qquad \text{for } \; t > 0. \tag{1.6}$$

With these initial and boundary conditions, we wish to determine the evolution of the concentration profiles of the impurities and the vacancies in the semiconductor as time progresses.

By introducing the nondimensional variables

$$\tilde{c} = \frac{c}{c^*}, \quad \tilde{v} = \frac{v}{v^*}, \quad \tilde{t} = \frac{t}{T} \text{ and } \tilde{x} = \frac{x}{\sqrt{D_c T}},$$

where T is a representative time scale, (1.1), (1.4), (1.5) and (1.6) reduce to the problem

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(v\frac{\partial c}{\partial x} - c\frac{\partial v}{\partial x}\right) \tag{1.7}$$

$$p\frac{\partial v}{\partial t} + q\frac{\partial c}{\partial t} = \frac{\partial^2 v}{\partial x^2} \tag{1.8}$$

$$c(x,0) = 0 \quad \text{and} \quad v(x,0) = 1 \qquad \text{for } x > 0 \tag{1.9}$$

$$c(0,t) = 1 \quad \text{and} \quad v(0,t) = 1 \qquad \text{for } t > 0 \tag{1.10}$$

in which we have dropped the tildes again and

$$p = \frac{v^*}{L}\frac{D_c}{D_h} \quad \text{and} \quad q = \frac{c^*}{L}\left(\frac{D_c}{D_h} - 1\right)$$

are both positive numbers.

In view of the invariance properties of the problem it is natural to look for a solution in self-similar form. Thus we set

$$c(x,t) = f(\eta) \quad \text{and} \quad v(x,t) = g(\eta),$$

where

$$\eta = \frac{x}{\sqrt{t}}.$$

Then substitution into (1.7) and (1.8) yields a coupled system of ordinary differential equations for f and g:

$$(f'g - fg')' + \frac{1}{2}\eta f' = 0 \tag{1.11}$$

$$g'' + \frac{p}{2}\eta g' + \frac{q}{2}\eta f' = 0, \tag{1.12}$$

whilst the initial conditions (1.9) become

$$f(\infty) = 0 \quad \text{and} \quad g(\infty) = 1. \tag{1.13}$$

Finally, the boundary conditions (1.10) yield for f and g

$$f(0) = 1 \quad \text{and} \quad g(0) = 1. \tag{1.14}$$

The object of this paper is to prove the existence of a solution (f, g) of the two point boundary value problem (1.11) - (1.14) and to establish a few global qualitative properties of the functions $f(\eta)$ and $g(\eta)$ as well as their asymptotic behaviour as $\eta \to \infty$.

To prove existence we shall use a shooting technique, replacing the conditions at infinity by additional conditions at the origin:

$$f'(0) = -\alpha \quad \text{and} \quad g'(0) = -\beta, \qquad \alpha, \beta \in \mathbf{R}. \tag{1.15}$$

Plainly, for every pair (α, β) there exists a unique local solution of (1.11), (1.12), (1.14) and (1.15). We shall show that it is possible to choose α and β in such a way that the resulting solution exists for all $\eta > 0$ and satisfies (1.13). This is done in Sections 2 and 3.

In the course of the proof of existence we shall find that f and g have the following properties:

$$f'(\eta) < 0 \quad \text{for} \quad 0 \le \eta < \infty \tag{1.16}$$

and there exists a number $\hat{\eta} > 0$ such that

$$g'(\eta) \begin{cases} < 0 & \text{for} \quad 0 \le \eta < \hat{\eta} \\ > 0 & \text{for} \quad \hat{\eta} < \eta < \infty, \end{cases} \tag{1.17}$$

so that the qualititive behaviour of f and g is as sketched in Firure 1.

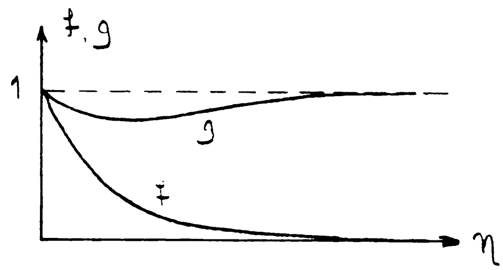

Fig. 1. The functions $f(\eta)$ and $g(\eta)$.

Finally, in Section 4 we shall study the asymptotic behaviour of $f(\eta)$ and $g(\eta)$ as $\eta \to \infty$. We shall show that there exists a constant $P > 0$ such that

$$f(\eta) \sim P\eta^{-1}e^{-\eta^2/4} \quad \text{as} \quad \eta \to \infty$$

and that

$$g(\eta) \sim \begin{cases} 1 + O(\eta e^{-p\eta^2/4}) & \text{if} \quad p < 1 \\ 1 - \dfrac{Pq}{4}\eta e^{-\eta^2/4} & \text{if} \quad p = 1 \\ 1 - \dfrac{Pq}{p-1} e^{-\eta^2/4} & \text{if} \quad p > 1 \end{cases} \quad \text{as} \quad \eta \to \infty.$$

2. Preliminary results

We begin by analyzing the behaviour of the solution (f, g) when (α, β) is chosen in the set

$$\mathcal{D} = \{(\alpha, \beta) : \alpha > 0,\ 0 \le \beta \le \frac{q}{1+q}\alpha\}.$$

For each $(\alpha, \beta) \in \mathcal{D}$ we denote the maximal interval of existence of (f, g) by $[0, \sigma(\alpha, \beta))$ and we write

$$\eta^*(\alpha, \beta) = \sup\{\eta \in (0, \sigma) : f > 0 \text{ on } (0, \eta)\}.$$

Lemma 2.1. *Let* $(\alpha, \beta) \in \mathcal{D}$. *Then*
(a) $f'(\eta) < 0$ *for* $0 \le \eta < \eta^*$;
(b) *if* $\eta^* = \infty$, *then* g' *has a unique zero* $\hat{\eta}$ *in* $(0, \infty)$ *and* $\inf\{g(\eta) : 0 \le \eta < \infty\} > 0$;
(c) *if* $\eta^* < \infty$, *then*

$$f(\eta^*) = 0, \quad f'(\eta^*) < 0 \quad \text{and} \quad g > 0 \text{ on } [0, \eta^*].$$

Proof. (a) Suppose for the sake of contradiction that there exists a point $\eta_0 \in (0, \eta^*)$ such that

$$f' < 0 \quad \text{on} \quad [0, \eta_0) \quad \text{and} \quad f'(\eta_0) = 0. \tag{2.1}$$

We assert that $g > 0$ on $[0, \eta_0)$. Clearly $g > 0$ near $\eta = 0$. Suppose that

$$\eta_1 = \sup\{\eta < \eta_0 : g > 0 \text{ on } [0, \eta)\} < \eta_0.$$

Then, by equation (1.12)

$$g''(\eta_1) = -\frac{p}{2}\eta_1 g'(\eta_1) - \frac{q}{2}\eta_1 f'(\eta_1) > 0.$$

On the other hand, from equation (1.11) we deduce that

$$f(\eta_1)g''(\eta_1) = \frac{1}{2}\eta_1 f'(\eta_1) < 0.$$

Since $f(\eta_1) > 0$ this yields a contradiction and so indeed

$$g(\eta) > 0 \quad \text{for} \quad 0 \le \eta < \eta_0. \tag{2.2}$$

At $\eta = \eta_0$ we have by (1.11)

$$fg'' = f''g \ge 0 \quad \text{since} \quad f'' \ge 0 \text{ and } g \ge 0.$$

Hence, because $f > 0$,

$$g''(\eta_0) \ge 0. \tag{2.3}$$

If we substitute this into (1.12) we obtain

$$g'(\eta_0) \leq 0. \tag{2.4}$$

Now multiply (1.12) by $e^{p\eta^2/4}$. This yields the equation

$$\left(g'(\eta)e^{p\eta^2/4}\right)' = -\frac{q}{2}\eta f'(\eta)e^{p\eta^2/4}.$$

Thus, since $f' < 0$ on $[0, \eta_0)$,

$$\left(g'(\eta)e^{p\eta^2/4}\right)' > 0 \quad \text{on} \quad (0, \eta_0)$$

and hence

$$g'(\eta_0)e^{p\eta_0^2/4} > g'(\eta)e^{p\eta^2/4} \quad \text{for} \quad 0 \leq \eta < \eta_0,$$

which means in view of (2.4) that

$$g'(\eta) < 0 \quad \text{for} \quad 0 \leq \eta < \eta_0. \tag{2.5}$$

On the other hand, if we subtract (1.12) from (1.11) we obtain

$$(f'g - fg')' = \frac{1}{q}g'' + \frac{p}{2q}\eta g',$$

which yields upon integration over $(0, \eta)$, together with the data at $\eta = 0$,

$$f'(\eta)g(\eta) - f(\eta)g'(\eta) = \frac{1+q}{q}\beta - \alpha + \frac{1}{q}g'(\eta) + \frac{p}{2q}\int_0^\eta tg'(t)dt. \tag{2.6}$$

Because $(\alpha, \beta) \in \mathcal{D}$ and $g' < 0$ by (2.5), it follows that the right hand side of (2.6) is negative for all $0 < \eta \leq \eta_0$. In particular, this implies that

$$fg' > f'g = 0 \quad \text{at} \quad \eta = \eta_0,$$

and so, because $f(\eta_0) > 0$,

$$g'(\eta_0) > 0.$$

This contradicts (2.5) and so proves Part (a).

Remark. If $\eta^* < \infty$, then by Part (a), $0 < f(\eta) < 1$ for $0 < \eta < \eta^*$ and it is clear that $\sigma > \eta^*$. On the other hand, if $\eta^* = \infty$, then of course $\sigma = \infty$ as well.

(b) Since $f' < 0$ on $[0, \infty)$ by Part (a), it follows from the argument used to prove (2.2) that

$$g(\eta) > 0 \quad \text{for all} \quad \eta > 0.$$

We assert that g' has a zero. Suppose to the contrary that

$$g'(\eta) < 0 \quad \text{for all} \quad \eta > 0.$$

Then

$$\lim_{\eta \to \infty} g(\eta) \text{ exists } = g(\infty) \geq 0.$$

¿From (1.11) and (1.12) we deduce that

$$f'' > 0 \text{ and } g'' > 0 \quad \text{on} \quad (0, \infty).$$

Hence,

$$\lim_{\eta \to \infty} f'(\eta) \text{ exists } = 0$$

and

$$\lim_{\eta \to \infty} g'(\eta) \text{ exists } = 0.$$

Thus

$$f'g - fg' \to 0 \quad \text{as} \quad \eta \to \infty$$

and we can conclude from (2.6) that

$$0 = \frac{1+q}{q}\beta - \alpha + \frac{p}{2q}\int_0^\infty tg'(t)dt. \tag{2.7}$$

Because by assumption $g'(\eta) < 0$ for all $\eta > 0$, (2.7) implies that $\beta > \frac{q}{1+q}\alpha$ and hence that $(\alpha, \beta) \notin \mathcal{D}$, a contradicition.

Thus, g' has a first zero, that is

$$\hat{\eta} = \sup\{\eta > 0 : g' < 0 \text{ on } [0, \eta)\} < \infty.$$

Suppose it has a second zero. Then at that zero $g'' \leq 0$. However, because $f' < 0$ it follows from (1.12) that at every zero of g',

$$g'' = -\frac{q}{2}\eta f' > 0,$$

so that we have a contradiction. Thus

$$g' > 0 \quad \text{on} \quad (\hat{\eta}, \infty).$$

(c) Suppose $\eta^* < \infty$. We assert that

$$f(\eta^*) = 0.$$

Suppose to the contrary that

$$f(\eta^*) > 0.$$

Then $\eta^* = \sigma$ and this can only be so if

$$g(\eta^*) = 0.$$

Again it follows from equation (1.12) that

$$g'(\eta) < 0 \quad \text{for} \quad 0 \leq \eta < \eta^*$$

and so, by (1.11) and (1.12),

$$f'' > 0 \;\text{ and }\; g'' > 0 \quad \text{on} \quad (0, \eta^*).$$

Thus, because $f'' > 0$,

$$f'(\eta) > -\alpha \quad \text{for} \quad 0 < \eta \leq \eta^*$$

and because $g'' > 0$,

$$\lim_{\eta \to \eta^*} g'(\eta) \text{ exists } = g'(\eta^*).$$

It follows that

$$\begin{aligned}\liminf_{\eta \to \eta^*} (f'g - fg') &\geq \liminf_{\eta \to \eta^*} (-fg') \\ &= |g'(\eta^*)| \liminf_{\eta \to \eta^*} f \\ &\geq 0. \end{aligned} \tag{2.8}$$

On the other hand, because $\beta \leq \frac{q}{1+q}\alpha$ and $g' < 0$, it follows from (2.6) that

$$\liminf_{\eta \to \eta^*} (f'g - fg') \leq \frac{p}{2q} \int_0^{\eta^*} t g'(t) dt < 0. \tag{2.9}$$

Because (2.8) and (2.9) are contradictory it follows that

$$g(\eta^*) > 0 \tag{2.10}$$

and so we can continue (f, g) beyond η^*, i.e. $\eta^* < \sigma$. ¿From this contradiction we conclude that

$$f(\eta^*) = 0. \tag{2.11}$$

Plainly, $f'(\eta^*) \leq 0$ and so to complete the proof of Part (c), we only have to rule out that $f'(\eta^*) = 0$. However, if $f'(\eta^*) = 0$, then the pair of functions $(\tilde{f}, \tilde{g})$ defined by

$$\tilde{f}(\eta) = 0, \quad \tilde{g}(\eta) = \rho(\eta), \qquad \eta \in [0, \infty), \tag{2.12}$$

where ρ is the solution of the problem

$$\rho'' + \frac{p}{2}\eta\rho' = 0, \quad \rho(\eta^*) = g(\eta^*), \quad \rho'(\eta^*) = g'(\eta^*),$$

would be a solution of (1.11) and (1.12). By uniquenesss $(f, g) = (\tilde{f}, \tilde{g})$ on $[0, \infty)$. Because $f(0) = 1 \neq \tilde{f}(0)$, we have reached a contradiction. Therefore we may conclude that $f'(\eta^*) < 0$.

This completes the proof of Lemma 2.1.

In the next three lemmas we further explore the case when $\eta^* = \infty$.

Lemma 2.2. *Let* $(\alpha, \beta) \in \mathcal{D}$ *and* $\eta^* = \infty$. *Then*

$$0 < f(\eta) < \min\{1, g(\eta)\} \quad \text{for all} \quad \eta > 0.$$

Proof. Since $\eta^* = \infty$ and $f' < 0$ on $[0, \infty)$ by Lemma 2.1(a) it follows that

$$0 < f(\eta) < 1 \quad \text{for all} \quad \eta > 0.$$

Thus it remains to show that $f < g$.

Because $f' < 0$, (1.11) yields

$$(f'g - fg')' > 0 \quad \text{on} \quad (0, \infty). \tag{2.13}$$

If we integrate (2.13) over $(\eta, \hat{\eta})$, where $\hat{\eta}$ is the unique zero of g', we obtain

$$f'g - fg' < 0 \quad \text{for} \quad 0 \leq \eta < \hat{\eta}.$$

Because $g' > 0$ on $(\hat{\eta}, \infty)$, we also have

$$f'g - fg' < 0 \quad \text{for} \quad \hat{\eta} \leq \eta < \infty.$$

Hence, since $f > 0$ and $g > 0$ on $[0, \infty)$,

$$\frac{f'}{f} < \frac{g'}{g} \quad \text{on} \quad [0, \infty),$$

or

$$f(\eta) < \frac{f(0)}{g(0)} g(\eta) = g(\eta) \quad \text{for all} \quad \eta > 0.$$

Lemma 2.3. *Let* $(\alpha, \beta) \in \mathcal{D}$ *and* $\eta^* = \infty$. *Then*

(a) $$\lim_{\eta \to \infty} g(\eta) \textit{ exists } = g(\infty);$$

(b) $$g'(\eta) = O(e^{-\kappa \eta^2}) \quad \textit{as} \quad \eta \to \infty$$

for some constant $\kappa > 0$, *and*

(c) $$g(\eta) = g(\infty) + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty.$$

Proof. (a) We use (1.12) to eliminate f' and f'' from (1.11). This yields the equation

$$g''' + \Big\{\frac{p\eta}{2} - \frac{1}{\eta} + \frac{\eta}{2g}(1+qf)\Big\}g'' + \frac{p\eta^2}{4g}g' = 0. \tag{2.14}$$

Setting $y = g''/g'$, which is well defined on the interval $(\hat{\eta}, \infty)$ where $g' > 0$, then turns (2.14) into a Riccati-type equation for y:

$$y' + y^2 + \Big\{\frac{p\eta}{2} - \frac{1}{\eta} + \frac{\eta}{2g}(1+qf)\Big\}y + \frac{p\eta^2}{4g} = 0, \quad \eta > \hat{\eta}. \tag{2.15}$$

Observe that by (1.12), $g''(\hat{\eta}) > 0$. Hence $y > 0$ in a right neighbourhood of $\eta = \hat{\eta}$. We shall show however that y cannot remain positive for all $\eta > \hat{\eta}$. For if $y(\eta) > 0$ for all $\eta > \hat{\eta}$, then by (2.15), $y'(\eta) < 0$ for η large enough so that

$$\lim_{\eta\to\infty} y(\eta) \text{ exists } = \overline{y} \geq 0.$$

It immediately follows from (2.15) that $\overline{y}$ cannot be positive. If $\overline{y} = 0$ then

$$\limsup_{\eta\to\infty} y'(\eta) \leq -\liminf_{p\eta\to\infty} \frac{p\eta^2}{4g(\eta)}. \tag{2.16}$$

Since $g' > 0$ on $(\hat{\eta}, \infty)$ it follows from (2.6) that g' is uniformly bounded on $[\hat{\eta}, \infty)$. This implies that $\eta^2/g(\eta) \to \infty$ as $\eta \to \infty$ and hence, by (2.16) that $y'(\eta) \to -\infty$ and $y(\eta) \to -\infty$ as $\eta \to \infty$. This contradict the positivity of y.

Thus, $y(\eta_1) = 0$ for some $\eta_1 > \hat{\eta}$ and, since by (2.15) $y' < 0$ when $y = 0$, it follows that $y(\eta) < 0$ for all $\eta > \eta_1$. Remembering that $g' > 0$ we conclude that $g'' < 0$ on (η_1, ∞).

We now write (2.6) for $\eta > \eta_1$ as

$$\frac{1}{q}g'(\eta) + \frac{p}{2q}\int_{\eta_1}^{\eta} tg'(t)dt < \alpha - \frac{1+q}{q}\beta - \frac{p}{2q}\int_0^{\eta_1} tg'(t)dt.$$

Because $g'' < 0$ for $\eta > \eta_1$ it follows that

$$g'(\eta)\Big(\frac{1}{q} + \frac{p}{2q}\int_{\eta_1}^{\eta} tdt\Big) < \text{constant} \quad \text{for} \quad \eta > \eta_1$$

and hence that

$$0 < g'(\eta) < C\eta^{-2} \quad \text{for} \quad \eta > \eta_1,$$

where C is some positive constant. Thus $g' \in L^1(\eta_1, \infty)$ and so $g(\eta)$ tends to a finite limit as $\eta \to \infty$.

To prove Part (b) we shall show that there exist constants $M > 0$ and $\tilde{\eta} > \eta_1$, such that

$$y(\eta) < -M\eta \quad \text{for all} \quad \eta > \tilde{\eta}. \tag{2.17}$$

Remembering that $y = g''/g'$ and that $g' > 0$, this implies that

$$\log \frac{g'(\eta)}{g'(\tilde{\eta})} < -\frac{1}{2}M(\eta^2 - \tilde{\eta}^2) \tag{2.18}$$

from which the assertion follows.

To prove (2.17) we introduce the function

$$h(\eta) = y(\eta) + M\eta$$

and we show that $h < 0$ on $(\tilde{\eta}, \infty)$ for some $\tilde{\eta} > 0$. Observe that if $h \geq 0$ and $\eta > \eta_1$, then because $y < 0$,

$$\begin{aligned} h'(\eta) &< -\frac{p\eta^2}{4g(\eta)} + \Big(\frac{p\eta}{2} + \frac{1+q}{2}\frac{\eta}{g(\eta)}\Big)M\eta + M \\ &< -\frac{p\eta^2}{4g(\infty)} + \frac{1}{2}\Big(p + \frac{1+q}{g(\hat{\eta})}\Big)M\eta^2 + M \\ &= -\frac{p\eta^2}{8g(\infty)} + M, \end{aligned} \tag{2.19}$$

if we choose

$$M = \frac{p}{4g(\infty)}\Big(p + \frac{1+q}{g(\hat{\eta})}\Big)^{-1}. \tag{2.20}$$

Set $\eta_2 = 1 + \sqrt{8Mg(\infty)/p}$. Then, if $h(\eta_2) \leq 0$, it follows from (2.19) that $h < 0$ on (η_2, ∞), so that we can take $\tilde{\eta} = \eta_2$. On the other hand, if $h(\eta_2) > 0$ then by (2.19), h must eventually vanish at some $\tilde{\eta} > \eta_2$ and remain negative for all $\eta > \tilde{\eta}$.

Finally, Part (c) is an immediate consequence of Part (b).

We conclude with corresponding estimates for f.

Lemma 2.4. *Let $(\alpha, \beta) \in \mathcal{D}$ and $\eta^* = \infty$. Then*

(a)
$$\lim_{\eta \to \infty} f(\eta) \text{ exists } = f(\infty) \geq 0;$$

(b)
$$f'(\eta) = O(e^{-\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty,$$

where the constant κ has been introduced in Lemma 2.3, and

(c)
$$f(\eta) = f(\infty) + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty.$$

Proof. (a) By Lemma 2.1(a), f is decreasing and by the definition of η^*, f is bounded below by zero. Therefore $f(\eta)$ tends to a nonnegative limit as η tends to infinity.

(b) Using (1.12) we write f' in terms of g' and g'':

$$f'(\eta) = -\frac{p}{q}g'(\eta) - \frac{2}{q\eta}g''(\eta).$$

Thus, since $f' < 0$ on $(0, \infty)$ and $g'' < 0$ on (η_1, ∞)

$$\begin{aligned}|f'(\eta)| &= \frac{p}{q}g'(\eta) + \frac{2}{q\eta}g''(\eta) \\ &< \frac{p}{q}g'(\eta) \qquad \text{for} \quad \eta > \eta_1.\end{aligned}$$

The desired asymptotic estimate now follows from Lemma 2.3(b).

(c) The estimate for $f(\eta)$ as $\eta \to \infty$ follows at once from Part (b).

3. The shooting

With Lemmas 2.1-2.4 in place we are now ready to carry out the shooting argument leading to the existence of a solution. We introduce the sets

$$\begin{aligned}\mathcal{A} &= \{(\alpha, \beta) \in \mathcal{D} : \eta^* < \infty\}, \\ \mathcal{B} &= \{(\alpha, \beta) \in \mathcal{D} : \eta^* = \infty \text{ and } f(\infty) > 0\}.\end{aligned}$$

Note that the set $\mathcal{B}$ is well defined because by Lemma 2.4, if $\eta^* = \infty$ then $f(\infty)$ exists.

Plainly

$$\mathcal{A} \cap \mathcal{B} = \emptyset. \tag{3.1}$$

In the following two lemmas we shall show that $\mathcal{A}$ and $\mathcal{B}$ are nonempty.

Lemma 3.1. *There exists a positive number α_1 such that*

$$\mathcal{D} \cap \{\alpha > \alpha_1\} \subset \mathcal{A}.$$

Proof. The proof relies on a scaling argument. Set $t = \alpha\eta$. Then (1.11) and (1.12) become

$$f''g - fg'' = -\frac{1}{2\alpha^2}tf' \tag{3.2}$$

$$g'' = -\frac{1}{2\alpha^2}t(qf' + pg'), \tag{3.3}$$

where primes now denote differentiation with respect to t. The initial values become

$$f(0)=1,\quad g(0)=1,\quad f'(0)=-1,\quad g'(0)=-\beta/\alpha. \tag{3.4}$$

It is evident that the initial value problem (3.2)-(3.4) is a regular perturbation of the problem

$$f''g-fg''=0 \tag{3.5}$$
$$g''=0 \tag{3.6}$$

$$f(0)=1,\quad g(0)=1,\quad f'(0)=-1,\quad g'(0)=-\theta, \tag{3.7}$$

where $0\le\theta\le 1/2$. The solution (f_0,g_0) of (3.5)-(3.7) is given by

$$f_0(t)=1-t,\quad g_0(t)=1-\theta t.$$

Note that f_0 vanishes at $t=1$ and that $g_0\ge 1-\theta\ge 1/2$ on $[0,1]$. Thus, for large values of α the function $f(t)$ in the solution (f,g) of (3.2)-(3.4) vanishes near $t=1$ so that for those values of α, $(\alpha,\beta)\in\mathcal{A}$.

Lemma 3.2. *There exists a positive number* α_0 *such that*

$$\mathcal{D}\cap\{\alpha<\alpha_0\}\subset\mathcal{B}.$$

Proof. If $\alpha=\beta=0$, the solution of (1.11), (1.12), (1.14) and (1.15) is given by $(f,g)=(1,1)$. Thus, for small values of α and β we may expect the corresponding solution (f,g) to be close to $(1,1)$, at least on bounded intervals. We shall show that this is indeed the case here, even uniformly on the entire half line $[0,\infty)$. Plainly this implies that for sufficiently small values of α and β, $(\alpha,\beta)\in\mathcal{B}$.

For convenience we set

$$f(\eta)=1+u(\eta)\quad\text{and}\quad g(\eta)=1+v(\eta). \tag{3.8}$$

Then after some rearrangement we obtain from (1.11) and (1.12) the following equations for u and v.

$$u''+\frac{\eta}{2}\frac{1+q+qu}{1+v}u'+\frac{\eta}{2}\frac{p+pu}{1+v}v'=0$$
$$v''+\frac{\eta}{2}qu'+\frac{\eta}{2}pv'=0.$$

We can write these equations compactly with $w(\eta)=\mathrm{col}(u(\eta),v(\eta))$ as

$$w''+\frac{\eta}{2}F(w)w'=0, \tag{3.9}$$

where

$$F(w)=A+\rho(w) \tag{3.10}$$

in which

$$A = \begin{pmatrix} 1+q & p \\ q & p \end{pmatrix} \quad \text{and} \quad \rho(w) = O(|w|) \quad \text{as} \quad w \to 0$$

and $|\cdot|$ denotes the Euclidian norm in $\mathbf{R}^2$. For every $p > 0$ and $q > 0$ the eigenvalues λ_1 and λ_2 of A are real, positive and distinct; we shall assume λ_1 to be the smaller one.

Wit the transformation

$$t = \frac{\eta^2}{4}, \quad y(t) = w'(\eta) \quad \text{and} \quad r(t) = \rho(w(\eta))$$

we can reduce (3.9), (3.10) to the familiar form

$$y' + \{A + r(t)\}y = 0,$$

which is equivalent woth the integral equation

$$y(t) = e^{-At}y(0) - \int_0^t e^{-A(t-s)}r(s)y(s)\,ds.$$

By standard theory there exists a constant $K > 0$ such that

$$|e^{-At}\xi| \le K|\xi|e^{-\lambda_1 t} \quad \text{for all} \quad \xi \in \mathbf{R}^2. \tag{3.11}$$

Thus, if we choose constants $\mu \in (0, \lambda_1)$ and $\delta > 0$ such that

$$|\rho(w)\xi| < \frac{\lambda_1 - \mu}{K}|\xi| \quad \text{for all} \quad \xi \in \mathbf{R}^2 \quad \text{if} \quad |w| < \delta, \tag{3.12}$$

then we obtain, using Gronwall's Lemma,

$$|w'(\eta)| \le K|w'(0)|e^{-\mu\eta^2/4} \quad \text{as long as} \quad |w(\eta)| < \delta. \tag{3.13}$$

This yields upon integration over $(0, \eta)$

$$|w(\eta)| \le \sqrt{2}\{|w(0)| + K|w'(0)| \int_0^\eta e^{-\mu\sigma^2/4} d\sigma\}, \tag{3.14}$$

still as long as $|w(\eta)| < \delta$. By choosing $w(0)$ and $w'(0)$ so small that

$$|w(0)| + 2K\sqrt{\frac{\pi}{\mu}}|w'(0)| < \frac{\delta}{\sqrt{2}} \tag{3.15}$$

this can be ensured for all $\eta > 0$. In fact, here $w(0) = 0$. Thus, for sufficiently small values of $w'(0) = -\text{col}(\alpha, \beta)$ the solution (f, g) exists for all $\eta > 0$ so that $\eta^* = \infty$, and $f(\infty) > 0$.

Lemma 3.3. *The sets $\mathcal{A}$ and $\mathcal{B}$ are open in $\mathcal{D}$.*

Proof. The fact that $\mathcal{A}$ is open in $\mathcal{D}$ follows at once from Lemma 2.1(c) and the continuous dependence of (f,g) on (α,β) on bounded intervals.

To prove that $\mathcal{B}$ is open in $\mathcal{D}$, let $(\overline{\alpha},\overline{\beta}) \in \mathcal{B}$ and let $(\overline{f},\overline{g})$ denote the corresponding solution of (1.11), (1.12), (1.14) and (1.15).

As in the proof of Lemma 3.2, we use vector notation, writing $\phi = \mathrm{col}(f,g)$ and $\overline{\phi} = \mathrm{col}(\overline{f},\overline{g})$. The equations (1.11) and (1.12) then become

$$\phi'' + \frac{\eta}{2} G(\phi)\phi' = 0, \tag{3.16}$$

where

$$G(\phi) = \begin{pmatrix} \dfrac{1+qf}{q} & \dfrac{pf}{p} \\ \dfrac{g}{q} & \dfrac{g}{p} \end{pmatrix}.$$

Write

$$f(\eta) = \overline{f}(\infty) + u(\eta) \quad \text{and} \quad g(\eta) = \overline{g}(\infty) + v(\eta).$$

Then

$$G(\phi) = A + \rho(w),$$

where

$$A = \begin{pmatrix} \dfrac{1+q\overline{f}}{q} & \dfrac{p\overline{f}}{p} \\ \dfrac{\overline{g}}{q} & \dfrac{\overline{g}}{p} \end{pmatrix} \quad \text{and} \quad \rho(w) = O(|w|) \quad \text{as} \quad w \to 0,$$

and $w = \mathrm{col}(u,v)$. It is readily verified that the eigenvalues λ_1 and λ_2 of A are real, positive and distinct. The smallest one will be denoted by λ_1.

We now proceed as in the proof of Lemma 3.2 to obtain the estimate

$$|w'(\eta)| \le K|w'(\eta_0)|e^{-\mu(\eta^2-\eta_0^2)/4} \quad \text{as long as} \quad |w(\eta)| < \delta, \tag{3.17}$$

where K, μ and δ are positive constants defined as in (3.11) and (3.12) and η_0 is a positive number to be chosen later. Integration over (η_0,η) then yields as in (3.14)

$$|w(\eta)| \le \sqrt{2}\{|w(\eta_0)| + K|w'(\eta_0)| \int_{\eta_0}^{\eta} e^{-\mu(\sigma^2-\eta_0^2)/4}\, d\sigma \}, \tag{3.18}$$

as long as $|w(\eta)| < \delta$. This can be achieved by choosing $w(\eta_0)$ and $w'(\eta_0)$ so, small that

$$|w(\eta_0)| + \frac{2K}{\mu\eta_0}|w'(\eta_0)| < \frac{\delta}{\sqrt{2}}.$$

This, in turn can be ensured by choosing η_0 sufficiently large and then (α,β) sufficiently close to $(\overline{\alpha},\overline{\beta})$. Thus, if we choose in addition $\delta < \overline{f}(\infty)$ we have shown that $(\alpha,\beta) \in \mathcal{B}$ when (α,β) is sufficiently close to $(\overline{\alpha},\overline{\beta})$.

Corollary 3.4. *The limits $f(\infty)$ and $g(\infty)$ depend continuously on (α, β) in $\mathcal{D} \setminus \mathcal{A}$.*

We are now ready to conclude the existence proof by means of a topological argument due to McLeod & Serrin [McLS], which states that the properties of the sets $\mathcal{A}$ and $\mathcal{B}$ ensure the existence of a continuum $\mathcal{C} \subset \mathcal{D}$ which joins the rays

$$\ell_1 = \{(\alpha, \beta) : \alpha > 0, \ \beta = 0\}$$
$$\ell_2 = \{(\alpha, \beta) : \alpha > 0, \ \beta = \frac{q}{1+q}\alpha\},$$

and has no points with $\mathcal{A}$ and $\mathcal{B}$ in common, that is

$$\mathcal{C} \cap (\mathcal{A} \cup \mathcal{B}) = \emptyset.$$

Lemma 3.5. *Let $(\alpha, \beta) \in \mathcal{C}$. Then*

$$f'(\eta) < 0 \ \textit{ for all } \ \eta \geq 0 \quad \textit{and} \quad f(\infty) = 0.$$

Proof. Because $(\alpha, \beta) \notin \mathcal{A}$, $\eta^* = \infty$ and hence, by Lemma 2.1(a), $f'(\eta) < 0$ for all $\eta \geq 0$. This implies by Lemma 2.4(a) that $f(\infty)$ exists and is nonnegative. If $f(\infty)$ were positive then $(\alpha, \beta) \in \mathcal{B}$ which we know is not true. Therefore $f(\infty) = 0$.

In the following two lemmas we consider the limit $g(\infty)$ on the two rays ℓ_1 and ℓ_2 when $(\alpha, \beta) \in \mathcal{C}$.

Lemma 3.6. *There exists a point $(\overline{\alpha}, 0) \in \mathcal{C}$ such that*

$$g(\infty) > 1.$$

Proof. We have shown in Lemmas 3.1 and 3.2 that there exist numbers $0 < \alpha_0 < \alpha_1 < \infty$ such that

$$\ell_1 \cap \{\alpha < \alpha_0\} \subset \mathcal{B} \quad \text{and} \quad \ell_1 \cap \{\alpha > \alpha_1\} \subset \mathcal{A}.$$

Hence, because the restrictions of $\mathcal{A}$ and $\mathcal{B}$ to ℓ_1 are both open there must be a point $(\overline{\alpha}, 0)$ on ℓ_1 which belongs to $\mathcal{C}$.

¿From equation (1.12) we deduce that $g'(\eta) > 0$ for all $\eta > 0$ and hence that $g(\infty) > 1$.

Lemma 3.7. *There exists a point $(\tilde{\alpha}, \tilde{\alpha}/2) \in \mathcal{C}$ such that*

$$g(\infty) \leq 1.$$

Proof. The fact that there exists a point $(\tilde{\alpha}, \tilde{\alpha}/2)$ on ℓ_2 which belongs to $\mathcal{C}$ follows exactly as in the proof of Lemma 3.6.

¿From (2.6) we obtain when $\beta = \frac{q}{1+q}\alpha$

$$f'(\eta)g(\eta) - f(\eta)g'(\eta) = \frac{1}{q}g'(\eta) + \frac{p}{2q}\int_0^\eta tg'(t)dt.$$

This yields after an integration by parts,

$$f'(\eta)g(\eta) = \{\frac{1}{q} + f(\eta)\}g'(\eta) + \frac{p}{2q}\Big(\eta g(\eta) - \int_0^\eta g(t)dt\Big). \tag{3.21}$$

Suppose that

$$\overline{\eta} = \sup\{\eta > 0 : g < 1 \text{ on } (0,\eta)\} < \infty.$$

Then $g'(\overline{\eta}) \geq 0$ and it follows from (3.21) that

$$f'(\overline{\eta}) > 0.$$

Since $f'(\eta) < 0$ for all $\eta > 0$ we have a contradiction. Thus $g(\eta) < 1$ for all $\eta > 0$ and $g(\infty) \leq 1$.

Because we are looking for a pair $(\alpha, \beta) \in \mathcal{C}$ such that $g(\infty) = 1$, the proof is completed if $g(\infty)$ is continuous on $\mathcal{C}$. This is proved in the following lemma.

Lemma 3.8. *The limit $g(\infty)$ is a continuous function of (α, β) on $\mathcal{C}$.*

Proof. By Corollary 3.4 $g(\infty)$ is a continuous function of (α, β) in $\mathcal{D} \setminus \mathcal{A}$. Because C is a continuum in $\mathcal{D} \setminus \mathcal{A}$ the result follows.

Thus, we have found that there exists a pair $(\alpha^*, \beta^*) \in \mathcal{C}$ so that the corresponding solution (f^*, g^*) has the required behaviour (1.13) at infinity: $f(\infty) = 0$ by Lemma 3.5 because (α^*, β^*) lies in $\mathcal{C}$ and $g(\infty) = 1$ because by Lemmas 3.6, 3.7 and 3.8 we can choose (α, β) in $\mathcal{C}$ so as to ensure this. This completes the proof of the existence of a solution of the problem (1.11) - (1.14).

4. Asymptotic behaviour

In this section we sharpen the asymptotic estimates obtained in Lemmas 2.3 and 2.4 for any solution (f, g) of (1.11) - (1.14):

$$f(\eta) = O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty \tag{4.1}$$

$$g(\eta) = 1 + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty. \tag{4.2}$$

Here κ is some positive constant which, according to (2.18) is given by $\kappa = M/2$, M in turn being given by (2.20). Since $g(\infty) = 1$ and $0 < g(\hat{\eta}) < 1$ it follows that $0 < \kappa < p/\{4(1 + 2q)\}$.

The main result of this section is contained in the following theorem.

Theorem 4.1. *Let (f,g) be a solution of Problem (1.11)-(1.14). Then there exists a constant $P>0$ such that as $\eta\to\infty$*

$$f(\eta)\sim P\eta^{-1}e^{-\eta^2/4},$$

and

$$g(\eta)\sim\begin{cases}1+O(\eta e^{-p\eta^2/4}) & \text{if} \quad p<1\\ 1-\dfrac{Pq}{4}\eta e^{-\eta^2/4} & \text{if} \quad p=1\\ 1-\dfrac{Pq}{p-1}\,e^{-\eta^2/4} & \text{if} \quad p>1.\end{cases}$$

Proof. To establish the asymptotic behaviour of $f(\eta)$ as $\eta\to\infty$ we write equation (1.11) as

$$f''+a(\eta)f'=b(\eta), \tag{4.3}$$

where

$$a(\eta)=\frac{\eta}{2g(\eta)} \quad \text{and} \quad b(\eta)=\frac{f(\eta)g''(\eta)}{g(\eta)}. \tag{4.4}$$

It follows from the asymptotic estimates in Lemma 2.3 and 2.4, together with the differential eqautions, that

$$a(\eta)=\frac{\eta}{2}+O(e^{-\kappa\eta^2}) \quad \text{as} \quad \eta\to\infty \tag{4.5}$$

and

$$b(\eta)=O(e^{-2\kappa\eta^2}) \quad \text{as} \quad \eta\to\infty \tag{4.6}$$

Solving equation (4.3) for f' we obtain

$$f'(\eta)=e^{-A(\eta)}\Big(-\alpha+\int_0^\eta e^{A(s)}b(s)\,ds\Big), \tag{4.7}$$

where

$$A(\eta)=\int_0^\eta a(s)\,ds.$$

Note that

$$\begin{aligned}A(\eta)&=\frac{\eta^2}{4}+\frac{1}{2}\int_0^\eta\Big(\frac{1}{g(s)}-1\Big)s\,ds\\ &=\frac{\eta^2}{4}+K+O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as} \quad \eta\to\infty,\end{aligned} \tag{4.8}$$

where

$$K=\frac{1}{2}\int_0^\infty\Big(\frac{1}{g(s)}-1\Big)s\,ds.$$

Clearly, in view of (4.2), the integral converges.

It follows from (4.6) and (4.8) that

$$e^{A(\eta)}b(\eta) = O(e^{(1-8\kappa)\eta^2/4}) \quad \text{as} \quad \eta \to \infty. \tag{4.9}$$

Therefore, if $8\kappa > 1$, the integral in (4.7) converges and we may conclude that

$$f'(\eta) = O(e^{-\eta^2/4}) \quad \text{as} \quad \eta \to \infty. \tag{4.10}$$

On the other hand, if $8\kappa < 1$, and the integral in (4.7) diverges, we deduce that

$$f'(\eta) = O(e^{-2\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty$$

and

$$f(\eta) = O(\eta^{-1}e^{-2\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty, \tag{4.11}$$

an improvement over (4.1). Using (4.11) rather than (4.1) to estimate $b(\eta)$, we obtain instead of (4.6)

$$b(\eta) = O(e^{-3\kappa\eta^2}) \quad \text{as} \quad \eta \to \infty \tag{4.12}$$

and instead of (4.9)

$$e^{A(\eta)}b(\eta) = O(e^{(1-12\kappa)\eta^2/4}) \quad \text{as} \quad \eta \to \infty. \tag{4.13}$$

If $12\kappa > 1$, (4.10) follows. If $12\kappa < 1$ we can repeat the above argument until after the n^{th} iteration $4(n+2)\kappa > 1$ and (4.10) follows. If at some stage in the process $4(n+2)\kappa = 1$, it is clear that one further iteration yields (4.10).

We can now refine (4.10) by returning to (4.7). Note that by Lemma 2.1, $f'(\eta) < 0$ so that by (4.7)

$$\int_0^\eta e^{A(s)}b(s)\,ds < \alpha \quad \text{for all} \quad \eta > 0.$$

Because $g''(\eta) < 0$ and so $b(\eta) < 0$ for large values of η, the integral is decreasing for large η so that

$$\int_0^\infty e^{A(s)}b(s)\,ds < \alpha \tag{4.14}$$

as well. Thus, because the integral in (4.14) is convergent by (4.10), we may conclude from (4.8) and (4.14) that there exists a constant $P > 0$ such that

$$f'(\eta) \sim -\frac{P}{2}e^{-\eta^2/4} \quad \text{as} \quad \eta \to \infty. \tag{4.15}$$

and consequently

$$f(\eta) \sim P\eta^{-1}e^{-\eta^2/4} \quad \text{as} \quad \eta \to \infty. \tag{4.16}$$

For the asymptotic behaviour of $g(\eta)$ we turn to equation (1.12). Solving it for g' we obtain

$$g'(\eta) = e^{-p\eta^2/4}\Big(-\beta - \frac{q}{2}\int_0^\eta e^{ps^2/4} f'(s)\,ds\Big). \tag{4.17}$$

We now distinguish three cases: $p < 1$, $p = 1$ and $p > 1$.

- When $p < 1$ the integral in (4.17) exists and so

$$g'(\eta) = O(e^{-p\eta^2/4}) \quad \text{as} \quad \eta \to \infty. \tag{4.18a}$$

- When $p = 1$ the integral in (4.17) is $O(\eta^2)$ as $\eta \to \infty$ and we find using l'Hôpital's rule that

$$g'(\eta) \sim \frac{Pq}{8}\eta^2 e^{-\eta^2/4} \quad \text{as} \quad \eta \to \infty. \tag{4.18b}$$

- When $p > 1$ the integral in (4.17) is $O(e^{(p-1)\eta^2/4})$ as $\eta \to \infty$ and we find that

$$g'(\eta) \sim \frac{Pq}{2(p-1)} e^{-\eta^2/4} \quad \text{as} \quad \eta \to \infty. \tag{4.18c}$$

The required estimates for $g(\eta)$ now follow once we integrate (4.18a-c) over (η, ∞). This completes the proof.

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