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**SELF-SIMILAR SOLUTIONS FOR DIFFUSION
IN SEMICONDUCTORS**

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1. Introduction

In this paper we continue our study of a system of nonlinear diffusion equations, initiated in [PT]. The system involved arises from a model for the solid-state diffusion by a substitutional mechanism, developed by Zahari & Tuck [ZT] and Hearne [H]. For a review of this model we also refer to King [K]. The system of equations obtained is

$$\frac{\partial c}{\partial t} = \frac{D_c}{v^*} \frac{\partial}{\partial x} \left(v \frac{\partial c}{\partial x} - c \frac{\partial v}{\partial x} \right) \quad (1.1)$$

$$\frac{\partial h}{\partial t} = \frac{D_h}{v^*} \frac{\partial}{\partial x} \left(v \frac{\partial h}{\partial x} - h \frac{\partial v}{\partial x} \right) \quad (1.2)$$

$$c + h + v = L \quad (1.3)$$

in which c , h and v denote the densities of respectively the impurity atoms, the host atoms and the vacancies in the lattice 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.

The density of the lattice sites L is assumed to be constant. Thus (1.3) can be used to eliminate the concentration h and so reduce the system to one involving two diffusion equations. The resulting equation for v is then

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

in which $D_v = D_h L / v^*$ 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.

In [PT] we discussed the infiltration of dopant into an initially pure semi-infinite slab of semiconductor ($c = 0$) in which the concentration of the vacancies is everywhere equal to its equilibrium value v^* .

In the present paper we also discuss a semi-infinite slab of semiconductor material. However, we now consider one in which dopant has first been implanted. Then, when for instance the material is heated, diffusion sets in and we are interested in the way the concentration profiles of the three constituents develop with time near the surface of the slab, when no dopant can leave or enter the material. Locally, we may take the initial profiles in the slab to be constant. Hence we set

$$c(x, 0) = c_0 \quad \text{and} \quad v(x, 0) = v_0 \quad \text{for} \quad x > 0, \quad (1.5)$$

in which c_0 and v_0 are positive constants. On the surface we assume that the vacancy concentration is kept at a constant value v_1 . Thus, on the face of the slab we have the two

boundary conditions

$$\left(v \frac{\partial c}{\partial x} - c \frac{\partial v}{\partial x}\right)(0, t) = 0 \quad \text{and} \quad v(0, t) = v_1 \quad \text{for} \quad t > 0. \quad (1.6)$$

To simplify the problem we introduce the nondimensional variables

$$\tilde{c} = \frac{c}{c_0}, \quad \tilde{v} = \frac{v}{v_1}, \quad \tilde{t} = \frac{t}{T} \quad \text{and} \quad \tilde{x} = x \sqrt{\frac{v^*}{D_c T v_1}},$$

where T is a representative time scale. We then obtain for (1.1), (1.4), (1.5) and (1.6) the problem

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

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

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

$$\left(v \frac{\partial c}{\partial x} - c \frac{\partial v}{\partial x}\right)(0, t) = 0 \quad \text{and} \quad v(0, t) = 1 \quad \text{for} \quad t > 0 \quad (1.10)$$

in which the tildes have been dropped and

$$p = \frac{v_1}{L} \frac{D_c}{D_h}, \quad q = \frac{c_0}{L} \left(\frac{D_c}{D_h} - 1 \right) \quad \text{and} \quad \sigma = \frac{v_0}{v_1}.$$

Thus p and q are positive numbers and σ may be positive or zero.

In view of the invariance properties of the equations and the data 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

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

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

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

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

whilst the initial conditions (1.9) become

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

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

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

In this paper we shall show that there exists a pair of positive functions (f, g) which satisfies (1.11) and (1.12) for all $\eta \geq 0$ and the boundary conditions (1.13) and (1.14) for any $\sigma > 0$. This is done by means of a shooting technique in which the conditions at infinity are replaced by additional conditions at the origin. It is then shown that these conditions can be chosen in such a way as to yield a solution of the initial value problem which has all the desired properties at infinity.

This shooting method involves a careful analysis of the solutions of the system (1.11), (1.12) which reveals some qualitative properties of solutions of (1.11) - (1.14) such as

(a) *There exists a point $\eta_0 > 0$ such that*

$$\begin{aligned} f' &> 0 \quad \text{on} \quad [0, \eta_0) \quad \text{and} \quad f' < 0 \quad \text{on} \quad (\eta_0, \infty) \quad \text{if} \quad \sigma > 1; \\ f' &< 0 \quad \text{on} \quad [0, \eta_0) \quad \text{and} \quad f' > 0 \quad \text{on} \quad (\eta_0, \infty) \quad \text{if} \quad \sigma < 1. \end{aligned}$$

(b) *We have*

$$\begin{aligned} g' &> 0 \quad \text{on} \quad [0, \infty) \quad \text{and} \quad g'' < 0 \quad \text{on} \quad (0, \infty) \quad \text{if} \quad \sigma > 1; \\ g' &< 0 \quad \text{on} \quad [0, \infty) \quad \text{and} \quad g'' > 0 \quad \text{on} \quad (0, \infty) \quad \text{if} \quad \sigma < 1. \end{aligned}$$

In Figure 1 typical graphs of f and g are sketched for $\sigma > 1$ and $0 < \sigma < 1$.

Fig. 1. Graphs of $f(\eta)$ and $g(\eta)$.

We conclude with an asymptotic analysis of the functions $f(\eta)$ and $g(\eta)$ which yields rates at which they approach their limits $f(\eta) = 1$ and $g(\eta) = \sigma$ when η tends to infinity.

Theorem. *Suppose that (f, g) is a solution of (1.11) - (1.14) for some $\sigma > 0$ ($\sigma \neq 1$). Then there exists a positive constant K such that*

$$\begin{aligned} f(\eta) &\sim 1 - K \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2/4} \quad \text{as} \quad \eta \rightarrow \infty \\ g(\eta) &\sim \sigma + \frac{Kq}{p - \lambda} \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2/4} \quad \text{as} \quad \eta \rightarrow \infty \end{aligned}$$

in which

$$\lambda = \frac{1}{2} \left(p + \frac{1+q}{\sigma} \right) - \frac{1}{2} \sqrt{\left(p + \frac{1+q}{\sigma} \right)^2 - \frac{4p}{\sigma}}.$$

When $\sigma = 1$, problem (1.11)-(1.14) only has the trivial solution $(f, g) = (1, 1)$.

Note that for all positive values of p, q and σ ,

$$0 < \lambda < p,$$

so that the asymptotic behaviour is indeed consistent with the properties (a) and (b) of f and g listed above.

For the flux $f'g - fg'$ we obtain when $\sigma \neq 1$

$$f'(\eta)g(\eta) - f(\eta)g'(\eta) \sim \frac{1}{2} \lambda K \left(\sigma + \frac{q}{p-\lambda} \right) \operatorname{sgn}(1-\sigma) e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty,$$

where K is the constant appearing in the estimates for f and g .

In the next section we prove a series of properties which will be essential in the proof of existence and in determining the asymptotic behaviour of solutions. In Section 3 we prove the existence of a solution when $\sigma > 1$ and in Section 4 we prove existence if $0 < \sigma < 1$. Finally, in Section 5, we establish the asymptotic behaviour of solutions.

2. Properties of solutions

We shall employ a topological shooting argument to prove our results. Thus, we consider the initial value problem for the system (1.11), (1.12) which we write with the function

$$H = f'g - fg'$$

as

$$\begin{cases} H' + \frac{1}{2}\eta f' = 0 & \eta > 0 \end{cases} \quad (2.1)$$

$$\begin{cases} g'' + \frac{p}{2}\eta g' + \frac{q}{2}\eta f' = 0 & \eta > 0. \end{cases} \quad (2.2)$$

At the origin we impose the conditions

$$H(0) = 0 \quad \text{and} \quad g(0) = 1 \quad (2.3)$$

and consistent with [PT] we add the conditions

$$f'(0) = \alpha, \quad g'(0) = \beta, \quad f(0) = \gamma. \quad (2.4)$$

Thus in this problem we have three parameters at our disposal: $\alpha, \beta \in \mathbf{R}$ and $\gamma > 0$, although in order to satisfy condition (2.3) we shall always require that

$$\alpha = \beta\gamma. \quad (2.5)$$

In Section 1 we indicated that the correct regimes for these parameters are

$$\alpha > 0, \beta > 0, 0 < \gamma < 1 \quad \text{if } \sigma > 1 \quad (2.6a)$$

$$\alpha < 0, \beta < 0, 1 < \gamma < \infty \quad \text{if } \sigma < 1. \quad (2.6b)$$

For each choice of (α, β, γ) we denote the maximal interval of existence of the solution (f, g) of (2.1) - (2.4) by $[0, \rho(\alpha, \beta, \gamma))$. Since we are only interested in solutions which make sense physically, that is if $f(\eta) > 0$ and $g(\eta) > 0$ for all $\eta \geq 0$, we define

$$\eta^* = \sup\{\eta \in (0, \rho) : fg > 0 \text{ on } (0, \eta)\}.$$

With these definitions in place we proceed with our analysis.

We begin with a few simple results which justify the choice of the parameter ranges in (2.5) and (2.6).

Lemma 2.1. *We have*

$$H(0) = 0, \quad H'(0) = 0 \quad \text{and} \quad H''(0) = -\frac{1}{2}f'(0).$$

Proof. It follows from (2.1) that $H'(0) = 0$. The third assertion follows from l'Hôpital's rule:

$$H''(0) = \lim_{\eta \rightarrow 0} \frac{H'(\eta)}{\eta} = -\frac{1}{2} \lim_{\eta \rightarrow 0} f'(\eta) = -\frac{1}{2}f'(0).$$

Lemma 2.2. *We have*

$$\begin{aligned} \beta < 0 &\Rightarrow g'(\eta) < 0 \text{ for } 0 \leq \eta < \eta^* \quad \text{and} \quad g''(\eta) > 0 \text{ for } 0 < \eta < \eta^* \\ \beta > 0 &\Rightarrow g'(\eta) > 0 \text{ for } 0 \leq \eta < \eta^* \quad \text{and} \quad g''(\eta) < 0 \text{ for } 0 < \eta < \eta^*. \end{aligned}$$

Proof. First of all, assume that $g'(0) < 0$. This implies by (2.4) that $f'(0) < 0$ as well. Suppose that

$$\eta_0 = \sup\{\eta \in (0, \eta^*) : g' < 0\} < \eta^*.$$

Then

$$0 < g(\eta_0) < 1, \quad g'(\eta_0) = 0 \quad \text{and} \quad g''(\eta_0) \geq 0.$$

But by (2.2),

$$g''(\eta_0) + \frac{q}{2}\eta_0 f'(\eta_0) = 0,$$

so that $f'(\eta_0) \leq 0$. If $f'(\eta_0) = 0$, then by uniqueness $(f(\eta), g(\eta)) = (f(\eta_0), g(\eta_0))$ for all $\eta \geq 0$ so that the initial condition for g would not be satisfied. Thus we have

$$g''(\eta_0) > 0 \quad \text{and} \quad f'(\eta_0) < 0. \quad (2.7)$$

We assert that

$$f'(\eta) < 0 \quad \text{for } 0 \leq \eta \leq \eta_0. \quad (2.8)$$

If not, then by (2.7) f' must change sign on $(0, \eta_0)$ at least twice and so there must exist a point $\eta_1 \in (0, \eta_0)$ such that

$$f'(\eta_1) = 0 \quad \text{and} \quad f''(\eta_1) \leq 0.$$

From (2.1) we conclude that $g''(\eta_1) \leq 0$, which implies by (2.2) that $g'(\eta_1) \geq 0$. This contradicts the definition of η_0 and thus proves (2.8).

It follows from (2.8) that $H' > 0$ on $(0, \eta_0]$. Hence

$$H(\eta_0) > H(0) = 0,$$

and so

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

This contradicts (2.8) and therefore we can conclude that

$$g'(\eta) < 0 \quad \text{for all } \eta \in [0, \eta^*). \quad (2.9)$$

Next we prove the convexity of the graph of g . From (2.2) we deduce that $g''(0) = 0$. However, if we differentiate (2.2) we obtain

$$g''' + \frac{1}{2}(pg' + qf') + \frac{1}{2}\eta(pg'' + qf'') = 0. \quad (2.10)$$

Thus, because $g'(0) < 0$ and $f'(0) < 0$ we see that $g'''(0) > 0$ so that $g''(\eta) > 0$ for η small. Set

$$\hat{\eta} = \sup\{\eta \in (0, \eta^*) : g'' > 0 \text{ on } (0, \eta)\}.$$

To force a contradiction we suppose that $\hat{\eta} < \eta^*$. Then

$$g''(\hat{\eta}) = 0 \quad \text{and} \quad g'''(\hat{\eta}) \leq 0. \quad (2.11)$$

We now compute g''' from (2.10). By (2.2)

$$qf' + pg' = 0 \quad \text{at } \eta = \hat{\eta} \quad (2.12)$$

so that

$$g'''(\hat{\eta}) = -\frac{1}{2}\hat{\eta}qf''(\hat{\eta}). \quad (2.13)$$

By (2.1) we have in turn

$$f''g = -\frac{1}{2}\eta f' \quad \text{at } \eta = \hat{\eta}. \quad (2.14)$$

Because $g' < 0$ by (2.9), it follows from (2.12) that $f' > 0$ and so, from (2.14) that $f'' < 0$. Putting this into (2.13) we find that $g''' > 0$ at $\eta = \hat{\eta}$. This contradicts the inequality in (2.11) and thus completes the proof of the first assertion.

The proof of the second assertion is the same.

The following lemma is an immediate consequence of Lemma 2.2.

Lemma 2.3. *We have*

$$\sigma < 1 \text{ (}>\text{)} \Rightarrow g'(0) < 0 \text{ (}>\text{)}.$$

Remark 1. We have now justified the parameter regimes for $f'(0)$ and $g'(0)$ described by (2.5) and (2.6). We note that if $\sigma = 0$ then necessarily $g'(0) = 0$. For if $g'(0) > 0$ then Lemma 2.3 states that $g'(\eta) > 0$ for all $\eta \geq 0$ so that $g(\infty) = 1$ is impossible. Likewise, if $g'(0) < 0$ then $g(\infty) = 1$ is not possible. If $g'(0) = 0$, then (2.4) implies that $f'(0) = 0$ and it follows by uniqueness that $f' = 0$ and $g' = 0$ on $[0, \infty)$ and so $f = \gamma$ and $g = 1$ for all $\eta \geq 0$. The boundary condition for f at infinity can then only hold if $\gamma = 1$. As we proceed with our analysis it will become evident that (2.6a) and (2.6b) describe the correct range for the values of γ as well.

About the function H we can now prove

Lemma 2.4. *We have*

$$\alpha < 0 \text{ (}> 0\text{)} \Rightarrow H(\eta) > 0 \text{ (< 0)} \text{ for all } \eta \in (0, \eta^*).$$

Proof. Suppose that $\alpha < 0$. Then by Lemma 2.1, $H''(0) > 0$ and hence $H(\eta) > 0$ for $\eta > 0$ small. Suppose, however that $H(\eta)$ vanishes at some $\eta_1 \in (0, \eta^*)$. Suppose η_1 is the first zero of H . Then at η_1 we have

$$H'(\eta_1) \leq 0 \quad \text{and so} \quad f'(\eta_1) \geq 0 \tag{2.15}$$

by (2.1), but also

$$H(\eta_1) = 0 \quad \text{and so} \quad f'(\eta_1)g(\eta_1) = f(\eta_1)g(\eta_1) \geq 0 \tag{2.16}$$

by Lemma 2.2. Plainly (2.15) and (2.16) contradict one another.

The assertion involving $\alpha > 0$ is proved in the same way.

Lemma 2.4 enables us to compare f and g .

Lemma 2.5. *We have*

$$\alpha < 0 \text{ (}>\text{)} \Rightarrow f(\eta) > \gamma g(\eta) \text{ (<)} \text{ for } 0 < \eta < \eta^*.$$

Proof. Suppose that $\alpha < 0$. Then by Lemma 2.4,

$$f'g - fg' > 0 \quad \text{on} \quad (0, \eta^*)$$

and so

$$\log \frac{f(\eta)}{g(\eta)} > \log \frac{f(0)}{g(0)}, \quad (2.17)$$

from which the assertion follows. The one for $\alpha > 0$ is proved the same way.

Lemma 2.6. *Let (f, g) be a solution of (2.1) - (2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then*

$$\begin{aligned} g(\eta) &< 1 + \frac{2\beta}{\sqrt{p}} \arctan\left(\frac{\sqrt{p}}{2}\eta\right) & \text{if } \beta > 0 \\ g(\eta) &> 1 - \frac{2\beta}{\sqrt{p}} \arctan\left(\frac{\sqrt{p}}{2}\eta\right) & \text{if } \beta < 0. \end{aligned}$$

Proof. Suppose that $\beta > 0$. We combine (2.1) and (2.2) to yield

$$H' = \frac{1}{q}g'' + \frac{p}{2q}\eta g'. \quad (2.18)$$

When we integrate this equation over $(0, \eta)$ we obtain, using the initial conditions (2.3) and (2.4)

$$H(\eta) = \frac{1}{q}g'(\eta) - \frac{\beta}{q} + \frac{p}{2q} \int_0^\eta t g'(t) dt \quad (2.19)$$

or

$$g'(\eta) + \frac{p}{2} \int_0^\eta t g'(t) dt = \beta + qH(\eta) < \beta,$$

because by Lemma 2.4, $H(\eta) < 0$ for all $\eta > 0$. Since by Lemma 2.2, $g'' < 0$ we deduce that

$$g'(\eta) \left(1 + \frac{p}{4}\eta^2\right) < \beta.$$

Hence

$$g'(\eta) \leq \frac{4\beta}{4 + p\eta^2} \quad \text{for } \eta \geq 0,$$

so that

$$g(\eta) \leq 1 + \frac{2\beta}{\sqrt{p}} \arctan\left(\frac{\sqrt{p}}{2}\eta\right).$$

The argument for $\beta < 0$ proceeds the same way.

In the following lemma we derive a second bound for f .

Lemma 2.7. *Suppose that $\alpha > 0$ ($<$). Then*

$$f(\eta) > \gamma \quad (<) \quad \text{for all } \eta \in (0, \eta^*).$$

Proof. Suppose that $\alpha < 0$ and assume that

$$\eta_\gamma = \sup\{\eta > 0 : f < \gamma \text{ on } (0, \eta)\} < \eta^*.$$

Then from (2.1) we obtain

$$H(\eta_\gamma) + \frac{1}{2}\eta_\gamma\gamma - \frac{1}{2}\int_0^{\eta_\gamma} f(s) ds = 0.$$

Since

$$\int_0^{\eta_\gamma} f(s) ds < \eta_\gamma\gamma,$$

it follows that

$$H(\eta_\gamma) < 0.$$

However, if $\alpha < 0$, then, by (2.5) $\beta < 0$ and so, by Lemmas 2.3 and 2.4, $H(\eta) > 0$ for all $\eta > 0$. Thus we have arrived at a contradiction.

Lemma 2.7 means in particular that if (f, g) is a solution of (1.11)-(1.14), then

$$\sigma > 1 (< 1) \Rightarrow \gamma < 1 (> 1). \quad (2.20)$$

It also implies that

$$\alpha > 0 \Rightarrow \eta^* = \infty \quad (2.21)$$

because now $f(\eta)g(\eta) > \gamma$ for all $\eta \in (0, \eta^*)$, which implies that $\eta^* = \infty$.

Before we can say more about the shape of the graph of f we need some information about the behaviour of $f(\eta)$ as $\eta \rightarrow \infty$.

Lemma 2.8. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then*

$$(a) \quad \begin{aligned} \lim_{\eta \rightarrow \infty} f(\eta) \text{ exists} &= f(\infty) \\ \lim_{\eta \rightarrow \infty} g(\eta) \text{ exists} &= g(\infty), \end{aligned}$$

$$(b) \quad f'(\eta) \rightarrow 0, \quad g'(\eta) \rightarrow 0 \quad \text{as } \eta \rightarrow \infty,$$

$$(c) \quad H(\eta) \rightarrow 0 \quad \text{as } \eta \rightarrow \infty.$$

Proof. Suppose that $\alpha < 0$. From Lemma 2.2 and the positivity of g we conclude that

$$g(\eta) \rightarrow g(\infty) \quad \text{and} \quad g'(\eta) \rightarrow 0 \quad \text{as } \eta \rightarrow \infty. \quad (2.22)$$

As regards f we note that it has a critical point if H has one. In view of (2.17) and Lemma 2.2 this can only be an isolated maximum. This in turn implies by (2.16) that f can only

have an isolated minimum. Thus either way, f is monotonic for large η . Since by Lemma 2.2 and 2.6

$$\gamma g(\eta) < f(\eta) < \gamma \quad (2.23)$$

it follows that

$$\lim_{\eta \rightarrow \infty} f(\eta) \text{ exists} = f(\infty).$$

Before turning to f' , we consider the limiting behaviour of H . Because $g' < 0$ by Lemma 2.2 it follows from (2.1) and (2.2) that

$$\lim_{\eta \rightarrow \infty} \{H(\eta) - \frac{1}{q}g'(\eta)\} \text{ exists} = L$$

where $L \in [-\infty, \infty)$. This means in view of (2.22) that

$$\lim_{\eta \rightarrow \infty} H(\eta) = L.$$

Because by Lemma 2.4. $H(\eta) > 0$ for all $\eta > 0$, we conclude that $0 \leq L < \infty$.

Remembering (2.22) again, we observe that

$$\lim_{\eta \rightarrow \infty} f'(\eta)g(\eta) = L$$

which, using (2.22) once more, implies that

$$\lim_{\eta \rightarrow \infty} f'(\eta) \text{ exists} = f'(\infty).$$

As we have shown that $f(\infty)$ exists, it follows that $f'(\infty) = 0$. This means that $L = 0$ and hence that $H(\infty) = 0$.

Similar arguments prove the case $\alpha > 0$. We should note for later reference that

$$\gamma < f(\eta) < \gamma g(\eta) \quad \text{for} \quad 0 < \eta < \infty \quad (2.24)$$

in this case.

With the results of Lemma 2.8 we can further describe the graph of f .

Lemma 2.9. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then the graph of f has precisely one isolated critical point: a minimum if $\alpha < 0$ and a maximum if $\alpha > 0$.*

Proof. Since $H(0) = 0$ by (2.5) and $H(\infty) = 0$ by Lemma 2.8, H must have at least one critical point. As we observed before, this must be an isolated maximum (minimum) if $\alpha < 0$ ($\alpha > 0$) and it is therefore unique. Thus, remembering (2.16) we conclude that f has one and only one critical point and that this is a minimum (maximum) if $\alpha < 0$ ($\alpha > 0$).

If $\alpha < 0$ the proof is almost the same, except that to prove that $g(\infty)$ exists we now use the upper bound of Lemma 2.6.

In the following lemma we derive rates of convergence for the limits obtained in Lemma 2.8.

Lemma 2.11. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then there exists a constant $\kappa > 0$ such that*

$$\begin{aligned} (a) \quad & f'(\eta) = O(e^{-\kappa\eta^2}) \quad \text{and} \quad g'(\eta) = O(e^{-\kappa\eta^2}) \quad \text{as } \eta \rightarrow \infty, \\ (b) \quad & f(\eta) = f(\infty) + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as } \eta \rightarrow \infty \\ & g(\eta) = g(\infty) + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as } \eta \rightarrow \infty. \end{aligned}$$

Proof. Suppose $\alpha > 0$. We differentiate (2.2) and use (2.1) to eliminate f' and f'' from the resulting equation. This yields

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

Set $y = g''/g'$. This function is well defined and negative by Lemma 2.2. When we substitute it into (2.22) we obtain a Riccati-type equation in y :

$$y' + y^2 + \left\{ \frac{p\eta}{2} - \frac{1}{\eta} + \frac{\eta}{2g}(1 + qf) \right\} y + \frac{p\eta^2}{4g} = 0. \quad (2.25)$$

We shall show that there exist constants $M > 0$ and $\eta_1 > 0$ such that

$$y < -M\eta \quad \text{for } \eta > \eta_1. \quad (2.26)$$

Indeed, if this is so, then

$$\log \frac{g'(\eta)}{g'(\eta_1)} < -\frac{1}{2}M(\eta^2 - \eta_1^2) \quad \text{for } \eta > \eta_1,$$

from which the assertion about g' follows.

To prove (2.26) we introduce the function,

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

in which the constant M will be chosen later, and we shall show that $h < 0$ on (η_1, ∞) for some $\eta_1 > 0$. Observe that if $h \geq 0$ and $\eta > 0$. Then because $y < 0$,

$$\begin{aligned} h'(\eta) &< -\frac{p\eta^2}{4g(\eta)} + \left\{ \frac{p\eta}{2} + \frac{1 + q\gamma g(\infty)}{2} \frac{\eta}{g(\eta)} \right\} M\eta + M \\ &< -\frac{p\eta^2}{4g(\infty)} + \frac{1}{2}(p + q\gamma g(\infty) + 1)M\eta^2 + M \\ &< -\frac{p\eta^2}{8g(\infty)} + M \end{aligned} \quad (2.27)$$

if we choose $M = p/\{4g(\infty)(p + q\gamma g(\infty) + 1)\}$. It follows from (2.27) that $h(\eta) < 0$ for η large enough. This completes the estimate for g' .

To estimate f' , we use (2.2), which we write as

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

Recall that when $\alpha > 0$, $g' > 0$, $g'' < 0$ on $(0, \infty)$ and $f' < 0$ on (η_2, ∞) for some $\eta_2 > 0$. Hence

$$|f'| = \frac{p}{q}g' + \frac{2}{q\eta}g'' < \frac{p}{q}g' \quad \text{for } \eta > \eta_2.$$

from which the desired estimate follows.

Integrating f' and g' over (η, ∞) we obtain the remaining estimates.

When $\alpha < 0$, the proof is exactly the same. The only possible difficulty arises in (2.27) when $g(\infty) = 0$. However, $g < 1$ in this case, so that (2.27) simplifies to

$$\begin{aligned} h'(\eta) &< \frac{1}{g(\eta)} \left\{ -\frac{p\eta^2}{4} + \frac{1}{2}[p\eta g(\eta) + (1 + q\gamma)\eta]M\eta + Mg \right\} \\ &< \frac{1}{g(\eta)} \left\{ -\frac{p\eta^2}{4} + \frac{1}{2}(p + q\gamma + 1)M\eta^2 + M \right\} \\ &= \frac{1}{g(\eta)} \left\{ -\frac{p\eta^2}{8} + M \right\} \end{aligned}$$

if we choose $M = p/\{4(p + q\gamma + 1)\}$. Again it follows that $h(\eta) < 0$ for η large enough and the proof continues as in the case $\alpha > 0$.

The asymptotic behaviour of $f(\eta)$ established in Lemma 2.11 enables us to extend Lemma 2.7 to $\eta = \infty$ if $\eta^* = \infty$.

Lemma 2.7a. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then*

$$f(\infty) > \gamma \quad (<) \quad \text{if } \alpha > 0 \quad (<).$$

Proof. Suppose that $\alpha > 0$. Then by Lemma 2.7, $f(\eta) > \gamma$ for all $\eta > 0$ and so $f(\infty) \geq \gamma$. Thus, it remains to prove strict inequality.

Suppose to the contrary that $f(\infty) = \gamma$ and write

$$\varphi(\eta) = f(\eta) - \gamma.$$

Equation (2.1) can then be written as

$$H' + \frac{1}{2}\eta\varphi'(\eta) = 0,$$

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

$$H(\eta) + \frac{1}{2}\eta\varphi(\eta) = \frac{1}{2} \int_0^\eta \varphi(s) ds.$$

If we now let η tend to infinity, the terms on the left hand side tend to zero by Lemmas 2.8 and 2.11. This implies that

$$\int_0^\infty \varphi(s) ds = 0.$$

Because $\varphi(\eta) > 0$ for all $\eta > 0$ by Lemma 2.7, this is impossible and we must conclude that $f(\infty) > \gamma$.

When $\alpha < 0$ the argument is the same.

3. The shooting: $\sigma > 1$

We are now ready to carry out the shooting arguments leading to the existence of a solution. In this section we shall consider the case $\sigma > 1$, and in Section 4, the details are given for $0 < \sigma < 1$.

We shall find it convenient to work with the parameters β and γ which leaves α determined via (2.5). Thus, we impose the initial values

$$f(0) = \gamma, \quad f'(0) = \beta\gamma \quad \text{and} \quad g(0) = 1, \quad g'(0) = \beta. \quad (3.1)$$

Since we take $\sigma > 1$ in this section, it follows from Lemma 2.3 that we need only consider positive values of β and from (2.21) that $\eta^* = \infty$.

We introduce the sets

$$\mathcal{D}_+ = \{(\gamma, \beta) \in \mathbf{R}^2 : 0 \leq \gamma \leq 1, \beta \geq 0\}$$

and

$$\begin{aligned} \mathcal{A}_+ &= \{(\gamma, \beta) \in \mathcal{D}_+ : g(\infty) < \sigma\} \\ \mathcal{B}_+ &= \{(\gamma, \beta) \in \mathcal{D}_+ : g(\infty) > \sigma\}. \end{aligned}$$

Because by Lemma 2.8 the limit $g(\infty)$ always exists, these sets are well defined.

It is clear that if $\beta = 0$, the solution is given by $(f, g) = (\gamma, 1)$ so that $g(\infty) = 1 < \sigma$. Thus $(\gamma, 0) \in \mathcal{A}_+$ if $0 \leq \gamma \leq 1$ (see Fig. 2.)

Fig. 2. The $\gamma\beta$ -plane ($\sigma > 1$).

In the next lemma we show that on the other hand $(\gamma, \beta) \in \mathcal{B}_+$ if β is large enough.

Lemma 3.1. *There exists a constant $\hat{\beta}$ such that if $0 \leq \gamma \leq 1$ and $\beta > \hat{\beta}$, then $(\alpha, \beta) \in \mathcal{B}_+$.*

Proof. We use a scaling argument and set $t = \beta\eta$. Then (2.1) and (2.2) become

$$f''g - fg'' = \frac{1}{2\beta^2} t f' \quad (3.2)$$

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

where primes now denote differentiation with respect to t . For the initial values we obtain

$$f(0) = \gamma, \quad f'(0) = \gamma \quad \text{and} \quad g(0) = 1, \quad g'(0) = 1. \quad (3.4)$$

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

$$f''g - fg'' = 0, \quad g'' = 0 \quad (3.5)$$

$$f(0) = \gamma, \quad f'(0) = \gamma, \quad g(0) = 1, \quad g'(0) = 1. \quad (3.6)$$

The solution (f_0, g_0) of this problem is given by

$$f_0(t) = \gamma + \gamma t \quad \text{and} \quad g_0(t) = 1 + t. \quad (3.7)$$

Note that

$$g_0(t) > \sigma \quad \text{if} \quad t > \sigma - 1.$$

Thus, for large values of β (independent of $\gamma \in (0, 1)$) the function $g(\eta)$ exceeds σ at some finite value of η and therefore $g(\infty) > \sigma$. This completes the proof.

We next show that the sets $\mathcal{A}_+$ and $\mathcal{B}_+$ are open in $\mathcal{D}_+$. By standard theory the functions f and g depend continuously on the parameters β and γ on finite intervals. However, here we need to show that $g(\infty)$ depends continuously on β and γ . This will be proved in the next lemma. The proof closely follows that of an analogous lemma in [PT]. For completeness we conclude it here.

Lemma 3.2. *The limits $\gamma(\infty)$ and $g(\infty)$ depend continuously on $(\gamma, \beta) \in \mathcal{D}_+$.*

Proof. Let $(\gamma^*, \beta^*) \in \mathcal{D}_+$ and let (f^*, g^*) denote the corresponding solution of (2.1)-(2.5) with initial values $(\gamma^*, \gamma^*\beta^*, 1, \beta^*)$. With the vector notation $\phi = \text{col}(f, g)$ the equations (2.1) and (2.2) can be written as

$$\phi'' + \frac{\eta}{2} G(\phi) \phi' = 0 \quad (3.8)$$

where

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

Now write

$$f(\eta) = f^*(\infty) + u(\eta), \quad g(\eta) = g^*(\infty) + v(\eta)$$

and $w = \text{col}(u, v)$. Then an elementary computation shows that

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

where

$$A = \begin{pmatrix} \frac{1 + qf^*}{g^*} & \frac{pf^*}{g^*} \\ \frac{q}{p} & \frac{p}{p} \end{pmatrix} \quad \text{and} \quad \rho(w) = O(|w|) \quad \text{as} \quad w \rightarrow 0.$$

Thus, w satisfies

$$w'' + \frac{1}{2}\eta\{A + \rho(w)\}w' = 0. \quad (3.9)$$

To bring this equation into standard form, we write

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

Then (3.9) becomes

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

and so

$$y(t) = e^{-At}y(0) - \int_0^t e^{-A(t-s)}r(s)y(s)ds \quad (3.10)$$

It is readily verified that the eigenvalues of A are real, positive and distinct. The smaller of these we denote by λ_1 . Then by standard theory there exists a constant $K > 0$ such that

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

Choose now constants $\mu \in (0, \lambda_1)$ and $\delta > 0$ such that

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

It then follows from (3.10) - (3.12) and an application of Grownwall's lemma that

$$|w'(\eta)| \leq K|w'(\eta_0)|e^{-\mu(\eta^2 - \eta_0^2)/4} \quad \text{as long as} \quad |w'(\eta)| < \delta \quad (3.13)$$

in which η_0 is a number yet to be determined.

Integration of (3.13) over (η_0, η) yields

$$|w(\eta)| \leq \sqrt{2}\{|w(\eta_0)| + K|w'(\eta_0)| \int_{\eta_0}^{\eta} e^{-\mu(\sigma^2 - \eta_0^2)/4} d\sigma\} \quad (3.14)$$

as long as $|w(\eta)| < \delta$. This can be achieved for all $\eta > \eta_0$ if we choose $w(\eta_0)$ 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 achieved by choosing η_0 sufficiently large and $(\gamma, \beta) \in \mathcal{D}_+$ sufficiently close to (γ^*, β^*) .

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

According to a result of McLeod & Serrin the properties of $\mathcal{A}_+$ and $\mathcal{B}_+$ which we have now established allow us to conclude that there exists a continuum $\mathcal{C}_+$ in the set $\mathcal{D}_+ \setminus (\mathcal{A}_+ \cup \mathcal{B}_+)$, which joins the lines $\{\gamma = 0, \beta > 0\}$ and $\{\gamma = 1, \beta > 0\}$. It is clear from the definitions of $\mathcal{A}_+$ and $\mathcal{B}_+$ and the fact that $g(\infty)$ exists, that

$$(\gamma, \beta) \in \mathcal{C}_+ \Rightarrow g(\infty) = \sigma.$$

We now pass along $\mathcal{C}_+$ from $\gamma = 0$ to $\gamma = 1$. Near $\gamma = 0$ we have

Lemma 3.4. *There exists a number $\beta_0 > 0$ such that if $(\gamma, \beta) \in \mathcal{C}_+ \cap \{\beta < \beta_0\}$, then $f(\infty) < 1$.*

Proof. If we eliminate g'' from (2.1) by means of (2.2), we obtain the equation

$$f'' + \frac{\eta}{2g}(1 + qf)f' + \frac{\eta}{2g}pg'f = 0.$$

Since $g > 1$ and $g' < \beta$ on $(0, \infty)$ we may conclude that if $\gamma = 0$ and so $f(0) = 0$ and $f'(0) = 0$, then $f(\eta) = 0$ for all $\eta \geq 0$ and in particular $f(\infty) = 0 < 1$. The assertion now follows from the continuous dependence of $f(\infty)$ on (γ, β) proved in Lemma 3.2.

For $\gamma = 1$, we have by Lemma 2.7a

Lemma 3.5. *If $(\gamma, \beta) \in \mathcal{C}_+ \cap \{\gamma = 1\}$, then $f(\infty) > 1$.*

Thus, as we pass along $\mathcal{C}_+$ from $\gamma = 0$ to $\gamma = 1$, $f(\infty)$ changes continuously from a value less than one to a value greater than one. Therefore, there must exist a point $(\gamma_0, \beta_0) \in \mathcal{C}_+ \cap \{0 < \gamma < 1\}$ such that $f(\infty) = 1$. Since $g(\infty) = \sigma$ for any point on $\mathcal{C}_+$, the solution (f_0, g_0) which corresponds to (γ_0, β_0) satisfies the two conditions at infinity. This completes the proof.

4. The shooting: $0 < \sigma < 1$

As in Section 3 we find it convenient to work with the parameters β and γ and thus we write the initial conditions again as

$$f(0) = \gamma, \quad f'(0) = \beta\gamma, \quad g(0) = 1, \quad g'(0) = \beta. \quad (4.1)$$

Since $\sigma < 1$ in this section, it follows from Lemma 2.3 that

$$\beta < 0 \quad \text{and} \quad \gamma > 1. \quad (4.2)$$

However we can no longer assume that $f(\eta)g(\eta) > 0$ for all $\eta \geq 0$, i.e., it may happen that $\eta^* < \infty$. In the next lemma we shall obtain an a priori bound for γ .

Lemma 4.1. *Let (f, g) be a solution of (1.11)-(1.14). Then*

$$\begin{aligned}\gamma &< \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q} \quad \text{if } \sigma < 1, \\ \gamma &> \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q} \quad \text{if } \sigma > 1.\end{aligned}$$

Proof. We combine equations (1.11) and (1.12) to

$$(f'g - fg')' = \frac{1}{q}g'' + \frac{p}{2q}\eta g'. \quad (4.3)$$

This yields upon integration over (η, ∞) .

$$f'g - fg' = \frac{1}{q}g' - \frac{p}{2q} \int_{\eta}^{\infty} sg'(s)ds, \quad (4.4)$$

or, when we divide by g^2 ,

$$\left(\frac{f}{g}\right)' = -\frac{1}{q} \left(\frac{1}{g}\right)' - \frac{p}{2q} \frac{1}{g^2} \int_{\eta}^{\infty} sg'(s)ds. \quad (4.5)$$

When we integrate (4.5) finally over $(0, \infty)$, we obtain in view of our boundary conditions (1.13) and (1.14)

$$\frac{1}{\sigma} - \gamma = -\frac{1}{q} \left(\frac{1}{\sigma} - 1\right) - \frac{p}{2q} \int_0^{\infty} \frac{1}{g^2(t)} \left(\int_t^{\infty} sg'(s)ds\right) dt.$$

Suppose that $\sigma < 1$. Then $g' < 0$ by Lemma 2.2 and we conclude that

$$\frac{1}{\sigma} - \gamma > -\frac{1}{q} \left(\frac{1}{\sigma} - 1\right)$$

or

$$\gamma < \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q}.$$

Thus, it follows from (4.2) and Lemma 4.1 that we have to look for a pair (γ, β) in the set

$$\mathcal{D}_- = \{(\gamma, \beta) : 1 \leq \gamma \leq \gamma^*, \beta \leq 0\}$$

where $\gamma^* = \sigma^{-1}(1 + q^{-1}) - q^{-1}$.

We define the sets

$$\begin{aligned}\mathcal{A}_- &= \{(\gamma, \beta) \in \mathcal{D}_- : g(\infty) > \sigma\} \\ \mathcal{B}_- &= \{(\gamma, \beta) \in \mathcal{D}_- : g(\eta) < \sigma \text{ for some } 0 < \eta < \infty\}.\end{aligned}$$

If $\beta = 0$, then $(f, g) = (\gamma, 1)$ and so $g(\infty) = 1 > \sigma$. Therefore $(\gamma, 0) \in \mathcal{A}_-$ if $1 \leq \gamma \leq \gamma^*$ (See Fig. 3)

Fig. 3. The $\gamma\beta$ - plane ($\sigma < 1$).

Proceeding as in Section 3 we now show that $(\gamma, \beta) \in \mathcal{B}_-$ if β is large and negative.

Lemma 4.2. *There exists a constraint $\tilde{\beta} < 0$ such that if $1 \leq \gamma \leq \gamma^*$ and $\beta < \tilde{\beta}$, then $(\gamma, \beta) \in \mathcal{B}_-$.*

Proof. We use a scaling argument again. Set $t = -\beta\eta$. Then (2.1) - (2.5) become

$$f''g - f_g'' = -\frac{1}{2\beta^2}tf' \quad (4.6)$$

$$g'' = -\frac{1}{2\beta^2}t(qf' + pg') \quad (4.7)$$

$$f(0) = \gamma, \quad f'(0) = -\gamma, \quad g(0) = 1, \quad g'(0) = -1 \quad (4.8)$$

and it is clear, as in Section 3, that as $\beta \rightarrow \infty$, $(f, g) \rightarrow (f_0, g_0)$ on compact sets, where

$$f_0(t) = \gamma - \gamma t \quad \text{and} \quad g_0(t) = 1 - t.$$

Hence, for large negative values of β (independent of $\gamma \in [1, \gamma^*]$) g drops below σ so that (γ, β) then belongs to $\mathcal{B}_-$.

Lemma 4.3. *The sets $\mathcal{A}_-$ and $\mathcal{B}_-$ are open.*

Proof. To prove that $\mathcal{A}_-$ is open, we can proceed exactly as in the proof of Lemma 3.2. Because $g(\infty) > \sigma$, we know that $g(\eta) > \sigma$ for all $\eta \geq 0$ and hence that $\eta^* = \infty$.

To show that $\mathcal{B}_-$ is open we proceed differently. Suppose that $(\bar{\gamma}, \bar{\beta}) \in \mathcal{B}_-$, let $(\bar{f}, \bar{g})$ be the corresponding solution, and let $\bar{\eta} \in (0, \infty)$ be given by

$$\bar{g}(\bar{\eta}) = \sigma.$$

Since $\bar{g}' < 0$ we can choose numbers $\delta \in (0, \frac{1}{3}\sigma)$ and $\eta_\delta > \bar{\eta}$ such that

$$\bar{g}(\eta_\delta) = \sigma - 2\delta.$$

Thus, remembering Lemma 2.5, we have

$$\bar{f}(\eta) > \sigma - 2\delta \quad \text{and} \quad \bar{g}(\eta) \geq \sigma - 2\delta \quad \text{for} \quad 0 \leq \eta \leq \eta_\delta.$$

Therefore, by continuous dependence on initial data there exists a neighbourhood $\mathcal{N}$ of $(\bar{\gamma}, \bar{\beta})$ such that if $(\gamma, \beta) \in \mathcal{N}$, then

$$f(\eta) > \sigma - 3\delta \quad \text{and} \quad g(\eta) > \sigma - 3\delta \quad \text{for} \quad 0 \leq \eta \leq \eta_\delta$$

as well as

$$\sigma - \delta < g(\eta_\delta) < \sigma - 3\delta.$$

Thus $\mathcal{N} \subset \mathcal{B}_-$ and $\mathcal{B}_-$ is open.

As in Section 3 we may now appeal to the topological result of McLeod & Serrin [McLS] to conclude that there exists a continuum $\mathcal{C}_- \subset \mathcal{D}_- \setminus (\mathcal{A}_- \cup \mathcal{B}_-)$ which joins the half lines $\{\gamma = 1, \beta \leq 0\}$ and $\{\gamma = \gamma^*, \beta \leq 0\}$.

Lemma 4.4. *If $(\gamma, \beta) \in \mathcal{C}_-$, then $g(\infty) = \sigma$.*

Proof. Since $(\gamma, \beta) \notin \mathcal{B}_-$, we have $g(\eta) > \sigma$ for all $\eta \geq 0$. Remembering Lemma 2.4 this means that $\eta^* = \infty$. Thus, by Lemma 2.2

$$\lim_{\eta \rightarrow \infty} g(\eta) \text{ exists } \geq \sigma. \tag{4.9}$$

Because $(\gamma, \beta) \notin \mathcal{A}_-$, equality must hold in (4.9).

It remains to prove that $f(\infty) = 1$ for some $(\gamma, \beta) \in \mathcal{C}_-$. This follows from the continuity of $f(\infty)$ with respect to $(\gamma, \beta) \in \mathcal{C}_-$, which can be proved exactly as in Lemma 3.2, and the following two lemmas.

Lemma 4.5. *Let $(1, \beta) \in \mathcal{C}_-$. Then $f(\infty) < 1$.*

Proof. This follows immediately from Lemma 2.7a.

Lemma 4.6. *Let $(\gamma^*, \beta) \in \mathcal{C}_-$. Then $f(\infty) > 1$.*

Proof. For this we return to (4.5), which we integrate over $(0, \infty)$. This yields

$$\begin{aligned} \frac{f(\infty)}{\sigma} - \gamma^* &= \frac{1}{q} \left(1 - \frac{1}{\sigma}\right) - \frac{p}{2q} \int_0^\infty \frac{1}{g^2(t)} \left(\int_t^\infty s g'(s) ds \right) dt \\ &> \frac{1}{q} \left(1 - \frac{1}{\sigma}\right) \end{aligned}$$

because $g'(\eta) < 0$ for all $\eta \geq 0$. Hence

$$\frac{f(\infty)}{\sigma} > \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q} + \frac{1}{q} \left(1 - \frac{1}{\sigma}\right) = \frac{1}{\sigma},$$

or $f(\infty) > 1$.

Thus, with $f(\infty) < 1$ at one end and $f(\infty) > 1$ at the other end of $\mathcal{C}_-$, there must exist a point $(\bar{\gamma}, \bar{\beta}) \in \mathcal{C}_-$ for which $f(\infty) = 1$. This completes the proof.

5. Asymptotic behaviour

Let (f, g) be a solution of (1.11)-(1.14) in which σ is some prescribed positive number. By (1.13)

$$f(\eta) \rightarrow 1 \quad \text{and} \quad g(\eta) \rightarrow \sigma \quad \text{as} \quad \eta \rightarrow \infty. \quad (5.1)$$

In this section we shall obtain estimates for the rates of convergence in (5.1), refining the preliminary estimates derived in Lemma 2.11:

$$f(\eta) = 1 + O(\eta^{-1} e^{-\kappa \eta^2}) \quad \text{as} \quad \eta \rightarrow \infty \quad (5.2)$$

$$g(\eta) = \sigma + O(\eta^{-1} e^{-\kappa \eta^2}) \quad \text{as} \quad \eta \rightarrow \infty \quad (5.3)$$

in which κ is a positive number.

We shall prove

Theorem 5.1. *Suppose that (f, g) is a solution of (1.11) - (1.14) for some $\sigma > 0$ ($\sigma \neq 1$). Then there exists a positive constant K such that*

$$\begin{aligned} f(\eta) &\sim 1 - K \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2/4} \quad \text{as} \quad \eta \rightarrow \infty \\ g(\eta) &\sim \sigma + \frac{Kq}{p - \lambda} \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2/4} \quad \text{as} \quad \eta \rightarrow \infty \end{aligned}$$

in which

$$\lambda = \frac{1}{2} \left(p + \frac{1+q}{\sigma} \right) - \frac{1}{2} \sqrt{\left(p + \frac{1+q}{\sigma} \right)^2 - \frac{4p}{\sigma}}.$$

Proof. Write

$$f(\eta) = 1 + u(\eta) \quad \text{and} \quad g(\eta) = \sigma + v(\eta),$$

and set $w = \text{col}(u, v)$. Then, proceeding as in the proof of Lemma 3.2, we find that w satisfies

$$w'' + \frac{1}{2}\eta\{A + \rho(w)\}w' = 0,$$

where

$$A = \begin{pmatrix} \frac{1+q}{\sigma} & \frac{p}{\sigma} \\ q & p \end{pmatrix} \quad \text{and} \quad \rho(w) = O(|w|) \quad \text{as} \quad w \rightarrow 0. \quad (5.4)$$

In terms of the variables

$$t = \frac{\eta^2}{4}, \quad y(t) = w'(\eta), \quad r(t) = \rho(w(\eta)), \quad (5.5)$$

this equation can be written as

$$y' = -\{A + r(t)\}y. \quad (5.6)$$

Note that in view of (5.2)-(5.4),

$$r(t) = O(e^{-4\kappa t}) \quad \text{as} \quad t \rightarrow \infty.$$

The eigenvalues λ and μ of A are given by

$$\lambda, \mu = \frac{1}{2}\left(p + \frac{1+q}{\sigma}\right) \pm \frac{1}{2}\sqrt{\left(p + \frac{1+q}{\sigma}\right)^2 - \frac{4p}{\sigma}}.$$

Plainly, for all values of $p, q, \sigma \in \mathbf{R}^+$, λ and μ are real, positive and distinct; we shall order them so that $0 < \lambda < \mu$ and denote the corresponding eigenvectors by ξ and ζ . We can conclude from [CL, Theorem 8.1] that there exist two linearly independent solutions $\varphi(t)$ and $\psi(t)$ of (5.6) so that

$$\varphi(t) \sim e^{-\lambda t}\xi \quad \text{and} \quad \psi(t) \sim e^{-\mu t}\zeta \quad \text{as} \quad t \rightarrow \infty.$$

Since (5.6) is linear we can write its solutions as linear combinations of φ and ψ :

$$y(t) = a\varphi(t) + b\psi(t), \quad a, b \in \mathbf{R}. \quad (5.7)$$

Because $\lambda < \mu$, $y(t)$ will behave as $a\varphi(t)$ when $t \rightarrow \infty$ unless $a = 0$. We shall show that if $y(t)$ corresponds to the solution (f, g) of (1.11)-(1.14), then $a \neq 0$.

Thus, let y correspond to (f, g) and let $y = \text{col}(y_1, y_2)$. Then

$$y_1(t) = f'(\eta) \quad \text{and} \quad y_2(t) = g'(\eta).$$

By the analysis of Section 2, $f'(\eta)$ and $g'(\eta)$ have always different signs for η large enough. Thus

$$y_1(t)y_2(t) < 0 \quad \text{for } t \text{ large.} \quad (5.8)$$

Suppose that $a = 0$. Then

$$y(t) \sim be^{-\mu t}\zeta \quad \text{as } t \rightarrow \infty$$

and so, with $\zeta = \text{col}(\zeta_1, \zeta_2)$,

$$\text{sgn } y_1(t)y_2(t) = \text{sgn } \zeta_1\zeta_2$$

for large values of t . However

$$q\zeta_1 = (\mu - p)\zeta_2$$

and therefore

$$\zeta_1\zeta_2 = \frac{\mu - p}{q}\zeta_2^2. \quad (5.9)$$

By an elementary computation we find that

$$\lambda < p < \mu,$$

and so it follows from (5.9) that

$$\zeta_1\zeta_2 > 0.$$

Therefore, if $a = 0$, the solution $y(t)$ cannot satisfy (5.8) for large values of t and we must conclude that $a \neq 0$. This implies that

$$y(t) \sim ae^{-\lambda t}\xi \quad \text{as } t \rightarrow \infty$$

and

$$w'(\eta) \sim ae^{-\lambda\eta^2/4}\xi \quad \text{as } \eta \rightarrow \infty.$$

Thus, since $\xi = \text{col}(1, -q/(p - \lambda))$, we have shown that

$$f'(\eta) \sim ae^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty \quad (5.10)$$

$$g'(\eta) \sim -a \frac{q}{p - \lambda} e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty \quad (5.11)$$

in which a is a constant different from zero. The estimates for $f(\eta)$ and $g(\eta)$ now follow upon integration of (5.10) and (5.11) over (η, ∞) . They are

$$f(\eta) \sim 1 - \frac{2a}{\lambda} \eta^{-1} e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty \quad (5.12)$$

$$g(\eta) \sim \sigma + \frac{2a}{\lambda} \frac{q}{p - \lambda} \eta^{-1} e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty. \quad (5.13)$$

Remark. Using the estimates (5.10) - (5.13) we obtain for $H(\eta)$ the asymptotic estimate

$$H(\eta) \sim a \left(\sigma + \frac{q}{p - \lambda} \right) e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty. \quad (5.14)$$

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**SELF-SIMILAR SOLUTIONS FOR DIFFUSION
IN SEMICONDUCTORS**

By

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Self-similar solutions for diffusion in semiconductors

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1. Introduction

In this paper we continue our study of a system of nonlinear diffusion equations, initiated in [PT]. The system involved arises from a model for the solid-state diffusion by a substitutional mechanism, developed by Zahari & Tuck [ZT] and Hearne [H]. For a review of this model we also refer to King [K]. The system of equations obtained is

$$\frac{\partial c}{\partial t} = \frac{D_c}{v^*} \frac{\partial}{\partial x} \left(v \frac{\partial c}{\partial x} - c \frac{\partial v}{\partial x} \right) \quad (1.1)$$

$$\frac{\partial h}{\partial t} = \frac{D_h}{v^*} \frac{\partial}{\partial x} \left(v \frac{\partial h}{\partial x} - h \frac{\partial v}{\partial x} \right) \quad (1.2)$$

$$c + h + v = L \quad (1.3)$$

in which c , h and v denote the densities of respectively the impurity atoms, the host atoms and the vacancies in the lattice 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.

The density of the lattice sites L is assumed to be constant. Thus (1.3) can be used to eliminate the concentration h and so reduce the system to one involving two diffusion equations. The resulting equation for v is then

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

in which $D_v = D_h L / v^*$ 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.

In [PT] we discussed the infiltration of dopant into an initially pure semi-infinite slab of semiconductor ($c = 0$) in which the concentration of the vacancies is everywhere equal to its equilibrium value v^* .

In the present paper we also discuss a semi-infinite slab of semiconductor material. However, we now consider one in which dopant has first been implanted. Then, when for instance the material is heated, diffusion sets in and we are interested in the way the concentration profiles of the three constituents develop with time near the surface of the slab, when no dopant can leave or enter the material. Locally, we may take the initial profiles in the slab to be constant. Hence we set

$$c(x, 0) = c_0 \quad \text{and} \quad v(x, 0) = v_0 \quad \text{for} \quad x > 0, \quad (1.5)$$

in which c_0 and v_0 are positive constants. On the surface we assume that the vacancy concentration is kept at a constant value v_1 . Thus, on the face of the slab we have the two

boundary conditions

$$\left(v \frac{\partial c}{\partial x} - c \frac{\partial v}{\partial x}\right)(0, t) = 0 \quad \text{and} \quad v(0, t) = v_1 \quad \text{for} \quad t > 0. \quad (1.6)$$

To simplify the problem we introduce the nondimensional variables

$$\tilde{c} = \frac{c}{c_0}, \quad \tilde{v} = \frac{v}{v_1}, \quad \tilde{t} = \frac{t}{T} \quad \text{and} \quad \tilde{x} = x \sqrt{\frac{v^*}{D_c T v_1}},$$

where T is a representative time scale. We then obtain for (1.1), (1.4), (1.5) and (1.6) the problem

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

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

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

$$\left(v \frac{\partial c}{\partial x} - c \frac{\partial v}{\partial x}\right)(0, t) = 0 \quad \text{and} \quad v(0, t) = 1 \quad \text{for} \quad t > 0 \quad (1.10)$$

in which the tildes have been dropped and

$$p = \frac{v_1}{L} \frac{D_c}{D_h}, \quad q = \frac{c_0}{L} \left(\frac{D_c}{D_h} - 1 \right) \quad \text{and} \quad \sigma = \frac{v_0}{v_1}.$$

Thus p and q are positive numbers and σ may be positive or zero.

In view of the invariance properties of the equations and the data 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

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

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

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

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

whilst the initial conditions (1.9) become

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

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

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

In this paper we shall show that there exists a pair of positive functions (f, g) which satisfies (1.11) and (1.12) for all $\eta \geq 0$ and the boundary conditions (1.13) and (1.14) for any $\sigma > 0$. This is done by means of a shooting technique in which the conditions at infinity are replaced by additional conditions at the origin. It is then shown that these conditions can be chosen in such a way as to yield a solution of the initial value problem which has all the desired properties at infinity.

This shooting method involves a careful analysis of the solutions of the system (1.11), (1.12) which reveals some qualitative properties of solutions of (1.11) - (1.14) such as

(a) *There exists a point $\eta_0 > 0$ such that*

$$\begin{aligned} f' &> 0 \text{ on } [0, \eta_0) \quad \text{and} \quad f' < 0 \text{ on } (\eta_0, \infty) \quad \text{if } \sigma > 1; \\ f' &< 0 \text{ on } [0, \eta_0) \quad \text{and} \quad f' > 0 \text{ on } (\eta_0, \infty) \quad \text{if } \sigma < 1. \end{aligned}$$

(b) *We have*

$$\begin{aligned} g' &> 0 \text{ on } [0, \infty) \quad \text{and} \quad g'' < 0 \text{ on } (0, \infty) \quad \text{if } \sigma > 1; \\ g' &< 0 \text{ on } [0, \infty) \quad \text{and} \quad g'' > 0 \text{ on } (0, \infty) \quad \text{if } \sigma < 1. \end{aligned}$$

In Figure 1 typical graphs of f and g are sketched for $\sigma > 1$ and $0 < \sigma < 1$.

Fig. 1. Graphs of $f(\eta)$ and $g(\eta)$.

We conclude with an asymptotic analysis of the functions $f(\eta)$ and $g(\eta)$ which yields rates at which they approach their limits $f(\eta) = 1$ and $g(\eta) = \sigma$ when η tends to infinity.

Theorem. *Suppose that (f, g) is a solution of (1.11) - (1.14) for some $\sigma > 0$ ($\sigma \neq 1$). Then there exists a positive constant K such that*

$$\begin{aligned} f(\eta) &\sim 1 - K \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2 / 4} \quad \text{as } \eta \rightarrow \infty \\ g(\eta) &\sim \sigma + \frac{Kq}{p - \lambda} \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2 / 4} \quad \text{as } \eta \rightarrow \infty \end{aligned}$$

in which

$$\lambda = \frac{1}{2} \left(p + \frac{1+q}{\sigma} \right) - \frac{1}{2} \sqrt{\left(p + \frac{1+q}{\sigma} \right)^2 - \frac{4p}{\sigma}}.$$

When $\sigma = 1$, problem (1.11)-(1.14) only has the trivial solution $(f, g) = (1, 1)$.

Note that for all positive values of p , q and σ ,

$$0 < \lambda < p,$$

so that the asymptotic behaviour is indeed consistent with the properties (a) and (b) of f and g listed above.

For the flux $f'g - fg'$ we obtain when $\sigma \neq 1$

$$f'(\eta)g(\eta) - f(\eta)g'(\eta) \sim \frac{1}{2} \lambda K \left(\sigma + \frac{q}{p-\lambda} \right) \text{sgn}(1-\sigma) e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty,$$

where K is the constant appearing in the estimates for f and g .

In the next section we prove a series of properties which will be essential in the proof of existence and in determining the asymptotic behaviour of solutions. In Section 3 we prove the existence of a solution when $\sigma > 1$ and in Section 4 we prove existence if $0 < \sigma < 1$. Finally, in Section 5, we establish the asymptotic behaviour of solutions.

2. Properties of solutions

We shall employ a topological shooting argument to prove our results. Thus, we consider the initial value problem for the system (1.11), (1.12) which we write with the function

$$H = f'g - fg'$$

as

$$\begin{cases} H' + \frac{1}{2}\eta f' = 0 & \eta > 0 \end{cases} \quad (2.1)$$

$$\begin{cases} g'' + \frac{p}{2}\eta g' + \frac{q}{2}\eta f' = 0 & \eta > 0. \end{cases} \quad (2.2)$$

At the origin we impose the conditions

$$H(0) = 0 \quad \text{and} \quad g(0) = 1 \quad (2.3)$$

and consistent with [PT] we add the conditions

$$f'(0) = \alpha, \quad g'(0) = \beta, \quad f(0) = \gamma. \quad (2.4)$$

Thus in this problem we have three parameters at our disposal: $\alpha, \beta \in \mathbf{R}$ and $\gamma > 0$, although in order to satisfy condition (2.3) we shall always require that

$$\alpha = \beta\gamma. \quad (2.5)$$

In Section 1 we indicated that the correct regimes for these parameters are

$$\alpha > 0, \beta > 0, 0 < \gamma < 1 \quad \text{if } \sigma > 1 \quad (2.6a)$$

$$\alpha < 0, \beta < 0, 1 < \gamma < \infty \quad \text{if } \sigma < 1. \quad (2.6b)$$

For each choice of (α, β, γ) we denote the maximal interval of existence of the solution (f, g) of (2.1) - (2.4) by $[0, \rho(\alpha, \beta, \gamma))$. Since we are only interested in solutions which make sense physically, that is if $f(\eta) > 0$ and $g(\eta) > 0$ for all $\eta \geq 0$, we define

$$\eta^* = \sup\{\eta \in (0, \rho) : fg > 0 \text{ on } (0, \eta)\}.$$

With these definitions in place we proceed with our analysis.

We begin with a few simple results which justify the choice of the parameter ranges in (2.5) and (2.6).

Lemma 2.1. *We have*

$$H(0) = 0, \quad H'(0) = 0 \quad \text{and} \quad H''(0) = -\frac{1}{2}f'(0).$$

Proof. It follows from (2.1) that $H'(0) = 0$. The third assertion follows from l'Hôpital's rule:

$$H''(0) = \lim_{\eta \rightarrow 0} \frac{H'(\eta)}{\eta} = -\frac{1}{2} \lim_{\eta \rightarrow 0} f'(\eta) = -\frac{1}{2}f'(0).$$

Lemma 2.2. *We have*

$$\begin{aligned} \beta < 0 &\Rightarrow g'(\eta) < 0 \text{ for } 0 \leq \eta < \eta^* \quad \text{and} \quad g''(\eta) > 0 \text{ for } 0 < \eta < \eta^* \\ \beta > 0 &\Rightarrow g'(\eta) > 0 \text{ for } 0 \leq \eta < \eta^* \quad \text{and} \quad g''(\eta) < 0 \text{ for } 0 < \eta < \eta^*. \end{aligned}$$

Proof. First of all, assume that $g'(0) < 0$. This implies by (2.4) that $f'(0) < 0$ as well. Suppose that

$$\eta_0 = \sup\{\eta \in (0, \eta^*) : g' < 0\} < \eta^*.$$

Then

$$0 < g(\eta_0) < 1, \quad g'(\eta_0) = 0 \quad \text{and} \quad g''(\eta_0) \geq 0.$$

But by (2.2),

$$g''(\eta_0) + \frac{q}{2}\eta_0 f'(\eta_0) = 0,$$

so that $f'(\eta_0) \leq 0$. If $f'(\eta_0) = 0$, then by uniqueness $(f(\eta), g(\eta)) = (f(\eta_0), g(\eta_0))$ for all $\eta \geq 0$ so that the initial condition for g would not be satisfied. Thus we have

$$g''(\eta_0) > 0 \quad \text{and} \quad f'(\eta_0) < 0. \quad (2.7)$$

We assert that

$$f'(\eta) < 0 \quad \text{for } 0 \leq \eta \leq \eta_0. \quad (2.8)$$

If not, then by (2.7) f' must change sign on $(0, \eta_0)$ at least twice and so there must exist a point $\eta_1 \in (0, \eta_0)$ such that

$$f'(\eta_1) = 0 \quad \text{and} \quad f''(\eta_1) \leq 0.$$

From (2.1) we conclude that $g''(\eta_1) \leq 0$, which implies by (2.2) that $g'(\eta_1) \geq 0$. This contradicts the definition of η_0 and thus proves (2.8).

It follows from (2.8) that $H' > 0$ on $(0, \eta_0]$. Hence

$$H(\eta_0) > H(0) = 0,$$

and so

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

This contradicts (2.8) and therefore we can conclude that

$$g'(\eta) < 0 \quad \text{for all } \eta \in [0, \eta^*). \quad (2.9)$$

Next we prove the convexity of the graph of g . From (2.2) we deduce that $g''(0) = 0$. However, if we differentiate (2.2) we obtain

$$g''' + \frac{1}{2}(pg' + qf') + \frac{1}{2}\eta(pg'' + qf'') = 0. \quad (2.10)$$

Thus, because $g'(0) < 0$ and $f'(0) < 0$ we see that $g'''(0) > 0$ so that $g''(\eta) > 0$ for η small. Set

$$\hat{\eta} = \sup\{\eta \in (0, \eta^*) : g'' > 0 \text{ on } (0, \eta)\}.$$

To force a contradiction we suppose that $\hat{\eta} < \eta^*$. Then

$$g''(\hat{\eta}) = 0 \quad \text{and} \quad g'''(\hat{\eta}) \leq 0. \quad (2.11)$$

We now compute g''' from (2.10). By (2.2)

$$qf' + pg' = 0 \quad \text{at } \eta = \hat{\eta} \quad (2.12)$$

so that

$$g'''(\hat{\eta}) = -\frac{1}{2}\hat{\eta}qf''(\hat{\eta}). \quad (2.13)$$

By (2.1) we have in turn

$$f''g = -\frac{1}{2}\eta f' \quad \text{at } \eta = \hat{\eta}. \quad (2.14)$$

Because $g' < 0$ by (2.9), it follows from (2.12) that $f' > 0$ and so, from (2.14) that $f'' < 0$. Putting this into (2.13) we find that $g''' > 0$ at $\eta = \hat{\eta}$. This contradicts the inequality in (2.11) and thus completes the proof of the first assertion.

The proof of the second assertion is the same.

The following lemma is an immediate consequence of Lemma 2.2.

Lemma 2.3. *We have*

$$\sigma < 1 (>) \Rightarrow g'(0) < 0 (>).$$

Remark 1. We have now justified the parameter regimes for $f'(0)$ and $g'(0)$ described by (2.5) and (2.6). We note that if $\sigma = 0$ then necessarily $g'(0) = 0$. For if $g'(0) > 0$ then Lemma 2.3 states that $g'(\eta) > 0$ for all $\eta \geq 0$ so that $g(\infty) = 1$ is impossible. Likewise, if $g'(0) < 0$ then $g(\infty) = 1$ is not possible. If $g'(0) = 0$, then (2.4) implies that $f'(0) = 0$ and it follows by uniqueness that $f' = 0$ and $g' = 0$ on $[0, \infty)$ and so $f = \gamma$ and $g = 1$ for all $\eta \geq 0$. The boundary condition for f at infinity can then only hold if $\gamma = 1$. As we proceed with our analysis it will become evident that (2.6a) and (2.6b) describe the correct range for the values of γ as well.

About the function H we can now prove

Lemma 2.4. *We have*

$$\alpha < 0 (> 0) \Rightarrow H(\eta) > 0 (< 0) \text{ for all } \eta \in (0, \eta^*).$$

Proof. Suppose that $\alpha < 0$. Then by Lemma 2.1, $H''(0) > 0$ and hence $H(\eta) > 0$ for $\eta > 0$ small. Suppose, however that $H(\eta)$ vanishes at some $\eta_1 \in (0, \eta^*)$. Suppose η_1 is the first zero of H . Then at η_1 we have

$$H'(\eta_1) \leq 0 \quad \text{and so} \quad f'(\eta_1) \geq 0 \tag{2.15}$$

by (2.1), but also

$$H(\eta_1) = 0 \quad \text{and so} \quad f'(\eta_1)g(\eta_1) = f(\eta_1)g(\eta_1) \geq 0 \tag{2.16}$$

by Lemma 2.2. Plainly (2.15) and (2.16) contradict one another.

The assertion involving $\alpha > 0$ is proved in the same way.

Lemma 2.4 enables us to compare f and g .

Lemma 2.5. *We have*

$$\alpha < 0 (>) \Rightarrow f(\eta) > \gamma g(\eta) (<) \text{ for } 0 < \eta < \eta^*.$$

Proof. Suppose that $\alpha < 0$. Then by Lemma 2.4,

$$f'g - fg' > 0 \quad \text{on} \quad (0, \eta^*)$$

and so

$$\log \frac{f(\eta)}{g(\eta)} > \log \frac{f(0)}{g(0)}, \quad (2.17)$$

from which the assertion follows. The one for $\alpha > 0$ is proved the same way.

Lemma 2.6. *Let (f, g) be a solution of (2.1) - (2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then*

$$\begin{aligned} g(\eta) &< 1 + \frac{2\beta}{\sqrt{p}} \arctan\left(\frac{\sqrt{p}}{2}\eta\right) & \text{if } \beta > 0 \\ g(\eta) &> 1 - \frac{2\beta}{\sqrt{p}} \arctan\left(\frac{\sqrt{p}}{2}\eta\right) & \text{if } \beta < 0. \end{aligned}$$

Proof. Suppose that $\beta > 0$. We combine (2.1) and (2.2) to yield

$$H' = \frac{1}{q}g'' + \frac{p}{2q}\eta g'. \quad (2.18)$$

When we integrate this equation over $(0, \eta)$ we obtain, using the initial conditions (2.3) and (2.4)

$$H(\eta) = \frac{1}{q}g'(\eta) - \frac{\beta}{q} + \frac{p}{2q} \int_0^\eta t g'(t) dt \quad (2.19)$$

or

$$g'(\eta) + \frac{p}{2} \int_0^\eta t g'(t) dt = \beta + qH(\eta) < \beta,$$

because by Lemma 2.4, $H(\eta) < 0$ for all $\eta > 0$. Since by Lemma 2.2, $g'' < 0$ we deduce that

$$g'(\eta) \left(1 + \frac{p}{4}\eta^2\right) < \beta.$$

Hence

$$g'(\eta) \leq \frac{4\beta}{4 + p\eta^2} \quad \text{for } \eta \geq 0,$$

so that

$$g(\eta) \leq 1 + \frac{2\beta}{\sqrt{p}} \arctan\left(\frac{\sqrt{p}}{2}\eta\right).$$

The argument for $\beta < 0$ proceeds the same way.

In the following lemma we derive a second bound for f .

Lemma 2.7. *Suppose that $\alpha > 0$ ($<$). Then*

$$f(\eta) > \gamma \quad (<) \quad \text{for all } \eta \in (0, \eta^*).$$

Proof. Suppose that $\alpha < 0$ and assume that

$$\eta_\gamma = \sup\{\eta > 0 : f < \gamma \text{ on } (0, \eta)\} < \eta^*.$$

Then from (2.1) we obtain

$$H(\eta_\gamma) + \frac{1}{2}\eta_\gamma\gamma - \frac{1}{2}\int_0^{\eta_\gamma} f(s) ds = 0.$$

Since

$$\int_0^{\eta_\gamma} f(s) ds < \eta_\gamma\gamma,$$

it follows that

$$H(\eta_\gamma) < 0.$$

However, if $\alpha < 0$, then, by (2.5) $\beta < 0$ and so, by Lemmas 2.3 and 2.4, $H(\eta) > 0$ for all $\eta > 0$. Thus we have arrived at a contradiction.

Lemma 2.7 means in particular that if (f, g) is a solution of (1.11)-(1.14), then

$$\sigma > 1 (< 1) \Rightarrow \gamma < 1 (> 1). \quad (2.20)$$

It also implies that

$$\alpha > 0 \Rightarrow \eta^* = \infty \quad (2.21)$$

because now $f(\eta)g(\eta) > \gamma$ for all $\eta \in (0, \eta^*)$, which implies that $\eta^* = \infty$.

Before we can say more about the shape of the graph if f we need some information about the behaviour of $f(\eta)$ as $\eta \rightarrow \infty$.

Lemma 2.8. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then*

$$(a) \quad \begin{aligned} \lim_{\eta \rightarrow \infty} f(\eta) \text{ exists} &= f(\infty) \\ \lim_{\eta \rightarrow \infty} g(\eta) \text{ exists} &= g(\infty), \end{aligned}$$

$$(b) \quad f'(\eta) \rightarrow 0, \quad g'(\eta) \rightarrow 0 \quad \text{as } \eta \rightarrow \infty,$$

$$(c) \quad H(\eta) \rightarrow 0 \quad \text{as } \eta \rightarrow \infty.$$

Proof. Suppose that $\alpha < 0$. From Lemma 2.2 and the positivity of g we conclude that

$$g(\eta) \rightarrow g(\infty) \quad \text{and} \quad g'(\eta) \rightarrow 0 \quad \text{as } \eta \rightarrow \infty. \quad (2.22)$$

As regards f we note that it has a critical point if H has one. In view of (2.17) and Lemma 2.2 this can only be an isolated maximum. This in turn implies by (2.16) that f can only

have an isolated minimum. Thus either way, f is monotonic for large η . Since by Lemma 2.2 and 2.6

$$\gamma g(\eta) < f(\eta) < \gamma \quad (2.23)$$

it follows that

$$\lim_{\eta \rightarrow \infty} f(\eta) \text{ exists} = f(\infty).$$

Before turning to f' , we consider the limiting behaviour of H . Because $g' < 0$ by Lemma 2.2 it follows from (2.1) and (2.2) that

$$\lim_{\eta \rightarrow \infty} \{H(\eta) - \frac{1}{q}g'(\eta)\} \text{ exists} = L$$

where $L \in [-\infty, \infty)$. This means in view of (2.22) that

$$\lim_{\eta \rightarrow \infty} H(\eta) = L.$$

Because by Lemma 2.4. $H(\eta) > 0$ for all $\eta > 0$, we conclude that $0 \leq L < \infty$.

Remembering (2.22) again, we observe that

$$\lim_{\eta \rightarrow \infty} f'(\eta)g(\eta) = L$$

which, using (2.22) once more, implies that

$$\lim_{\eta \rightarrow \infty} f'(\eta) \text{ exists} = f'(\infty).$$

As we have shown that $f(\infty)$ exists, it follows that $f'(\infty) = 0$. This means that $L = 0$ and hence that $H(\infty) = 0$.

Similar arguments prove the case $\alpha > 0$. We should note for later reference that

$$\gamma < f(\eta) < \gamma g(\eta) \quad \text{for} \quad 0 < \eta < \infty \quad (2.24)$$

in this case.

With the results of Lemma 2.8 we can further describe the graph of f .

Lemma 2.9. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then the graph of f has precisely one isolated critical point: a minimum if $\alpha < 0$ and a maximum if $\alpha > 0$.*

Proof. Since $H(0) = 0$ by (2.5) and $H(\infty) = 0$ by Lemma 2.8, H must have at least one critical point. As we observed before, this must be an isolated maximum (minimum) if $\alpha < 0$ ($\alpha > 0$) and it is therefore unique. Thus, remembering (2.16) we conclude that f has one and only one critical point and that this is a minimum (maximum) if $\alpha < 0$ ($\alpha > 0$).

If $\alpha < 0$ the proof is almost the same, except that to prove that $g(\infty)$ exists we now use the upper bound of Lemma 2.6.

In the following lemma we derive rates of convergence for the limits obtained in Lemma 2.8.

Lemma 2.11. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then there exists a constant $\kappa > 0$ such that*

$$\begin{aligned} (a) \quad & f'(\eta) = O(e^{-\kappa\eta^2}) \quad \text{and} \quad g'(\eta) = O(e^{-\kappa\eta^2}) \quad \text{as } \eta \rightarrow \infty, \\ (b) \quad & f(\eta) = f(\infty) + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as } \eta \rightarrow \infty \\ & g(\eta) = g(\infty) + O(\eta^{-1}e^{-\kappa\eta^2}) \quad \text{as } \eta \rightarrow \infty. \end{aligned}$$

Proof. Suppose $\alpha > 0$. We differentiate (2.2) and use (2.1) to eliminate f' and f'' from the resulting equation. This yields

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

Set $y = g''/g'$. This function is well defined and negative by Lemma 2.2. When we substitute it into (2.22) we obtain a Riccati-type equation in y :

$$y' + y^2 + \left\{ \frac{p\eta}{2} - \frac{1}{\eta} + \frac{\eta}{2g}(1 + qf) \right\} y + \frac{p\eta^2}{4g} = 0. \quad (2.25)$$

We shall show that there exist constants $M > 0$ and $\eta_1 > 0$ such that

$$y < -M\eta \quad \text{for } \eta > \eta_1. \quad (2.26)$$

Indeed, if this is so, then

$$\log \frac{g'(\eta)}{g'(\eta_1)} < -\frac{1}{2}M(\eta^2 - \eta_1^2) \quad \text{for } \eta > \eta_1,$$

from which the assertion about g' follows.

To prove (2.26) we introduce the function,

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

in which the constant M will be chosen later, and we shall show that $h < 0$ on (η_1, ∞) for some $\eta_1 > 0$. Observe that if $h \geq 0$ and $\eta > 0$. Then because $y < 0$,

$$\begin{aligned} h'(\eta) &< -\frac{p\eta^2}{4g(\eta)} + \left\{ \frac{p\eta}{2} + \frac{1 + q\gamma g(\infty)}{2} \frac{\eta}{g(\eta)} \right\} M\eta + M \\ &< -\frac{p\eta^2}{4g(\infty)} + \frac{1}{2}(p + q\gamma g(\infty) + 1)M\eta^2 + M \\ &< -\frac{p\eta^2}{8g(\infty)} + M \end{aligned} \quad (2.27)$$

if we choose $M = p/\{4g(\infty)(p + q\gamma g(\infty) + 1)\}$. It follows from (2.27) that $h(\eta) < 0$ for η large enough. This completes the estimate for g' .

To estimate f' , we use (2.2), which we write as

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

Recall that when $\alpha > 0$, $g' > 0$, $g'' < 0$ on $(0, \infty)$ and $f' < 0$ on (η_2, ∞) for some $\eta_2 > 0$. Hence

$$|f'| = \frac{p}{q}g' + \frac{2}{q\eta}g'' < \frac{p}{q}g' \quad \text{for } \eta > \eta_2.$$

from which the desired estimate follows.

Integrating f' and g' over (η, ∞) we obtain the remaining estimates.

When $\alpha < 0$, the proof is exactly the same. The only possible difficulty arises in (2.27) when $g(\infty) = 0$. However, $g < 1$ in this case, so that (2.27) simplifies to

$$\begin{aligned} h'(\eta) &< \frac{1}{g(\eta)} \left\{ -\frac{p\eta^2}{4} + \frac{1}{2}[p\eta g(\eta) + (1 + q\gamma)\eta]M\eta + Mg \right\} \\ &< \frac{1}{g(\eta)} \left\{ -\frac{p\eta^2}{4} + \frac{1}{2}(p + q\gamma + 1)M\eta^2 + M \right\} \\ &= \frac{1}{g(\eta)} \left\{ -\frac{p\eta^2}{8} + M \right\} \end{aligned}$$

if we choose $M = p/\{4(p + q\gamma + 1)\}$. Again it follows that $h(\eta) < 0$ for η large enough and the proof continues as in the case $\alpha > 0$.

The asymptotic behaviour of $f(\eta)$ established in Lemma 2.11 enables us to extend Lemma 2.7 to $\eta = \infty$ if $\eta^* = \infty$.

Lemma 2.7a. *Let (f, g) be a solution of (2.1)-(2.5) which exists for all $\eta \geq 0$ and $\eta^* = \infty$. Then*

$$f(\infty) > \gamma \quad (<) \quad \text{if } \alpha > 0 \quad (<).$$

Proof. Suppose that $\alpha > 0$. Then by Lemma 2.7, $f(\eta) > \gamma$ for all $\eta > 0$ and so $f(\infty) \geq \gamma$. Thus, it remains to prove strict inequality.

Suppose to the contrary that $f(\infty) = \gamma$ and write

$$\varphi(\eta) = f(\eta) - \gamma.$$

Equation (2.1) can then be written as

$$H' + \frac{1}{2}\eta\varphi'(\eta) = 0,$$

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

$$H(\eta) + \frac{1}{2}\eta\varphi(\eta) = \frac{1}{2} \int_0^\eta \varphi(s) ds.$$

If we now let η tend to infinity, the terms on the left hand side tend to zero by Lemmas 2.8 and 2.11. This implies that

$$\int_0^\infty \varphi(s) ds = 0.$$

Because $\varphi(\eta) > 0$ for all $\eta > 0$ by Lemma 2.7, this is impossible and we must conclude that $f(\infty) > \gamma$.

When $\alpha < 0$ the argument is the same.

3. The shooting: $\sigma > 1$

We are now ready to carry out the shooting arguments leading to the existence of a solution. In this section we shall consider the case $\sigma > 1$, and in Section 4, the details are given for $0 < \sigma < 1$.

We shall find it convenient to work with the parameters β and γ which leaves α determined via (2.5). Thus, we impose the initial values

$$f(0) = \gamma, \quad f'(0) = \beta\gamma \quad \text{and} \quad g(0) = 1, \quad g'(0) = \beta. \quad (3.1)$$

Since we take $\sigma > 1$ in this section, it follows from Lemma 2.3 that we need only consider positive values of β and from (2.21) that $\eta^* = \infty$.

We introduce the sets

$$\mathcal{D}_+ = \{(\gamma, \beta) \in \mathbf{R}^2 : 0 \leq \gamma \leq 1, \beta \geq 0\}$$

and

$$\begin{aligned} \mathcal{A}_+ &= \{(\gamma, \beta) \in \mathcal{D}_+ : g(\infty) < \sigma\} \\ \mathcal{B}_+ &= \{(\gamma, \beta) \in \mathcal{D}_+ : g(\infty) > \sigma\}. \end{aligned}$$

Because by Lemma 2.8 the limit $g(\infty)$ always exists, these sets are well defined.

It is clear that if $\beta = 0$, the solution is given by $(f, g) = (\gamma, 1)$ so that $g(\infty) = 1 < \sigma$. Thus $(\gamma, 0) \in \mathcal{A}_+$ if $0 \leq \gamma \leq 1$ (see Fig. 2.)

Fig. 2. The $\gamma\beta$ -plane ($\sigma > 1$).

In the next lemma we show that on the other hand $(\gamma, \beta) \in \mathcal{B}_+$ if β is large enough.

Lemma 3.1. *There exists a constant $\hat{\beta}$ such that if $0 \leq \gamma \leq 1$ and $\beta > \hat{\beta}$, then $(\alpha, \beta) \in \mathcal{B}_+$.*

Proof. We use a scaling argument and set $t = \beta\eta$. Then (2.1) and (2.2) become

$$f''g - fg'' = \frac{1}{2\beta^2} t f' \quad (3.2)$$

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

where primes now denote differentiation with respect to t . For the initial values we obtain

$$f(0) = \gamma, \quad f'(0) = \gamma \quad \text{and} \quad g(0) = 1, \quad g'(0) = 1. \quad (3.4)$$

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

$$f''g - fg'' = 0, \quad g'' = 0 \quad (3.5)$$

$$f(0) = \gamma, \quad f'(0) = \gamma, \quad g(0) = 1, \quad g'(0) = 1. \quad (3.6)$$

The solution (f_0, g_0) of this problem is given by

$$f_0(t) = \gamma + \gamma t \quad \text{and} \quad g_0(t) = 1 + t. \quad (3.7)$$

Note that

$$g_0(t) > \sigma \quad \text{if} \quad t > \sigma - 1.$$

Thus, for large values of β (independent of $\gamma \in (0, 1)$) the function $g(\eta)$ exceeds σ at some finite value of η and therefore $g(\infty) > \sigma$. This completes the proof.

We next show that the sets $\mathcal{A}_+$ and $\mathcal{B}_+$ are open in $\mathcal{D}_+$. By standard theory the functions f and g depend continuously on the parameters β and γ on finite intervals. However, here we need to show that $g(\infty)$ depends continuously on β and γ . This will be proved in the next lemma. The proof closely follows that of an analogous lemma in [PT]. For completeness we conclude it here.

Lemma 3.2. *The limits $\gamma(\infty)$ and $g(\infty)$ depend continuously on $(\gamma, \beta) \in \mathcal{D}_+$.*

Proof. Let $(\gamma^*, \beta^*) \in \mathcal{D}_+$ and let (f^*, g^*) denote the corresponding solution of (2.1)-(2.5) with initial values $(\gamma^*, \gamma^*\beta^*, 1, \beta^*)$. With the vector notation $\phi = \text{col}(f, g)$ the equations (2.1) and (2.2) can be written as

$$\phi'' + \frac{\eta}{2} G(\phi) \phi' = 0 \quad (3.8)$$

where

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

Now write

$$f(\eta) = f^*(\infty) + u(\eta), \quad g(\eta) = g^*(\infty) + v(\eta)$$

and $w = \text{col}(u, v)$. Then an elementary computation shows that

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

where

$$A = \begin{pmatrix} \frac{1 + qf^*}{g^*_q} & \frac{pf^*}{g^*_p} \end{pmatrix} \quad \text{and} \quad \rho(w) = O(|w|) \quad \text{as} \quad w \rightarrow 0.$$

Thus, w satisfies

$$w'' + \frac{1}{2}\eta\{A + \rho(w)\}w' = 0. \quad (3.9)$$

To bring this equation into standard form, we write

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

Then (3.9) becomes

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

and so

$$y(t) = e^{-At}y(0) - \int_0^t e^{-A(t-s)}r(s)y(s)ds \quad (3.10)$$

It is readily verified that the eigenvalues of A are real, positive and distinct. The smaller of these we denote by λ_1 . Then by standard theory there exists a constant $K > 0$ such that

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

Choose now constants $\mu \in (0, \lambda_1)$ and $\delta > 0$ such that

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

It then follows from (3.10) - (3.12) and an application of Grownwall's lemma that

$$|w'(\eta)| \leq K|w'(\eta_0)|e^{-\mu(\eta^2 - \eta_0^2)/4} \quad \text{as long as} \quad |w'(\eta)| < \delta \quad (3.13)$$

in which η_0 is a number yet to be determined.

Integration of (3.13) over (η_0, η) yields

$$|w(\eta)| \leq \sqrt{2}\{|w(\eta_0)| + K|w'(\eta_0)| \int_{\eta_0}^{\eta} e^{-\mu(\sigma^2 - \eta_0^2)/4} d\sigma\} \quad (3.14)$$

as long as $|w(\eta)| < \delta$. This can be achieved for all $\eta > \eta_0$ if we choose $w(\eta_0)$ 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 achieved by choosing η_0 sufficiently large and $(\gamma, \beta) \in \mathcal{D}_+$ sufficiently close to (γ^*, β^*) .

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

According to a result of McLeod & Serrin the properties of $\mathcal{A}_+$ and $\mathcal{B}_+$ which we have now established allow us to conclude that there exists a continuum $\mathcal{C}_+$ in the set $\mathcal{D}_+ \setminus (\mathcal{A}_+ \cup \mathcal{B}_+)$, which joins the lines $\{\gamma = 0, \beta > 0\}$ and $\{\gamma = 1, \beta > 0\}$. It is clear from the definitions of $\mathcal{A}_+$ and $\mathcal{B}_+$ and the fact that $g(\infty)$ exists, that

$$(\gamma, \beta) \in \mathcal{C}_+ \Rightarrow g(\infty) = \sigma.$$

We now pass along $\mathcal{C}_+$ from $\gamma = 0$ to $\gamma = 1$. Near $\gamma = 0$ we have

Lemma 3.4. *There exists a number $\beta_0 > 0$ such that if $(\gamma, \beta) \in \mathcal{C}_+ \cap \{\beta < \beta_0\}$, then $f(\infty) < 1$.*

Proof. If we eliminate g'' from (2.1) by means of (2.2), we obtain the equation

$$f'' + \frac{\eta}{2g}(1 + qf)f' + \frac{\eta}{2g}pg'f = 0.$$

Since $g > 1$ and $g' < \beta$ on $(0, \infty)$ we may conclude that if $\gamma = 0$ and so $f(0) = 0$ and $f'(0) = 0$, then $f(\eta) = 0$ for all $\eta \geq 0$ and in particular $f(\infty) = 0 < 1$. The assertion now follows from the continuous dependence of $f(\infty)$ on (γ, β) proved in Lemma 3.2.

For $\gamma = 1$, we have by Lemma 2.7a

Lemma 3.5. *If $(\gamma, \beta) \in \mathcal{C}_+ \cap \{\gamma = 1\}$, then $f(\infty) > 1$.*

Thus, as we pass along $\mathcal{C}_+$ from $\gamma = 0$ to $\gamma = 1$, $f(\infty)$ changes continuously from a value less than one to a value greater than one. Therefore, there must exist a point $(\gamma_0, \beta_0) \in \mathcal{C}_+ \cap \{0 < \gamma < 1\}$ such that $f(\infty) = 1$. Since $g(\infty) = \sigma$ for any point on $\mathcal{C}_+$, the solution (f_0, g_0) which corresponds to (γ_0, β_0) satisfies the two conditions at infinity. This completes the proof.

4. The shooting: $0 < \sigma < 1$

As in Section 3 we find it convenient to work with the parameters β and γ and thus we write the initial conditions again as

$$f(0) = \gamma, \quad f'(0) = \beta\gamma, \quad g(0) = 1, \quad g'(0) = \beta. \quad (4.1)$$

Since $\sigma < 1$ in this section, it follows from Lemma 2.3 that

$$\beta < 0 \quad \text{and} \quad \gamma > 1. \quad (4.2)$$

However we can no longer assume that $f(\eta)g(\eta) > 0$ for all $\eta \geq 0$, i.e., it may happen that $\eta^* < \infty$. In the next lemma we shall obtain an a priori bound for γ .

Lemma 4.1. *Let (f, g) be a solution of (1.11)-(1.14). Then*

$$\begin{aligned}\gamma &< \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q} \quad \text{if } \sigma < 1, \\ \gamma &> \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q} \quad \text{if } \sigma > 1.\end{aligned}$$

Proof. We combine equations (1.11) and (1.12) to

$$(f'g - fg')' = \frac{1}{q}g'' + \frac{p}{2q}\eta g'. \quad (4.3)$$

This yields upon integration over (η, ∞) .

$$f'g - fg' = \frac{1}{q}g' - \frac{p}{2q} \int_{\eta}^{\infty} sg'(s)ds, \quad (4.4)$$

or, when we divide by g^2 ,

$$\left(\frac{f}{g}\right)' = -\frac{1}{q} \left(\frac{1}{g}\right)' - \frac{p}{2q} \frac{1}{g^2} \int_{\eta}^{\infty} sg'(s)ds. \quad (4.5)$$

When we integrate (4.5) finally over $(0, \infty)$, we obtain in view of our boundary conditions (1.13) and (1.14)

$$\frac{1}{\sigma} - \gamma = -\frac{1}{q} \left(\frac{1}{\sigma} - 1\right) - \frac{p}{2q} \int_0^{\infty} \frac{1}{g^2(t)} \left(\int_t^{\infty} sg'(s)ds\right) dt.$$

Suppose that $\sigma < 1$. Then $g' < 0$ by Lemma 2.2 and we conclude that

$$\frac{1}{\sigma} - \gamma > -\frac{1}{q} \left(\frac{1}{\sigma} - 1\right)$$

or

$$\gamma < \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q}.$$

Thus, it follows from (4.2) and Lemma 4.1 that we have to look for a pair (γ, β) in the set

$$\mathcal{D}_- = \{(\gamma, \beta) : 1 \leq \gamma \leq \gamma^*, \beta \leq 0\}$$

where $\gamma^* = \sigma^{-1}(1 + q^{-1}) - q^{-1}$.

We define the sets

$$\begin{aligned}\mathcal{A}_- &= \{(\gamma, \beta) \in \mathcal{D}_- : g(\infty) > \sigma\} \\ \mathcal{B}_- &= \{(\gamma, \beta) \in \mathcal{D}_- : g(\eta) < \sigma \text{ for some } 0 < \eta < \infty\}.\end{aligned}$$

If $\beta = 0$, then $(f, g) = (\gamma, 1)$ and so $g(\infty) = 1 > \sigma$. Therefore $(\gamma, 0) \in \mathcal{A}_-$ if $1 \leq \gamma \leq \gamma^*$ (See Fig. 3)

Fig. 3. The $\gamma\beta$ - plane ($\sigma < 1$).

Proceeding as in Section 3 we now show that $(\gamma, \beta) \in \mathcal{B}_-$ if β is large and negative.

Lemma 4.2. *There exists a constraint $\tilde{\beta} < 0$ such that if $1 \leq \gamma \leq \gamma^*$ and $\beta < \tilde{\beta}$, then $(\gamma, \beta) \in \mathcal{B}_-$.*

Proof. We use a scaling argument again. Set $t = -\beta\eta$. Then (2.1) - (2.5) become

$$f''g - f_g'' = -\frac{1}{2\beta^2}tf' \quad (4.6)$$

$$g'' = -\frac{1}{2\beta^2}t(qf' + pg') \quad (4.7)$$

$$f(0) = \gamma, f'(0) = -\gamma, g(0) = 1, g'(0) = -1 \quad (4.8)$$

and it is clear, as in Section 3, that as $\beta \rightarrow \infty$, $(f, g) \rightarrow (f_0, g_0)$ on compact sets, where

$$f_0(t) = \gamma - \gamma t \quad \text{and} \quad g_0(t) = 1 - t.$$

Hence, for large negative values of β (independent of $\gamma \in [1, \gamma^*]$) g drops below σ so that (γ, β) then belongs to $\mathcal{B}_-$.

Lemma 4.3. *The sets $\mathcal{A}_-$ and $\mathcal{B}_-$ are open.*

Proof. To prove that $\mathcal{A}_-$ is open, we can proceed exactly as in the proof of Lemma 3.2. Because $g(\infty) > \sigma$, we know that $g(\eta) > \sigma$ for all $\eta \geq 0$ and hence that $\eta^* = \infty$.

To show that $\mathcal{B}_-$ is open we proceed differently. Suppose that $(\bar{\gamma}, \bar{\beta}) \in \mathcal{B}_-$, let $(\bar{f}, \bar{g})$ be the corresponding solution, and let $\bar{\eta} \in (0, \infty)$ be given by

$$\bar{g}(\bar{\eta}) = \sigma.$$

Since $\bar{g}' < 0$ we can choose numbers $\delta \in (0, \frac{1}{3}\sigma)$ and $\eta_\delta > \bar{\eta}$ such that

$$\bar{g}(\eta_\delta) = \sigma - 2\delta.$$

Thus, remembering Lemma 2.5, we have

$$\bar{f}(\eta) > \sigma - 2\delta \quad \text{and} \quad \bar{g}(\eta) \geq \sigma - 2\delta \quad \text{for} \quad 0 \leq \eta \leq \eta_\delta.$$

Therefore, by continuous dependence on initial data there exists a neighbourhood $\mathcal{N}$ of $(\bar{\gamma}, \bar{\beta})$ such that if $(\gamma, \beta) \in \mathcal{N}$, then

$$f(\eta) > \sigma - 3\delta \quad \text{and} \quad g(\eta) > \sigma - 3\delta \quad \text{for} \quad 0 \leq \eta \leq \eta_\delta$$

as well as

$$\sigma - \delta < g(\eta_\delta) < \sigma - 3\delta.$$

Thus $\mathcal{N} \subset \mathcal{B}_-$ and $\mathcal{B}_-$ is open.

As in Section 3 we may now appeal to the topological result of McLeod & Serrin [McLS] to conclude that there exists a continuum $\mathcal{C}_- \subset \mathcal{D}_- \setminus (\mathcal{A}_- \cup \mathcal{B}_-)$ which joins the half lines $\{\gamma = 1, \beta \leq 0\}$ and $\{\gamma = \gamma^*, \beta \leq 0\}$.

Lemma 4.4. *If $(\gamma, \beta) \in \mathcal{C}_-$, then $g(\infty) = \sigma$.*

Proof. Since $(\gamma, \beta) \notin \mathcal{B}_-$, we have $g(\eta) > \sigma$ for all $\eta \geq 0$. Remembering Lemma 2.4 this means that $\eta^* = \infty$. Thus, by Lemma 2.2

$$\lim_{\eta \rightarrow \infty} g(\eta) \text{ exists } \geq \sigma. \tag{4.9}$$

Because $(\gamma, \beta) \notin \mathcal{A}_-$, equality must hold in (4.9).

It remains to prove that $f(\infty) = 1$ for some $(\gamma, \beta) \in \mathcal{C}_-$. This follows from the continuity of $f(\infty)$ with respect to $(\gamma, \beta) \in \mathcal{C}_-$, which can be proved exactly as in Lemma 3.2, and the following two lemmas.

Lemma 4.5. *Let $(1, \beta) \in \mathcal{C}_-$. Then $f(\infty) < 1$.*

Proof. This follows immediately from Lemma 2.7a.

Lemma 4.6. *Let $(\gamma^*, \beta) \in \mathcal{C}_-$. Then $f(\infty) > 1$.*

Proof. For this we return to (4.5), which we integrate over $(0, \infty)$. This yields

$$\begin{aligned} \frac{f(\infty)}{\sigma} - \gamma^* &= \frac{1}{q} \left(1 - \frac{1}{\sigma}\right) - \frac{p}{2q} \int_0^\infty \frac{1}{g^2(t)} \left(\int_t^\infty s g'(s) ds \right) dt \\ &> \frac{1}{q} \left(1 - \frac{1}{\sigma}\right) \end{aligned}$$

because $g'(\eta) < 0$ for all $\eta \geq 0$. Hence

$$\frac{f(\infty)}{\sigma} > \frac{1}{\sigma} \left(1 + \frac{1}{q}\right) - \frac{1}{q} + \frac{1}{q} \left(1 - \frac{1}{\sigma}\right) = \frac{1}{\sigma},$$

or $f(\infty) > 1$.

Thus, with $f(\infty) < 1$ at one end and $f(\infty) > 1$ at the other end of $\mathcal{C}_-$, there must exist a point $(\bar{\gamma}, \bar{\beta}) \in \mathcal{C}_-$ for which $f(\infty) = 1$. This completes the proof.

5. Asymptotic behaviour

Let (f, g) be a solution of (1.11)-(1.14) in which σ is some prescribed positive number. By (1.13)

$$f(\eta) \rightarrow 1 \quad \text{and} \quad g(\eta) \rightarrow \sigma \quad \text{as} \quad \eta \rightarrow \infty. \quad (5.1)$$

In this section we shall obtain estimates for the rates of convergence in (5.1), refining the preliminary estimates derived in Lemma 2.11:

$$f(\eta) = 1 + O(\eta^{-1} e^{-\kappa \eta^2}) \quad \text{as} \quad \eta \rightarrow \infty \quad (5.2)$$

$$g(\eta) = \sigma + O(\eta^{-1} e^{-\kappa \eta^2}) \quad \text{as} \quad \eta \rightarrow \infty \quad (5.3)$$

in which κ is a positive number.

We shall prove

Theorem 5.1. *Suppose that (f, g) is a solution of (1.11) - (1.14) for some $\sigma > 0$ ($\sigma \neq 1$). Then there exists a positive constant K such that*

$$\begin{aligned} f(\eta) &\sim 1 - K \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2 / 4} \quad \text{as} \quad \eta \rightarrow \infty \\ g(\eta) &\sim \sigma + \frac{Kq}{p - \lambda} \operatorname{sgn}(\sigma - 1) \eta^{-1} e^{-\lambda \eta^2 / 4} \quad \text{as} \quad \eta \rightarrow \infty \end{aligned}$$

in which

$$\lambda = \frac{1}{2} \left(p + \frac{1+q}{\sigma} \right) - \frac{1}{2} \sqrt{\left(p + \frac{1+q}{\sigma} \right)^2 - \frac{4p}{\sigma}}.$$

Proof. Write

$$f(\eta) = 1 + u(\eta) \quad \text{and} \quad g(\eta) = \sigma + v(\eta),$$

and set $w = \text{col}(u, v)$. Then, proceeding as in the proof of Lemma 3.2, we find that w satisfies

$$w'' + \frac{1}{2}\eta\{A + \rho(w)\}w' = 0,$$

where

$$A = \begin{pmatrix} \frac{1+q}{\sigma} & \frac{p}{\sigma} \\ q & p \end{pmatrix} \quad \text{and} \quad \rho(w) = O(|w|) \quad \text{as} \quad w \rightarrow 0. \quad (5.4)$$

In terms of the variables

$$t = \frac{\eta^2}{4}, \quad y(t) = w'(\eta), \quad r(t) = \rho(w(\eta)), \quad (5.5)$$

this equation can be written as

$$y' = -\{A + r(t)\}y. \quad (5.6)$$

Note that in view of (5.2)-(5.4),

$$r(t) = O(e^{-4\kappa t}) \quad \text{as} \quad t \rightarrow \infty.$$

The eigenvalues λ and μ of A are given by

$$\lambda, \mu = \frac{1}{2}\left(p + \frac{1+q}{\sigma}\right) \pm \frac{1}{2}\sqrt{\left(p + \frac{1+q}{\sigma}\right)^2 - \frac{4p}{\sigma}}.$$

Plainly, for all values of $p, q, \sigma \in \mathbf{R}^+$, λ and μ are real, positive and distinct; we shall order them so that $0 < \lambda < \mu$ and denote the corresponding eigenvectors by ξ and ζ . We can conclude from [CL, Theorem 8.1] that there exist two linearly independent solutions $\varphi(t)$ and $\psi(t)$ of (5.6) so that

$$\varphi(t) \sim e^{-\lambda t}\xi \quad \text{and} \quad \psi(t) \sim e^{-\mu t}\zeta \quad \text{as} \quad t \rightarrow \infty.$$

Since (5.6) is linear we can write its solutions as linear combinations of φ and ψ :

$$y(t) = a\varphi(t) + b\psi(t), \quad a, b \in \mathbf{R}. \quad (5.7)$$

Because $\lambda < \mu$, $y(t)$ will behave as $a\varphi(t)$ when $t \rightarrow \infty$ unless $a = 0$. We shall show that if $y(t)$ corresponds to the solution (f, g) of (1.11)-(1.14), then $a \neq 0$.

Thus, let y correspond to (f, g) and let $y = \text{col}(y_1, y_2)$. Then

$$y_1(t) = f'(\eta) \quad \text{and} \quad y_2(t) = g'(\eta).$$

By the analysis of Section 2, $f'(\eta)$ and $g'(\eta)$ have always different signs for η large enough. Thus

$$y_1(t)y_2(t) < 0 \quad \text{for } t \text{ large.} \quad (5.8)$$

Suppose that $a = 0$. Then

$$y(t) \sim be^{-\mu t} \zeta \quad \text{as } t \rightarrow \infty$$

and so, with $\zeta = \text{col}(\zeta_1, \zeta_2)$,

$$\text{sgn } y_1(t)y_2(t) = \text{sgn } \zeta_1 \zeta_2$$

for large values of t . However

$$q\zeta_1 = (\mu - p)\zeta_2$$

and therefore

$$\zeta_1 \zeta_2 = \frac{\mu - p}{q} \zeta_2^2. \quad (5.9)$$

By an elementary computation we find that

$$\lambda < p < \mu,$$

and so it follows from (5.9) that

$$\zeta_1 \zeta_2 > 0.$$

Therefore, if $a = 0$, the solution $y(t)$ cannot satisfy (5.8) for large values of t and we must conclude that $a \neq 0$. This implies that

$$y(t) \sim ae^{-\lambda t} \xi \quad \text{as } t \rightarrow \infty$$

and

$$w'(\eta) \sim ae^{-\lambda\eta^2/4} \xi \quad \text{as } \eta \rightarrow \infty.$$

Thus, since $\xi = \text{col}(1, -q/(p - \lambda))$, we have shown that

$$f'(\eta) \sim ae^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty \quad (5.10)$$

$$g'(\eta) \sim -a \frac{q}{p - \lambda} e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty \quad (5.11)$$

in which a is a constant different from zero. The estimates for $f(\eta)$ and $g(\eta)$ now follow upon integration of (5.10) and (5.11) over (η, ∞) . They are

$$f(\eta) \sim 1 - \frac{2a}{\lambda} \eta^{-1} e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty \quad (5.12)$$

$$g(\eta) \sim \sigma + \frac{2a}{\lambda} \frac{q}{p - \lambda} \eta^{-1} e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty. \quad (5.13)$$

Remark. Using the estimates (5.10) - (5.13) we obtain for $H(\eta)$ the asymptotic estimate

$$H(\eta) \sim a \left(\sigma + \frac{q}{p - \lambda} \right) e^{-\lambda\eta^2/4} \quad \text{as } \eta \rightarrow \infty. \quad (5.14)$$

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