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The development of travelling waves in quadratic and cubic autocatalysis with unequal diffusion rates. I. Permanent form travelling waves

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We study the isothermal autocatalytic system, $A + nB \rightarrow (n+1)B$, where $n = 1$ or 2 for quadratic or cubic autocatalysis respectively. In addition, we allow the chemical species, A and B, to have unequal diffusion rates. The propagating reaction–diffusion waves that may develop from a local initial input of the autocatalyst, B, are considered in one spatial dimension. We find that travelling wave solutions exist for all propagation speeds $v \geqslant v_n^*$, where v_n^* is a function of the ratio of the diffusion rates of the species A and B and represents the minimum propagation speed. It is also shown that the concentration of the autocatalyst, B, decays exponentially ahead of the wavefront for quadratic autocatalysis. However, for cubic autocatalysis, although the concentration of the autocatalyst decays exponentially ahead of the wavefront for travelling waves which propagate at speed $v = v_2^*$, this rate of decay is only algebraic for faster travelling waves with $v > v_2^*$. This difference in decay rate has implications for the selection of the long time wave speed when such travelling waves are generated from an initial-value problem.

1. Introduction

In this paper we consider two model, isothermal, autocatalytic, chemical reaction schemes. The first scheme is based on the quadratic autocatalytic step

$$A + B \rightarrow 2B, \quad \text{rate} \quad k_1 ab, \tag{1}$$

while the second scheme is based on the cubic autocatalytic step

$$A + 2B \rightarrow 3B, \quad \text{rate} \quad k_2 ab^2. \tag{2}$$

Here a and b are the concentrations of the reactant, A, and the autocatalyst, B, respectively, and k_1 and k_2 are constant reaction rates. The autocatalytic steps (1)

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and (2) have been used in several successful models of real chemical systems. The quadratic step (1) arises in models of the Belousov–Zhabotinskii reaction and also gas-phase, radical chain branching, oxidation reactions, such as the carbon-monoxide–oxygen, and hydrogen–oxygen systems (Gray *et al.* 1984; Merkin *et al.* 1985). Almost isothermal flames in the carbon-sulphide–oxygen reaction, which arise from quadratic branching, can be described in terms of the cubic autocatalytic step (2) (Voronkov & Semenov 1939). The cubic rate law also provides a good model for both the iodate–arsenous acid reaction (Saul & Showalter 1984) and hydroxylamine–nitrate reaction (Gowland & Stedman 1983). On a theoretical level, Aris *et al.* (1988) have shown that the chemically implausible termolecular step can be replaced by a series of elementary, bimolecular steps which lead to the cubic rate law (2). Autocatalytic rate laws also arise in enzyme reactions such as glycolysis (Sel'kov 1968).

Observations show that chemical systems for which quadratic or cubic autocatalysis forms a key step can support propagating chemical wavefronts, when the reaction mixture is unstirred (see, for example, Zaikin & Zhabotinskii 1970; Hanna *et al.* 1982). These wavefronts, or travelling waves, arise via a combination of reaction and diffusion. Physically, the typical situation which leads to the development of travelling waves is that which arises when a quantity of the autocatalyst, B, is introduced locally into an expanse of the reactant, A, which is initially at uniform concentration. The developing reaction is often observed to generate wavefronts, which propagate outward from the initial reaction zone. It is this phenomenon that we address in the present paper. For analytical convenience, we restrict attention to the case of one-dimensional slab geometry, with the coordinate $\bar{x}$ measuring distance.

The equations that govern the reaction and diffusion of the species A and B under reaction schemes (1) and (2) are

$$\partial a/\partial \bar{t} = D_{\mathrm{A}}(\partial^2 a/\partial \bar{x}^2) - k_n ab^n, \tag{3a}$$

$$\partial b/\partial \bar{t} = D_{\mathrm{B}}(\partial^2 b/\partial \bar{x}^2) + k_n ab^n. \tag{3b}$$

Here D_{A} and D_{B} are the constant diffusion rates of the reactant, A, and the autocatalyst, B, respectively, and $\bar{t}$ is time, Under quadratic autocatalysis $n = 1$, while for cubic autocatalysis $n = 2$. The initial conditions to be considered are

$$a(\bar{x}, 0) = a_0, \quad b(\bar{x}, 0) = b_0 g(\bar{x}), \quad |\bar{x}| < \infty, \tag{4a}$$

where $g(\bar{x})$ is a given, non-negative function of $\bar{x}$, with a maximum value of unity, and $g(\bar{x}) \to 0$ as $|x| \to \infty$. Here a_0 and b_0 are the positive, constant, initial concentration of A and maximum initial concentration of B respectively. In addition, we have the boundary conditions

$$a(\bar{x}, \bar{t}) \to a_0, \quad b(\bar{x}, \bar{t}) \to 0, \quad \text{as} \quad |\bar{x}| \to \infty. \tag{4b}$$

It is convenient to introduce dimensionless variables as

$$\alpha = a/a_0, \quad \beta = b/a_0, \quad t = k_n a_0^n \bar{t}, \quad x = (k_n a_0^n / D_{\mathrm{A}})^{\frac{1}{2}} \bar{x}, \tag{5}$$

in terms of which equation (3), together with initial and boundary conditions (4), becomes

$$\partial\alpha/\partial t = (\partial^2\alpha/\partial x^2) - \alpha\beta^n, \tag{6a}$$

$$\partial\beta/\partial t = D(\partial^2\beta/\partial x^2) + \alpha\beta^n, \tag{6b}$$

where $D = D_B/D_A$ and

$$\alpha(x,0) = 1, \quad \beta(x,0) = \beta_0 g(x), \quad |x| < \infty, \tag{7a}$$

$$\alpha(x,t) \to 1, \quad \beta(x,t) \to 0, \quad \text{as} \quad |x| \to \infty. \tag{7b}$$

The dimensionless parameter $\beta_0 = b_0/a_0$ provides a measure of the maximum concentration of the initial input of the autocatalyst, while the dimensionless parameter, D, measures the rate of diffusion of the autocatalyst, B, relative to that of the reactant, A. In chemical systems that involve reactants of similar molecular weight it is a reasonable approximation to assume that the diffusion coefficients, D_A and D_B, are equal, which gives $D = 1$. This simplifying assumption was used by Billingham & Needham (1990) and Merkin & Needham (1989). However, enzyme reactions may involve large enzyme molecules and much smaller substrate molecules, which can lead to significantly different diffusion rates. It is also possible to immobilize enzymes in a gel or membrane, so that one diffusion coefficient is zero (see, for example, Kernevez *et al.* 1979). Equation (6) also arises in epidemiology, where α represents the number density of healthy individuals and β the number density of infected individuals (see, for example, Bailey 1975). Infected individuals may be significantly more or less mobile than healthy individuals. This situation again leads to a value for D that can be significantly different from unity. Thus it is of interest to consider the behaviour of solutions to the initial-value problem (6) and (7) when $D \neq 1$. In this paper we will assume only that $D > 0$.

An important preliminary to the study of the initial-value problem (6) and (7) is an investigation of the permanent form travelling wave solutions of equation (6*a*, *b*), which may be generated from the initial-value problem (6) and (7). We study these in the present paper and to this end we make the following definition.

Definition. A permanent form travelling wave solution of equation (6*a*, *b*) is a non-trivial, non-negative solution that depends only on the single variable $z = x - \gamma(t)$, where $\gamma(t)$ is the position of the wavefront, and satisfies the conditions $\alpha \to 1$, $\beta \to 0$ as $z \to +\infty$, and $\alpha \to \alpha_{-\infty}$, $\beta \to \beta_{-\infty}$ as $z \to -\infty$, where $\alpha_{-\infty}, \beta_{-\infty}$ are the uniform, non-negative concentrations behind the wavefront.

2. General properties of travelling wave solutions

The equations which govern permanent form travelling waves are obtained by looking for a solution of equation (6*a*, *b*) in the form $\alpha \equiv \alpha(z)$ and $\beta \equiv \beta(z)$ which becomes

$$\alpha_{zz} + v\alpha_z - \alpha\beta^n = 0, \tag{8a}$$

$$D\beta_{zz} + v\beta_z + \alpha\beta^n = 0, \tag{8b}$$

where $v(t) = \mathrm{d}\gamma/\mathrm{d}t$. However, since α and β are functions of z alone, equation (8*a*, *b*) shows that the front propagation speed, v, must be constant, after which the symmetry of the equation shows that we need only consider the case when $v > 0$. We now prove four elementary results which concern the travelling wave solutions of equation (8*a*, *b*).

Proposition 2.1. *A permanent form travelling wave solution of equation* (8*a*, *b*) *has* $\alpha > 0$ *and* $\beta > 0$ *for all* $-\infty < z < \infty$.

Proof. Let $\alpha(z)$, $\beta(z)$ be a permanent form travelling wave solution and suppose that there exists a z_0 such that $\alpha(z_0) = 0$. Then, since $\alpha(z)$ is non-negative, we have that

$\alpha_z(z_0) = 0$. Moreover, for the given $\beta(z)$, equation (8a) can be regarded as a second-order, linear, ordinary differential equation for $\alpha(z)$, which has no singular points for any $-\infty < z < \infty$. Thus any initial value problem for $\alpha(z)$ has a unique solution in $-\infty < z < \infty$ (see, for example, Burkhill 1968). Equation (8a) together with the above homogeneous conditions at z_0 form an initial value problem for $\alpha(z)$, which has the unique solution $\alpha(z) \equiv 0$ for $-\infty < z < \infty$. However, we must have $\alpha \to 1$ as $z \to \infty$ for a permanent form travelling wave solution. Hence, no such z_0 exists and $\alpha > 0$ for all $-\infty < z < \infty$. Following similar arguments, we readily establish the equivalent results for β. □

Proposition 2.2. *A permanent form travelling wave solution of equation* (8a, b) *has* $\alpha \to 0$, $\beta \to 1$ *as* $z \to -\infty$.

Proof. Let $\alpha(z)$, $\beta(z)$ be a permanent form travelling wave solution. As $z \to -\infty$, $\alpha \to \alpha_{-\infty}$ and hence $\alpha_z, \alpha_{zz} \to 0$. Thus, from equation (8$a$), we must have that $\alpha_{-\infty} = 0$ or $\beta_{-\infty} = 0$. After integrating equation (8a, b) with respect to z on the range $-\infty < z < \infty$ we obtain

$$\int_{-\infty}^{\infty} \alpha\beta^n \, dz = v(1-\alpha_{-\infty}), \quad \int_{-\infty}^{\infty} \alpha\beta^n \, dz = v\beta_{-\infty}. \tag{9a, b}$$

Equation (9a, b) shows that $\alpha_{-\infty} + \beta_{-\infty} = 1$, and hence $\alpha_{-\infty} = 0$, $\beta_{-\infty} = 1$ or $\alpha_{-\infty} = 1$, $\beta_{-\infty} = 0$. However, via (9b) and Proposition 2.1, $\beta_{-\infty} \neq 0$ and therefore $\alpha_{-\infty} = 0$, $\beta_{-\infty} = 1$ and the proposition is established. □

Proposition 2.3. *A permanent form travelling wave solution of equation* (8a, b) *is strictly monotone increasing in* α *and strictly monotone decreasing in* β, *with* $0 < \alpha < 1$ *and* $0 < \beta < 1$ *for* $-\infty < z < \infty$.

Proof. Let $\alpha(z)$, $\beta(z)$ be a permanent form travelling wave solution. Suppose $\alpha_z(z)$ has more than one zero in $-\infty < z < \infty$. Let z_n and z_{n+1} be two consecutive zeros of $\alpha_z(z)$ with $z_n < z_{n+1}$. Then, using equation (8a) and proposition 2.1, we have that $\alpha_{zz}(z_{n+1}) > 0$ and hence $\alpha_z(z) < 0$ for all $z_n < z < z_{n+1}$. Thus $\alpha_{zz}(z_n) \leqslant 0$. However, from equation (8a) and Proposition 2.1, we obtain $\alpha_{zz}(z_n) > 0$. This leads to a contradiction and we conclude that $\alpha_z(z)$ has at most one zero for $-\infty < z < \infty$. Suppose now that $\alpha_z(z)$ has exactly one zero in $-\infty < z < \infty$ at $z = z_0$. Since $\alpha_z(z_0) = 0$, equation (8a) and Proposition 2.1 shows that $\alpha_{zz}(z_0) > 0$, and hence $\alpha_z(z) < 0$ for all $-\infty < z < z_0$. Therefore, on integrating α_z with respect to z on the range $-\infty < z < z^*$, we obtain, on using proposition 2.2,

$$\int_{-\infty}^{z^*} \alpha_z \, dz = \alpha(z^*) < 0,$$

for any $-\infty < z^* < z_0$, which violates Proposition 2.1. Thus we conclude that $\alpha_z(z) \neq 0$ for any $-\infty < z < \infty$. Also, from proposition 2.2, $\alpha \to 0$ as $z \to -\infty$ and $\alpha \to 1$ as $z \to +\infty$, and so $\alpha(z)$ is strictly monotone increasing, with $0 < \alpha < 1$ for $-\infty < z < \infty$. A similar argument establishes the analogous result for $\beta(z)$. □

Proposition 2.4. *A permanent form travelling wave solution of equation* (8a, b) *has* $\alpha + \beta \gtreqqless 1$ *for* $-\infty < z < \infty$ *when* $D \gtreqqless 1$.

Proof. On addition, equation (8a, b) may be integrated once to yield, after application of the conditions in Proposition 2.2,

$$(\alpha+\beta)_z + v(\alpha+\beta) = v + (1-D)\,\beta_z \gtreqqless v \quad \text{for} \quad -\infty < z < \infty, \tag{10}$$

when $D \gtreqless 1$. By integrating this inequality and applying the condition $(\alpha+\beta)\rightarrow 1$ as $z\rightarrow-\infty$, the result is established. □

We also note that equation (10) may be integrated once more to give

$$\int_{-\infty}^{\infty}(1-\alpha-\beta)\,\mathrm{d}z=\frac{1-D}{v}, \tag{11}$$

after applying the appropriate boundary conditions as $z\rightarrow\pm\infty$. Together with Propositions 2.3 and 2.4, equation (11) shows that, at any $D\geqslant 0$, as $v\rightarrow\infty$, $\alpha+\beta\rightarrow 1$ uniformly for $-\infty<z<\infty$. It is now convenient to introduce the dependent variable, $w=\beta_z$, and write equations (8*b*) and (10) as the equivalent third-order system

$$\alpha_z=v(1-\alpha-\beta)-Dw, \tag{12a}$$

$$\beta_z=w, \tag{12b}$$

$$w_z=-D^{-1}(\alpha\beta^n+vw). \tag{12c}$$

A permanent form travelling wave solution of equation (8*a*, *b*) is equivalent to a solution of equation (12) in the domain $-\infty<z<\infty$, with $\alpha,\beta>0$ and which satisfies the conditions

$$\alpha\rightarrow 1,\quad \beta\rightarrow 0,\quad w\rightarrow 0\quad \text{as}\quad z\rightarrow+\infty, \tag{13a}$$

$$\alpha\rightarrow 0,\quad \beta\rightarrow 1,\quad w\rightarrow 0\quad \text{as}\quad z\rightarrow-\infty. \tag{13b}$$

For each fixed $D\geqslant 0$ this can be thought of as a nonlinear eigenvalue problem, with the positive propagation speed, v, being the eigenvalue.

From Proposition 2.4 when $D=1$, $\alpha+\beta\equiv 1$ and equation (8*a*, *b*) reduces to the single equation

$$\beta_{zz}+v\beta_z+\beta^n(1-\beta)=0, \tag{14}$$

or the equivalent second-order system,

$$\beta_z=w,\quad w_z=-\{\beta^n(1-\beta)+vw\}. \tag{15a, b}$$

For quadratic autocatalysis, $n=1$, equation (14) is the Fisher equation (Fisher 1937), while for cubic autocatalysis, $n=2$, equation (14) is the cubic Fisher equation. On applying a theorem given in Britton (1986) it is readily shown that equation (14) has permanent form travelling wave solutions for all $v\geqslant v_n^*$, where $v_1^*\in(0,2]$ and $v_2^*\in(0,1]$. A phase plane analysis of equation (15) shows that $v_1^*=2$ (see, for example, Murray 1977) and $v_2^*=1/\surd 2$ (Billingham & Needham 1990). However, these and other general results on second-order equations, such as (14), are not applicable to third-order systems, such as (12). Thus to obtain detailed information about the solutions of the eigenvalue problem posed by (12) and (13) when $D\neq 1$, we must consider the system (12) in the (α,β,w) phase space. We address first the case of quadratic autocatalysis with $n=1$.

3. Quadratic autocatalysis, $n=1$

When $n=1$, equation (12*a*, *b*, *c*) becomes

$$\alpha_z=v(1-\alpha-\beta)-Dw, \tag{16a}$$

$$\beta_z=w, \tag{16b}$$

$$w_z=-D^{-1}(\alpha\beta+vw). \tag{16c}$$

This system has just two finite equilibrium points in the (α, β, w) phase space at (0, 1, 0) and (1, 0, 0.). Thus a solution of equation (8a, b) which satisfies conditions (13a, b) is a directed integral path of equation (16a, b, c) which connects the point (0, 1, 0) to (1, 0, 0). We begin by examining the local behaviour in the neighbourhood of the two finite equilibrium points. Linearization of equation (16) about the point (0, 1, 0) shows that it is a simple equilibrium point with a two-dimensional stable manifold and a one-dimensional unstable manifold. The eigenvalues and associated eigenvectors are

$$\lambda_1 = -vD^{-1}, \qquad \boldsymbol{e}_{\lambda_1} = (0, -1, -\lambda_1)^{\mathrm{T}}, \tag{17a}$$

$$\lambda_2 = -\tfrac{1}{2}\{\surd(v^2+4)+v\}, \qquad \boldsymbol{e}_{\lambda_2} = (\lambda_2(D\lambda_2+v), -1, -\lambda_2)^{\mathrm{T}}, \tag{17b}$$

$$\lambda_3 = \tfrac{1}{2}\{\surd(v^2+4)-v\}, \qquad \boldsymbol{e}_{\lambda_3} = (\lambda_3(D\lambda_3+v), -1, -\lambda_3)^{\mathrm{T}}. \tag{17c}$$

Therefore the only integral path which satisfies condition (13b) and has $\alpha \geqslant 0$ as $z \to -\infty$ is the unstable manifold of the point (0, 1, 0) in $\alpha \geqslant 0$, which we label S_1. Linearization of equation (16) about the other equilibrium point (1, 0, 0) shows that it is a simple, stable equilibrium point with eigenvalues and associated eigenvectors given by

$$\mu_1 = -v, \qquad \boldsymbol{e}_{\mu_1} = (1, 0, 0)^{\mathrm{T}}, \tag{18a}$$

$$\mu_2 = -(1/2\mathrm{D})\{\surd(v^2-4D)+v\}, \qquad \boldsymbol{e}_{\mu_2} = (\{D\mu_2+v\}, -\{\mu_2+v\}, -\mu_2\{\mu_2+v\})^{\mathrm{T}}, \tag{18b}$$

$$\mu_3 = (1/2D)\{\surd(v^2-4D)-v\}, \qquad \boldsymbol{e}_{\mu_3} = (\{D\mu_3+v\}, -\{\mu_3+v\}, -\mu_3\{\mu_3+v\})^{\mathrm{T}}. \tag{18c}$$

When $v < 2\surd D$, the two eigenvalues μ_2 and μ_3 are complex conjugate, and, sufficiently close to the equilibrium point (1, 0, 0), all solutions are oscillatory and take both positive and negative values of β. However, a permanent form travelling wave solution must enter the point (1, 0, 0) and remain non-negative, which leads to the following result.

Proposition 3.1. *There exist no permanent form travelling wave solutions of equation* (16a, b, c) *for* $v < 2\surd D$.

This proposition establishes a necessary condition for the existence of a permanent form travelling wave solution of equation (16a, b, c). The following proposition establishes the sufficiency of this condition.

Proposition 3.2. *A unique permanent form travelling wave solution of equation* (16a, b, c) *exists for each* $v \geqslant 2\surd D$.

Proof. Define the region R by

$$R = \{(\alpha, \beta, w): 0 \leqslant \alpha \leqslant 1, 0 \leqslant \beta \leqslant 1, -(v\beta/2D) \leqslant w \leqslant 0\}. \tag{19}$$

An examination of equation (16a, b, c) shows that for each $v \geqslant 2\surd D$, all integral paths at the faces of R are directed strictly into R, whilst the integral paths at the edges are directed into or along the surface of R. Under these conditions it is readily deduced that any integral path which strictly enters R must remain within R. Moreover, since $\beta_z = w < 0$ within R, any integral path which starts within R, or strictly enters R, is monotone decreasing in β as z increases. However, the integral path must be bounded below by the edge of R along $\beta = 0$. The only remaining possibility is that the integral path enters the stable equilibrium point at (1,0, 0). Thus any integral path, which at $z = z^*$, say, is strictly within R, remains within R

for all $z > z^*$ and is asymptotic to the equilibrium point $(1, 0, 0)$ as $z \to \infty$. Now, via (17*c*), the unstable manifold, S_1, of the equilibrium point $(0, 1, 0)$ enters R. Therefore S_1 remains within R and connects with the equilibrium point $(1, 0, 0)$. This connection is unique, and must have $0 < \alpha < 1$, $0 < \beta < 1$ for all $-\infty < z < \infty$. Thus S_1 represents a unique, permanent form travelling wave solution and the result is established. □

Propositions 3.1 and 3.2 may be combined to give the following.

Proposition 3.3. *A permanent form travelling wave solution of equation* (16*a*, *b*, *c*) *exists if and only if* $v \geqslant v_1^*(D) = 2\sqrt{D}$ *and is unique.*

Note that this is consistent with the minimum propagation speed for Fisher's equation $v_1^*(1) = 2$, as mentioned in §2. Solutions of equation (16*a*, *b*, *c*) were obtained numerically via a fourth-order Runge–Kutta method, with initial values of α and β close to the equilibrium point $(0, 1, 0)$ on the unstable manifold, S_1, given by (17*c*). These numerical integrations of equations (16*a*, *b*, *c*) verify that β becomes negative, and hence that no permanent form travelling wave solution exists if $v < 2\sqrt{D}$. Several permanent form travelling wave solutions are shown in figure 1 for various values of v and D, with $v \geqslant 2\sqrt{D}$. We observe that the width of the wavefront increases with both v and D. The wavefront also becomes more asymmetric as $D \to 0$, with β decaying more rapidly than α as $z \to \infty$. This asymmetry decreases as v increases for fixed D, as indicated by equation (11). We now examine the asymptotic form of these travelling wave solutions for both $D \ll 1$ and $D \gg 1$.

$D \ll 1$. Equation (16*c*) indicates that for $D \ll 1$ and $v \gg D$, w changes rapidly except where $w \sim -\alpha\beta/v$, which thus forms a centre manifold for the system of equation (16), when $D \ll 1$. From arbitrary initial conditions w changes rapidly to reach this centre manifold, with w_z of $O(D^{-1})$, whilst α and β change only at $O(D)$. The remaining dynamics occur on the centre manifold. We note that the two equilibrium points at $(1, 0, 0)$ and $(0, 1, 0)$ lie in the centre manifold and thus, at leading order, the integral path which connects these points and represents the travelling wave solution will lie entirely in the centre manifold. To analyse the behaviour of this travelling wave solution we put $w = -\alpha\beta/v$ and substitute into equation (16) to obtain, at leading order in D,

$$\alpha_z = v(1-\alpha-\beta), \quad \beta_z = -\alpha\beta/v. \tag{20a, b}$$

This two-dimensional system has just two finite equilibrium points in the (α, β) phase plane, at $(1, 0)$ and $(0, 1)$. It is readily shown that for each $v > 0$, there exists a unique integral path which connects these points in $\alpha, \beta > 0$ and represents the leading order approximation, for $D \ll 1$, to the travelling wave solution. Of particular interest is the travelling wave with minimum propagation speed and we continue our analysis by examining the solutions of equation (20*a*, *b*) when $v = O(\sqrt{D})$. On linearization about the equilibrium point $(0, 1)$ we find that, on the unstable manifold, which forms part of the connecting path, $\alpha = O(v)$ and $\beta = O(1)$ as $z \to -\infty$. This suggests the change of variables $\alpha = vA$, $\beta = B$, where $A, B = O(1)$ at least as $z \to -\infty$. We now define region I to be that in which $A, B = O(1)$. At leading order in v, equation (20*a*, *b*) becomes

$$A_z = 1-B, \quad B_z = -AB. \tag{21a, b}$$

In the (A, B) phase plane, the system (21) has a unique finite equilibrium point at $(0, 1)$ which is a saddle.

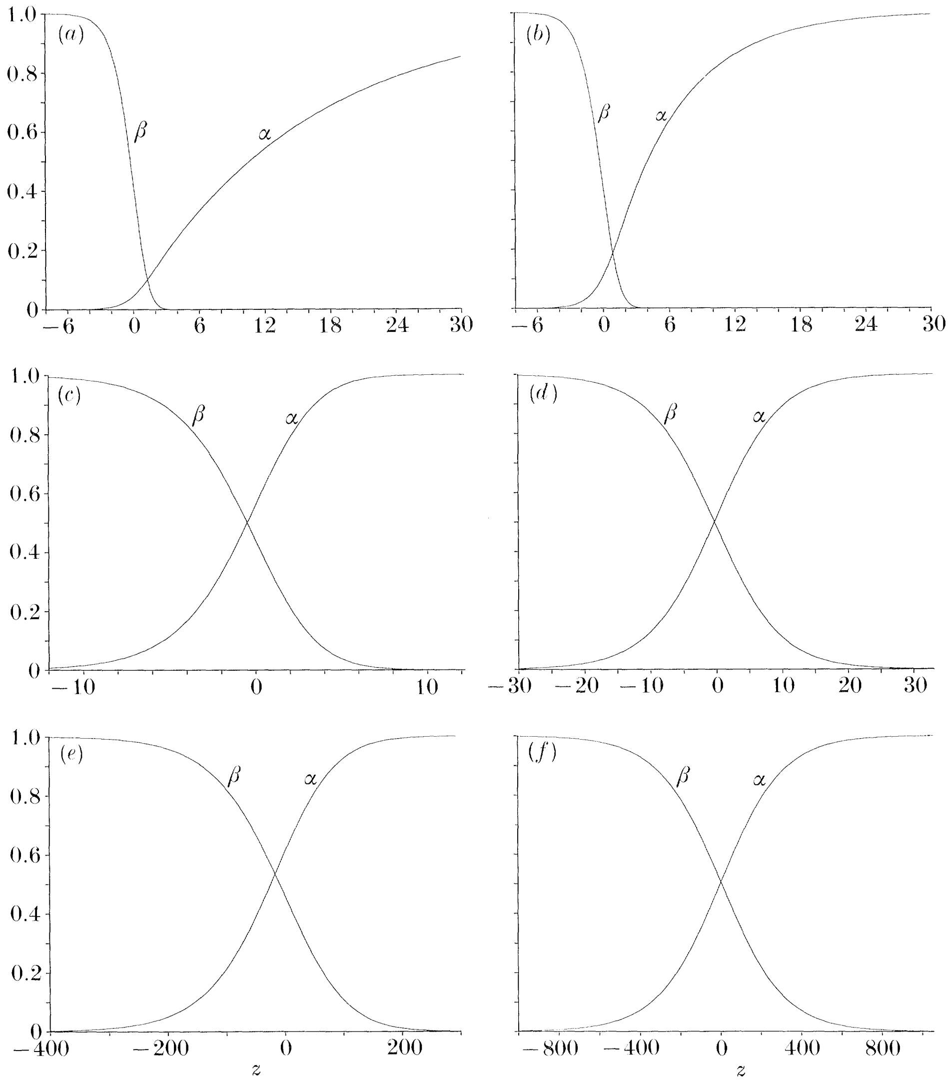

Figure 1. Graphs of the travelling wave solutions of equations (16), when: (*a*) $D = 0.001$, $v = 2\surd D$; (*b*) $D = 0.001$, $v = 5\surd D$; (*c*) $D = 1$, $v = 2\surd D$; (*d*) $D = 1$, $v = 5\surd D$; (*e*) $D = 1000$, $v = 2\surd D$; (*f*) $D = 1000$, $v = 5\surd D$.

We require the integral path which has $A \to 0$, $B \to 1$ as $z \to -\infty$. An examination of the phase portrait of equation (21*a*, *b*) shows that this path is unique, and has $A \to \infty$ and $B \to 0$ as $z \to \infty$. In particular, we have $A(z) \sim z + o(z^{-1})$, $B(z) \sim e^{-\frac{1}{2}(z^2+2)}$ as $z \to \infty$. Since $\alpha = vA \sim vz$ as $z \to \infty$, this approximation becomes non-uniform when $z = O(v^{-1})$ with $\alpha = O(1)$, $\beta = O(e^{-1/v^2})$. Thus we need to introduce a further region with $z \gg 1$, which we label region II, to complete the solution. In region II we let $\eta = vz$ and $\beta = e^{-\phi(\eta)/v^2}$, with η, ϕ of $O(1)$ as $v \to 0$. On substituting into (20), the leading order equations may be integrated immediately to give the solution, which matches as $\eta \to 0$ with the solution in region I, as

$$\alpha = 1 - e^{-\eta}, \quad \beta = \exp\{-(\eta - 1 + e^{-\eta})/v^2\}. \qquad (22a, b)$$

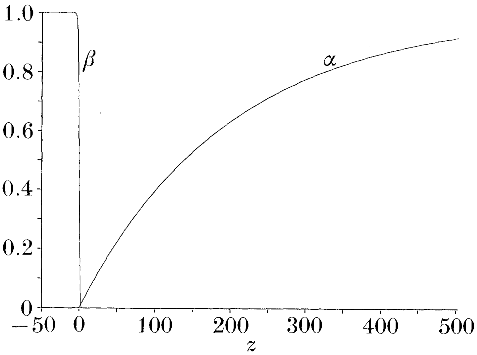

Figure 2. A graph of the travelling wave solution of equation (20) when $v = 0.005$.

This solution has $\alpha \to 1$, $\beta \to 0$ as $\eta \to \infty$, which now satisfies condition (13*a*). A numerical calculation of the travelling wave solution of equation (20) is illustrated in figure 2, when $v = 0.005$. The concentration α exhibits a slow exponential decay to its final value of unity over a region with length of $O(v^{-1})$, as indicated by equation (22*a*). The predicted rapid exponential decay of β, is also clearly visible. The travelling wave solutions with $D \ll 1$ and $v \ll 1$, shown in figure 1, display similar features.

$D \gg 1$. Equation (16) does not have any obvious leading order balance when $D \gg 1$. However, since a travelling wave solution exists only for $v \geqslant 2\sqrt{D}$, this suggests scaling both v and z with $\sqrt{D}$. A further consideration of equation (16) shows that w must be scaled with $D^{-\frac{1}{2}}$. We define appropriate scaled variables by

$$\hat{v}\sqrt{D} = v, \quad \hat{z}\sqrt{D} = z, \quad \hat{\alpha} = \alpha, \quad \hat{\beta} = \beta, \quad \hat{w} = w\sqrt{D}, \tag{23}$$

where $\hat{\alpha}$, $\hat{\beta}$, $\hat{w}$ and $\hat{v}$ are $O(1)$ as $D \to \infty$. In terms of these new variables, equation (16) becomes

$$D^{-1}\hat{\alpha}_{\hat{z}} = \hat{v}(1-\hat{\alpha}-\hat{\beta})-\hat{w}, \quad \hat{\beta}_{\hat{z}} = \hat{w}, \quad \hat{w}_{\hat{z}} = -(\hat{\alpha}\hat{\beta}+\hat{v}\hat{w}). \qquad (24\,a, b, c)$$

Equation (24*a*) indicates that for $D \gg 1$, $\hat{\alpha}$ changes rapidly, except where $\hat{w} \sim \hat{v}(1-\hat{\alpha}-\hat{\beta})$, which forms a centre manifold for the system (24). From arbitrary initial conditions, $\hat{\alpha}$ adjusts rapidly to reach the centre manifold. We note that the two equilibrium points at (0, 1, 0) and (1, 0, 0) lie in the centre manifold and thus, at leading order, the integral path which connects these points and represents the travelling wave solution will lie entirely in the centre manifold. To analyse the behaviour of the travelling wave solution we put $\hat{w} = \hat{v}(1-\hat{\alpha}-\hat{\beta})$ and substitute into equation (24) to obtain, at leading order as $D \to \infty$,

$$\hat{\alpha}_{\hat{z}} = \hat{\alpha}\hat{\beta}/\hat{v}, \quad \hat{\beta}_{\hat{z}} = \hat{v}(1-\hat{\alpha}-\hat{\beta}). \qquad (25\,a, b)$$

This second-order system has just two finite equilibrium points in the $(\hat{\alpha}, \hat{\beta})$ phase plane at (1, 0) and (0, 1), and it is readily shown that there exists a unique connection in $\hat{\alpha}, \hat{\beta} > 0$ between (0, 1) and (1, 0) for $\hat{v} \geqslant 2$, consistent with Proposition 3.3. An asymptotic approximation to this integral path is readily obtained for $\hat{v} \gg 1$, as

$$\hat{\alpha} \sim (\mathrm{e}^{\bar{z}}/1+\mathrm{e}^{\bar{z}}), \quad \hat{\beta} \sim (1/1+\mathrm{e}^{\bar{z}}), \quad \text{as} \quad \hat{v} \to \infty \tag{26}$$

where $\bar{z} = \hat{z}/\hat{v}$. Permanent form travelling wave solutions of equation (25) are illustrated in figure 3 for $\hat{v} = 2$ and $\hat{v} = 5$. These indicate that the asymptotic solution

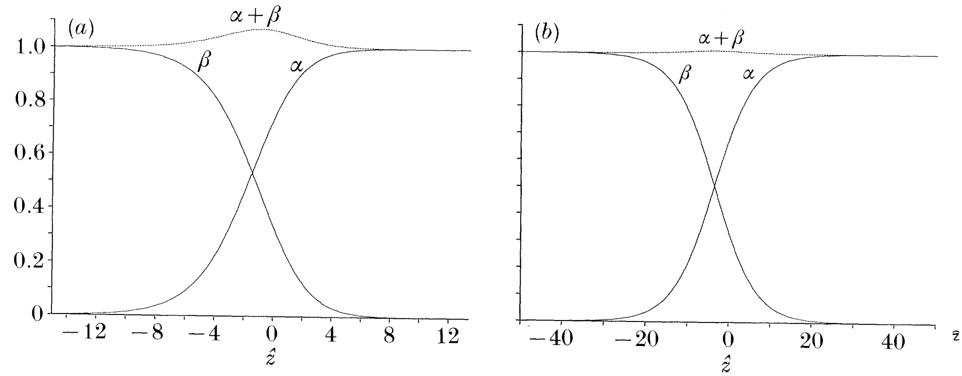

Figure 3. Graphs of the travelling wave solutions of equation (25) when: (*a*) $\hat{v} = 2$; (*b*) $\hat{v} = 5$.

(26) is attained for moderate values of $\hat{v}$. We can conclude that the width of the wavefront is of $O(\hat{v})$ and hence, for $D \gg 1$, the width of the wavefront for travelling wave solutions of equation (16) is of $O(v)$.

4. Cubic autocatalysis, $n = 2$

When $n = 2$, equation (12*a*, *b*, *c*) becomes

$$\alpha_z = v(1-\alpha-\beta)-Dw, \tag{27a}$$

$$\beta_z = w, \tag{27b}$$

$$w_z = -D^{-1}(\alpha\beta^2+vw). \tag{27c}$$

This system of equations has many features in common with the system (16). It has just two finite equilibrium points at (0, 1, 0) and (1, 0, 0) in the (α, β, w) phase space. A solution of equation (8*a*, *b*) which satisfies condition (13*a*, *b*) is a directed integral path of equation (27*a*, *b*, *c*) which connects the point (0, 1, 0) to (1, 0, 0). The point (0, 1, 0) is a simple equilibrium point with a two-dimensional stable manifold and a one-dimensional unstable manifold. The eigenvalues and associated eigenvectors are again given by (17*a*, *b*, *c*). The only integral path which satisfies condition (13*b*) and has $\alpha \geqslant 0$ as $z \to -\infty$ is the unstable manifold of (0,1,0) in $\alpha \geqslant 0$ which we again label S_1. However, the behaviour of the system (27) in the neighbourhood of the other equilibrium point (1, 0, 0) is entirely different from that of the system (16) and we now consider this behaviour in detail.

Linearization of equation (27) about the point (1, 0, 0) shows that it is a non-simple equilibrium point with eigenvalues and associated eigenvectors given by

$$\nu_1 = -v, \qquad \boldsymbol{e}_{\nu_1} = (1,0,0)^{\mathrm{T}}, \tag{28a}$$

$$\nu_2 = -vD^{-1}, \qquad \boldsymbol{e}_{\nu_2} = (0,-1,vD^{-1})^{\mathrm{T}}, \tag{28b}$$

$$\nu_3 = 0, \qquad \boldsymbol{e}_{\nu_3} = (1,-1,0)^{\mathrm{T}}. \tag{28c}$$

Hence the linearized equations do not give a classification of the local behaviour. However, an application of the centre manifold theorem (see, for example, Guckenheimer & Holmes 1983) shows that the equilibrium point has a unique, two-dimensional, invariant, stable manifold, locally tangent to the plane through (1, 0, 0) spanned by $\boldsymbol{e}_{\nu_1}$ and $\boldsymbol{e}_{\nu_2}$, which we label S_0, and a one-dimensional invariant, centre manifold, locally tangent to $\boldsymbol{e}_{\nu_3}$. We define the equation of the surface describing the stable manifold, S_0, to be $w \equiv w_s(\alpha, \beta)$. Since the surface, S_0, is composed of integral paths of the system (27), w_s must satisfy the partial differential equation

$$\{v(1-\alpha-\beta)-Dw_s\}\,\partial w_s/\partial\alpha + w_s\,\partial w_s/\partial\beta + D^{-1}(\alpha\beta^2+vw_s) = 0. \tag{29}$$

Also, from (28*a*, *b*) we know that $w_s(\alpha, \beta) \sim -vD^{-1}\beta$ as $\alpha \to 1$, $\beta \to 0$. On making the substitution $w_s(\alpha,\beta) = -vD^{-1}\beta + k_1\beta^2 + k_2\beta(\alpha-1) + k_3(\alpha-1)^2$ in equation (29) and equating coefficients of $(\alpha-1)^2$, $(\alpha-1)\beta$ and β^2, we obtain $k_1 = \frac{1}{2}v, k_2 = k_3 = 0$, so that, to a higher approximation,

$$w_s \sim -vD^{-1}\beta + \tfrac{1}{2}(\beta^2/v) + O((\alpha-1)^3, \beta^3) \quad \text{as} \quad \alpha \to 1, \quad \beta \to 0. \tag{30}$$

Since equation (27) has the exact solution, $\beta = w = 0$, $\alpha = 1 + k\,e^{-vz}$, where k is an arbitrary constant, the stable manifold, S_0, must contain the α-axis, and hence $w_s(\alpha, 0) = 0$ for $-\infty < \alpha < \infty$. Hence (30) gives a uniform representation of $w_s(\alpha, \beta)$ in the neighbourhood of the point (1, 0, 0) and further cubic terms need not be calculated. To calculate the equation of the curve describing the centre manifold we first write equation (27) in normal form as

$$y_{1z} = -vy_1 - v^{-1}(y_1 - x + 1)(y_2 + x)^2, \tag{31a}$$

$$y_{2z} = -(v/D)\,y_2 + v^{-1}(y_1 - x + 1)(y_2 + x)^2, \tag{31b}$$

$$x_z = -v^{-1}(y_1 - x + 1)(y_2 + x)^2, \tag{31c}$$

where $y_1 = \alpha + \beta + (D/v)w - 1$, $y_2 = -(D/v)w$, $x = \beta + (D/v)w$. The equation of the centre manifold is now readily obtained as $y_1 \sim -x^2/v^2$, $y_2 \sim Dx^2/v^2$, as $x \to 0$. In terms of the original variables, this becomes

$$\alpha = \alpha_c(t) \sim 1 - t - (t^2/v^2) \quad \beta = \beta_c(t) \sim t + (Dt^2/v^2), \quad w = w_c(t) \sim -t^2/v \quad \text{as} \quad t \to 0, \tag{32}$$

where t parametrizes the one-dimensional centre manifold.

Carr's theorem (see, for example, Guckenheimer & Holmes 1983) guarantees that any paths in the vicinity of (1, 0, 0), except those in the stable manifold, decay rapidly on to the centre manifold. Thus the dynamics on the centre manifold determines the nature of the equilibrium point (1, 0, 0). From equations (27*b*) and (32) we can see that on the centre manifold, close to the point (1, 0, 0), $\beta_z < 0$ in both $\beta > 0$ and $\beta < 0$. Therefore, locally, all paths which start on the side of S_0 which contains the centre manifold in $\beta > 0$ enter (1, 0, 0) along the centre manifold, while all paths which start on the other side of S_0 are swept away from (1, 0, 0) close to the centre manifold. All paths which enter (1, 0, 0) do so along the centre manifold, except those which form the stable manifold, S_0. Thus we have established that the non-simple equilibrium point (1, 0, 0) has a stable nodal region on the side of S_0 which contains the positive w-axis in the neighbourhood of the point (1, 0, 0) and an unstable region on the other side of S_0, for each $v > 0$. Since the behaviour in the neighbourhood of the point (1, 0, 0) is entirely different from that of the system (16), we do not, in the case of cubic autocatalysis, have a result analogous to Proposition 3.1, which gives a lower bound on the possible eigenvalues, v. However, the analogue of Proposition 3.2 still holds and we have the following sufficient condition.

Proposition 4.1. *A unique permanent form travelling wave solution of equation* (27*a*, *b*, *c*) *exists for each* $v \geqslant 2\sqrt{D}$.

Proof. This is identical to the proof of Proposition 3.1. □

However, we know that when $D = 1$ a permanent form travelling wave solution exists for all $v \geqslant v_2^*(1) = 1/\sqrt{2}$, so Proposition 4.1 does not provide a good upper bound on the minimum propagation speed. We now use a constructional method to show that a minimum propagation speed, $v_2^*(D)$, exists for all $D \geqslant 0$, and we calculate $v_2^*(D)$. This shows that Proposition 4.1 does not provide a good upper bound on $v_2^*(D)$ for any $D > 0$.

A solution of the original eigenvalue problem requires the directed integral path which leaves (0, 1, 0) as the unstable manifold, S_1, to enter (1, 0, 0) in $\beta > 0$, $\alpha > 0$. To decide whether S_1 enters (1, 0, 0) we consider the global behaviour of the stable manifold, S_0, of the equilibrium point (1, 0, 0) since this forms the boundary of the region in which paths enter (1, 0, 0). Firstly we prove the following result which concerns the behaviour of S_0.

Proposition 4.2. *When $\alpha > 0$ and $\beta \neq 0$ then $w_s(\alpha, \beta) > -(v/D)\,\beta$.*

Proof. Let the surface $\partial\bar{R}$ be the boundary of the region $\bar{R} = \{(\alpha, \beta, w): \alpha \geqslant 0, w \leqslant -(v/D)\,\beta\}$. From equation (27*a*), when $\alpha = 0$ and

$$w \leqslant -(v/D)\,\beta, \quad \text{then } \alpha_z = v - (v\beta + Dw) > 0.$$

Also from equation (27*b*, *c*) when $w = -(v/D)\,\beta$, $\alpha > 0$ and $\beta \neq 0$, then

$$w_z + (v/D)\,\beta_z = -\alpha\beta^2/D < 0.$$

Hence, apart from the α-axis, all integral paths which intersect $\partial\bar{R}$ are directed into $\bar{R}$. Now suppose that there exists an integral path which lies in S_0 (other than the integral path along the α-axis), and intersects the surface $\partial\bar{R}$ at least once. Let (α_0, β_0, w_0) be the final point of intersection before the integral path enters the equilibrium point (1, 0, 0). From the local behaviour of S_0 close to (1, 0, 0) given by (30), which shows that S_0 lies outside $\bar{R}$ in the neighbourhood of (1, 0, 0), this integral path must be directed out of $\bar{R}$ at (α_0, β_0, w_0), which leads to a contradiction. Thus any integral path which lies in S_0 (with the exception of the integral path along the α-axis) cannot intersect $\partial\bar{R}$. Since S_0 is entirely composed of integral paths, we deduce that S_0 itself cannot intersect $\partial\bar{R}$ at any point away from the α-axis. The local behaviour of S_0, given by (30), then shows that S_0 must remain outside the region $\bar{R}$ everywhere except along the α-axis, and the proposition is established. □

A direct consequence of this result is the following.

Corollary 4.3. *The stable manifold, S_0, of the point* (1, 0, 0) *is tangent to the plane $w = -(v/D)\,\beta$ along the α-axis, for $\alpha > 0$.*

We now define the closed region $\hat{R}$ by

$$\hat{R} = \{(\alpha, \beta, w): 0 \leqslant \alpha \leqslant 1, \quad 0 \leqslant \beta \leqslant 1, \quad -(v/D)\,\beta \leqslant w \leqslant 0\}, \tag{33}$$

and prove the following proposition.

Proposition 4.4. *The stable manifold, S_0, of the point* (1, 0, 0) *divides the closed region $\hat{R}$ into exactly two subregions.* □

Proof. From Corollary 4.3, S_0 must divide $\hat{R}$ into at least two subregions. In addition, two of these subregions must contain the segment of the α-axis in $\hat{R}$ within their bounding surfaces. We label the closed subregion of $\hat{R}$ which lies on the side of S_0 which contains the positive w-axis in the neighbourhood of the α-axis as R_1, and the closed subregion of $\hat{R}$ which lies on the side of S_0 which contains the negative w-axis in the neighbourhood of the α-axis as R_2. We now suppose that S_0 divides the region $\hat{R}$ into more than two subregions and label one of these other closed subregions

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as R_3. The closed subregion R_3 cannot contain any segment of the α-axis in its bounding surface, by the definition of R_1 and R_2, nor can it contain any point in the plane $w = -(v/D)\,\beta$, since within $\hat{R}$ this forms part of the boundary surface of the subregion R_2, by proposition 4.2. Hence, the subregion R_3 must be bounded by S_0 and at least one of the planes $w = 0$, $\alpha = 0$, $\alpha = 1$ and $\beta = 1$. From equations (27) and the definitions of S_0, no integral path is directed out of the bounding surface of R_3. Also, from equation (27*b*), $\beta_z < 0$ in R_3 and so any integral path which strictly enters R_3 must be monotone decreasing in β as z increases, and bounded below in β. However, the region R_3 contains no stable equilibrium point and thus such an integral path cannot exist, which leads to a contradiction and the result is established. □

Next we consider the line segments L_1 and L_2 which are defined by

$$L_1 = \{(\alpha,\ \beta,\ 0) : \alpha+\beta = 1,\ \alpha > 0,\ \beta > 0\}, \quad L_2 = \{(0,\ 1,\ w) : -v/D \leqslant w \leqslant 0\}. \qquad (34\,a,\ b)$$

Proposition 4.5. *The eigenvalue problem* (27), (13*a*, *b*) *has* (i) *a unique solution for each* $v > 0$, $D > 0$ *such that the line segment* L_1 *intersects* S_0 *at an even number of points* (*counting multiplicity*), (*ii*) *no solution for each* $v > 0$, $D > 0$ *such that the line segment* L_1 *intersects* S_0 *at an odd number of points* (*counting multiplicity*).

Proof. The closed region R_1 is bounded by S_0, the planes $w = 0$, $\alpha = 0$, $\alpha = 1$ and possibly $\beta = 1$. Thus from equations (27) and the definition of S_0, no integral path is directed out of the bounding surface of the region R_1. Also, from equation (27*b*), $\beta_z < 0$ in R_1, so any integral path which strictly enters or lies within R_1 is monotone decreasing in β as z increases and bounded below in β by the segment of the α-axis which lies within $\hat{R}$. The only possibility is that such an integral path enters the equilibrium point at (1, 0, 0). Thus any integral path which at $z = z^*$ is strictly within R_1 remains within R_1 for all $z > z^*$ and is asymptotic to the equilibrium point (1, 0, 0) as $z \to \infty$.

The closed region R_2 is bounded by S_0, the planes $\alpha = 0$, $\alpha = 1$, $\beta = 1$, $w = -(v/D)\,\beta$ and possibly $w = 0$. From equation (27) all integral paths which intersect the plane $w = -(v/D)\,\beta$ leave the region R_2, while on the remainder of the bounding surface of R_2, no integral path leaves R_2. From equation (27*b*) $\beta_z < 0$ in R_2 and so, from our knowledge of the behaviour of the system in the neighbourhood of the equilibrium point (1, 0, 0), any integral path which strictly enters R_2 must be monotone decreasing in β as z increases and leave R_2 through the plane $w = -(v/D)\,\beta$ to enter the region $\bar{R}$, where it remains. Hence no integral path which strictly enters the region R_2 can be asymptotic to the equilibrium point (1, 0, 0) as $z \to \infty$.

The eigenvalue problem (27) and (13*a*, *b*) has a unique solution if and only if the unstable manifold, S_1, of the point (0, 1, 0) enters the equilibrium point at (1, 0, 0). From (17*c*), S_1 enters the region $\hat{R}$ and hence must either strictly enter the subregion R_1, or strictly enter the subregion R_2, or lie in the stable manifold, S_0, of (1, 0, 0) which forms the common boundary of the subregions R_1 and R_2. If S_1 strictly enters the subregion R_1 or lies in S_0, then S_1 is asymptotic to the point (1, 0, 0) as $z \to \infty$, with $0 < \alpha < 1$ and $0 < \beta < 1$ for all $-\infty < z < \infty$, and thus represents the unique solution to the eigenvalue problem. If S_1 strictly enters the subregion R_2 then it cannot be asymptotic to the point (1, 0, 0) as $z \to \infty$ and no solution of the eigenvalue problem exists. If the equilibrium point (0, 1, 0) lies in the stable manifold, S_0, of (1, 0, 0) then S_1 lies in S_0, since S_1 must also be the unique, invariant, unstable manifold of (0, 1, 0) with respect to the dynamics on S_0. Hence if the point (0, 1, 0) lies in R_1 then S_1 strictly enters R_1, if (0, 1, 0) lies in S_0 then S_1 lies in S_0 and if (0, 1, 0) lies in R_2 then S_1 strictly enters R_2. However, by Proposition 4.4, if the point (0, 1, 0) lies in R_1 then L_1 must intersect S_0 at an even number of points and if (0, 1, 0) lies in the interior of R_2 then L_1 must intersect S_0 at an odd number of points and the result is established. □

To study the behaviour of S_0 and determine the eigenvalues of the problem (27) and (13 a, b) we define the function $g(v, D)$ to have the value $\bar{\beta}$ when S_0 intersects the line segment L_1 at the point $(1-\bar{\beta}, \bar{\beta}, 0)$ and to be $1-(D/v)\,\bar{w}$ when S_0 intersects the line segment L_2 at the point $(0, 1, \bar{w})$. We note that S_0 must intersect $L_1 \cup L_2$ at least once by proposition 4.2 and that $g(v, D)$ may be multivalued. However, since the right-hand sides of equation (27) are well-behaved functions of the parameters v and D as well as α, β and w, the solution depends continuously on v and D (see, for example, Hirsch & Smale 1974), and hence $g(v, D)$ is a continuous function in $v > 0$, $D > 0$. We now determine the behaviour of S_0, given by $w = w_s(\alpha, \beta)$, as β increases from zero, and hence determine $g(v, D)$. From corollary 4.3 we know that $w_s \sim -(v/D)\,\beta$ as $\beta \to 0^+$. This suggests that a convenient rescaling of the variable w_s can be made by defining $\alpha = \tilde{\alpha}$, $\beta = \tilde{\beta}$, $w = (v/D)\,\tilde{w}$. In terms of these new variables, equation (29) becomes

$$D(1-\tilde{\alpha}-\tilde{\beta}-\tilde{w}_s)\frac{\partial \tilde{w}_s}{\partial \tilde{\alpha}}+\tilde{w}_s\frac{\partial \tilde{w}_s}{\partial \tilde{\beta}}+\tilde{w}_s+\frac{D}{v^2}\tilde{\alpha}\tilde{\beta}^2 = 0. \tag{35}$$

We also have that
$$\tilde{w}_s(\tilde{\alpha}, \tilde{\beta}) \sim -\tilde{\beta}, \quad \text{as} \quad \tilde{\beta} \to 0^+. \tag{36}$$

We now consider the asymptotic forms of $\tilde{w}_s(\tilde{\alpha}, \tilde{\beta})$ and hence $g(v, D)$, when $v \gg 1$ and $0 < v \ll 1$, with D of $O(1)$.

$v \gg 1$. With $v \gg 1$, equation (35) suggest that we seek an asymptotic expansion of $\tilde{w}_s$ in the form $\tilde{w}_s(\tilde{\alpha}, \tilde{\beta}) = \tilde{w}_0(\tilde{\alpha}, \tilde{\beta}) + v^{-2}\tilde{w}_1(\tilde{\alpha}, \tilde{\beta}) + \dots$. At leading order, equation (35) becomes

$$D(\partial \tilde{w}_0/\partial \tilde{\alpha})(1-\tilde{\alpha}-\tilde{\beta}-\tilde{w}_0)+(\partial \tilde{w}_0/\partial \tilde{\beta})\,\tilde{w}_0+\tilde{w}_0 = 0. \tag{37}$$

This equation has the solution $\tilde{w}_0 = -\tilde{\beta}$, which satisfies the condition (36) as $\tilde{\beta} \to 0^+$. In terms of the original variables we have that $w_s(\alpha, \beta) = -(v/D)\,\beta + O(v^{-1})$, as $v \to \infty$. Hence, as $v \to \infty$, S_0 asymptotes to the plane $w = -(v/D)\,\beta$ and does not intersect the line segment L_1. Thus we obtain case (i) of Proposition 4.5 and a unique solution of the eigenvalue problem exists for $v \gg 1$. This result is consistent with Proposition 4.1. We also note that $g(v, D) \to 2$, as $v \to \infty$, and is singled-valued.

$0 < v \ll 1$. In this case a balance of terms is not obtained in equation (35) as $v \to 0^+$. This suggests that a rescaling is required. Condition (36) indicates that the rescaling of $\tilde{w}$ and $\tilde{\beta}$ should be of the same order. The appropriate scaled variables which give a leading order balance are then found to be $\tilde{\alpha} = \hat{\alpha}$, $\tilde{\beta} = (v^2/D)\,\hat{\beta}$, $\tilde{w}_s = (v^2/D)\,\hat{w}_s$. In terms of these new variables, equation (35) and condition (36) become

$$D\{1-\hat{\alpha}-(v^2/D)\,(\hat{\beta}+\hat{w}_s)\}\,\partial \hat{w}_s/\partial \hat{\alpha}+\hat{w}_s\,\partial \hat{w}_s/\partial \hat{\beta}+\hat{w}_s+\hat{\alpha}\hat{\beta}^2 = 0, \tag{38}$$

$$\hat{w}_s \sim -\hat{\beta}, \quad \text{as} \quad \hat{\beta} \to 0^+. \tag{39}$$

With $0 < v \ll 1$ equation (38) suggests that we seek an asymptotic expansion of $\hat{w}_s$ in the form $\hat{w}_s(\hat{\alpha}, \hat{\beta}) = \hat{w}_0(\hat{\alpha}, \hat{\beta}) + v^2\hat{w}_1(\hat{\alpha}, \hat{\beta}) + \dots$, as $v \to 0^+$. At leading order, equation (38) becomes

$$D(1-\hat{\alpha})\,\partial \hat{w}_0/\partial \hat{\alpha}+\hat{w}_0\,\partial \hat{w}_0/\partial \hat{\beta}+\hat{w}_0+\hat{\alpha}\hat{\beta}^2 = 0. \tag{40}$$

This equation has no obvious solution which satisfies condition (39). However, in terms of the scaled variables, the plane $\alpha+\beta = 1$ becomes $\hat{\alpha}+(v^2/D)\,\hat{\beta} = 1$ and, at leading order in v^2, $\hat{\alpha} = 1$. Hence to determine the leading order form of the

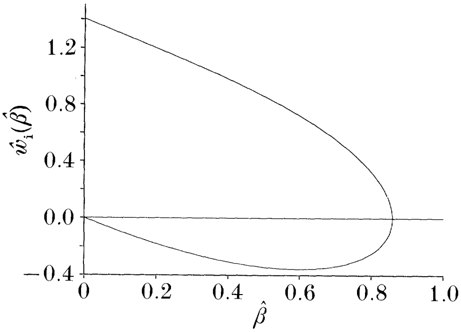

Figure 4. A graph of the function $\hat{w}_i(\hat{\beta})$, the curve of intersection of the stable manifold, S_0, with the plane $\hat{\alpha} = 1$.

intersection of the manifold S_0 with the plane $\alpha + \beta = 1$, given by $\hat{w} = \hat{w}_i(\hat{\beta})$, we set $\hat{\alpha} = 1$ in equation (40) to obtain

$$\mathrm{d}\hat{w}_i/\mathrm{d}\hat{\beta} = -1 - \hat{\beta}^2/\hat{w}_i. \tag{41}$$

A numerical integration of equation (41) using a fourth-order Runge–Kutta method with initial conditions $\hat{w}_i = -10^{-6}$, $\hat{\beta} = 10^{-6}$, shows that $\hat{w}_i$ crosses the $\hat{\beta}$-axis at $\hat{\beta} = \beta^* \approx 0.859$ and that $\hat{w}_i \to \infty$ as $\hat{\beta} \to -\infty$. A graph of $\hat{w}_i(\hat{\beta})$ is shown in figure 4. Hence, as $v \to 0^+$, S_0 intersects the line segment L_1 at only one point. Thus we obtain case (ii) of proposition 4.5 and the eigenvalue problem has no solution for $0 < v \ll 1$. We also note that $g(v, D) \sim \beta^* v^2/D$, as $v \to 0^+$, and is single-valued.

$v = O(1)$. Between its asymptotic forms for $v \gg 1$ and $0 < v \ll 1$, we compute $g(v, D)$ numerically. By integrating equation (27) from $z = 0$ to $z = z_0$ for sufficiently large, positive z_0, with initial conditions $(\alpha(0), \beta(0), w(0)) \in L_1 \cup L_2$, it is possible to determine whether the point $(\alpha(0), \beta(0), w(0))$ lies in the region R_1 or the region R_2, since integral paths that enter the region R_1 asymptote to the point (1, 0, 0), while integral paths that enter the region R_2 leave R_2 through the plane $w = -(v/D)\beta$. By performing this integration for a range of initial conditions on $L_1 \cup L_2$, for fixed v and D, the points of intersection of S_0 with $L_1 \cup L_2$ are easily identified since they lie on the common boundary of R_1 and R_2, and hence $g(v, D)$ can be calculated. However, this method of calculating $g(v, D)$ is computationally very inefficient, since a large number of numerical integrations of equation (27) must be performed for each pair of values of v and D. Calculations of $g(v, D)$ obtained by this method indicate that, for fixed D, $g(v, D)$ has a single-valued inverse. We can therefore calculate $g(v, D)$ precisely and in a computationally efficient manner by fixing D and for each of a range of points lying in $L_1 \cup L_2$ using a bisection search technique to locate the unique value of v for which this point lies in S_0. Graphs of $g(v, D)$ against v obtained in this way are shown in figure 5 for a range of fixed values of D. In each of these graphs, $g(v, D) \to 0$ as $v \to 0^+$ and $g(v, D) \to 2$ as $v \to \infty$, consistent with the asymptotic forms obtained for $v \gg 1$ and $v \ll 1$. For each $D \geqslant 1$, $g(v, D)$ is monotone increasing with v, while for each $0 < D < 1$, $g(v, D)$ has a single folded region where $g(v, D)$ is triple valued. Thus, for each $D \geqslant 1$, S_0 always intersects $L_1 \cup L_2$ at a unique point, while for each $0 < D < 1$, S_0 meets $L_1 \cup L_2$ at three points for a range of values of v. However, S_0 never intersects L_1 at more than two points. These numerical results complete our constructional proof of the following proposition, which is a consequence of Proposition 4.5.

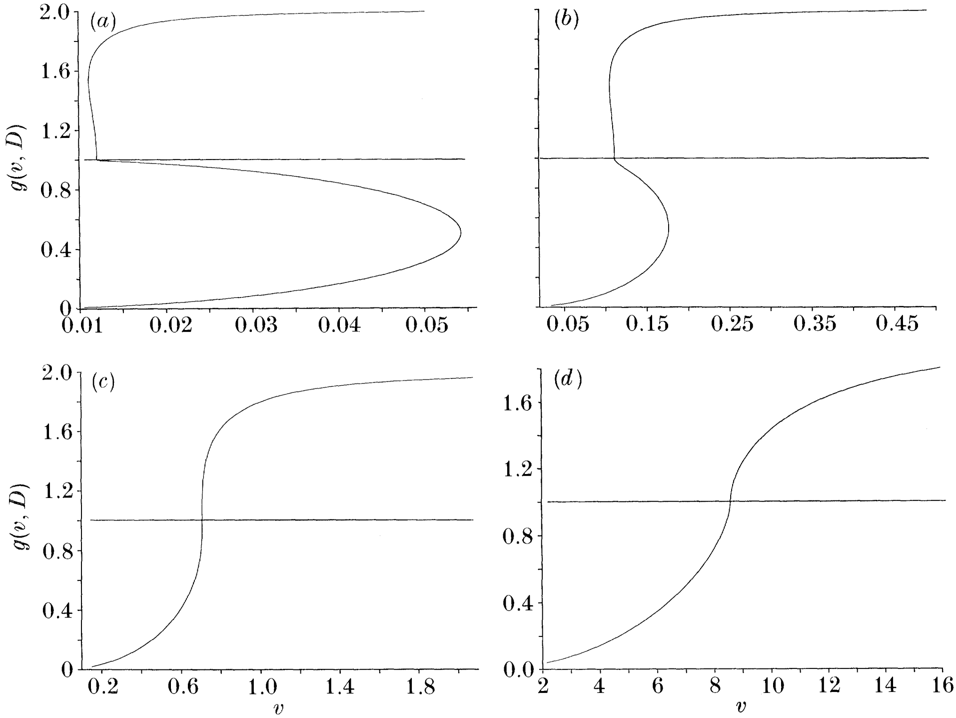

Figure 5. Graphs of the function $g(v, D)$ against v, when: (a) $D = 0.01$; (b) $D = 0.1$; (c) $D = 1$; (d) $D = 100$.

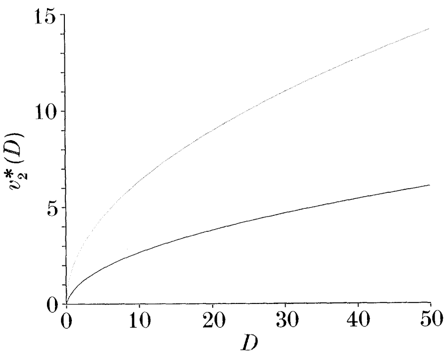

Figure 6. A graph of the minimum propagation speed, $v_2^*(D)$, shown as the solid line. The broken line is the upper bound on $v_2^*(D)$, given by Proposition 4.1.

Proposition 4.6. *The eigenvalue problem* (27) *and* (13*a*, *b*) *has a unique solution if and only if* $v \geqslant v_2^*(D)$, *where* $v_2^*(D)$ *is the unique, positive solution of* $g(v, D) = 1$ *for each* $D > 0$.

A graph of $v_2^*(D)$ against D, as calculated by the above numerical procedure, is shown in figure 6, which indicates that $v_2^*(D)$ is of $O(D)$ for $D \ll 1$, and $v_2^*(D)$ is of $O(\sqrt{D})$ for $D \gg 1$. The graph also shows the upper bound on v_2^*, given by proposition 4.1. Some typical travelling wave solutions of equation (27*a*, *b*, *c*) are illustrated in figure 7. These were obtained numerically by the method used in §3 for the case of

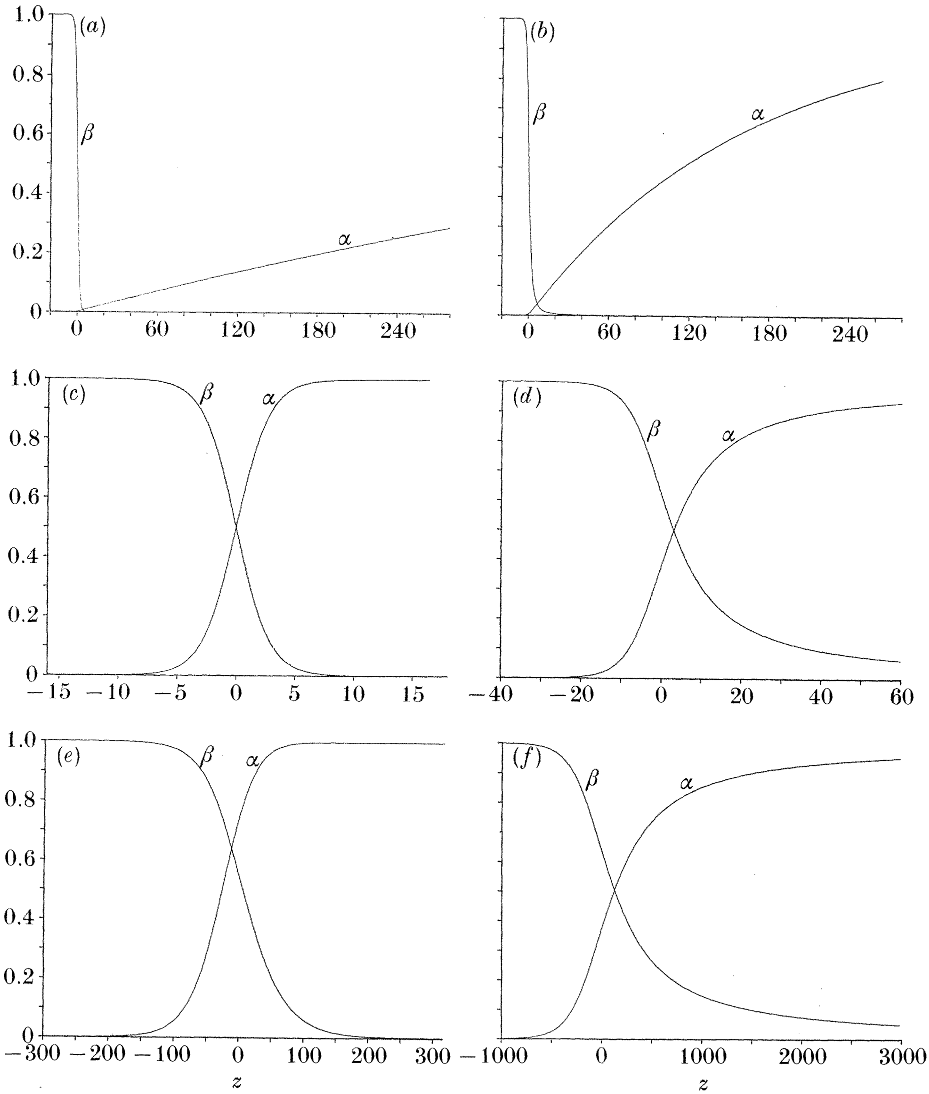

Figure 7. Graphs of the travelling wave solutions of equation (27), when: (*a*) $D = 0.001$, $v = v_2^* \approx 0.00122$; (*b*) $D = 0.001$, $v = 5v_2^*$; (*c*) $D = 1$, $v = v_2^* = \surd\frac{1}{2}$; (*d*) $D = 1$, $v = 5v_2^*$; (*e*) $D = 1000$, $v = v_2^* \approx 27.28857$; (*f*) $D = 1000$, $v = 5v_2^*$.

quadratic autocatalysis, $n = 1$. The solutions show that the wavefront width increases with both v and D, and that the wavefront becomes more asymmetric as $D \rightarrow 0$, with β decaying more rapidly than α as $z \rightarrow \infty$, as in the quadratic case. However, there is now an obvious difference in the rate of decay of $1-\alpha$ and β as $z \rightarrow \infty$ between the minimum speed travelling wave solutions and the faster travelling wave solutions. This important difference will be examined in §5, but first we complete our analysis of equation (27) by studying the asymptotic behaviour of the permanent form travelling wave solution for $0 < D \ll 1$ and $D \gg 1$.

$D \ll 1$. Equation (27*c*) indicates that for $D \ll 1$ and $v \gg D$, w changes rapidly except where $w \sim \alpha\beta^2/v$. However, our numerical results suggests that $v_2^* = O(D)$ for $D \ll 1$, so it is not helpful to construct a centre manifold in this case. Expressions

(17c) indicate that $\alpha = O(D)$, $\beta = O(1)$, $w = O(1)$ as $z \to -\infty$, when $v = O(D)$ and $D \ll 1$. This suggests the change of variables $\alpha = D\tilde{A}$, $\beta = \tilde{B}$, $w = \tilde{W}$, $v = D\tilde{v}$, where $\tilde{A}$, $\tilde{B}$, $\tilde{W} = O(1)$ at least as $z \to -\infty$. We define region I to be that in which $\tilde{A}$, $\tilde{B}$, $\tilde{W} = O(1)$. At leading order in D, equations (27a, b, c) become

$$\tilde{A}_z = \tilde{v}(1-\tilde{B}) - \tilde{W}, \quad \tilde{B}_z = \tilde{W}, \quad \tilde{W}_z = -\tilde{v}\tilde{W} - \tilde{A}\tilde{B}^2. \qquad (42a, b, c)$$

We analyse this system in the $(\tilde{A}, \tilde{B}, \tilde{W})$ phase space. The system has a unique finite equilibrium point at (0, 1, 0), with a two-dimensional stable manifold and a one-dimensional unstable manifold. The only integral path which satisfies condition (13b) as $z \to -\infty$ is the unstable manifold of the point (0,1,0) in $\tilde{A} \geqslant 0$. The system also has a solution $\tilde{A} = \tilde{v}z + \text{const.}$, $\tilde{B} = \tilde{W} = 0$, which is represented by the $\tilde{A}$-axis. We note that, for fixed $\tilde{A}$, equation (42b, c) is identical to the leading order form of equation (15a, b) when $|\beta| \ll 1$. Equation (15a, b) was analysed in Billingham & Needham (1990), where it was shown that the point $\beta = w = 0$ is a saddle-node with a saddle region and a nodal region separated by a stable manifold. Integral paths that enter the nodal region or the stable manifold asymptote to the equilibrium point, while integral paths that enter the saddle region are swept away from the equilibrium point into the region $\beta < 0$. These results indicate that, for the present system (42), the unstable manifold of the point (0, 1, 0) may enter either a 'nodal' region of the $\tilde{A}$-axis, to which it will then become asymptotic, or a 'saddle' region of the $\tilde{A}$-axis, when it will be swept away into the region $\tilde{B} < 0$ and not represent a solution of the eigenvalue problem. Numerical integrations of equation (42) using a fourth-order Runge–Kutta method, with initial conditions lying on the unstable manifold of (0, 1, 0) show that, for $\tilde{v} < \tilde{v}^* \approx 1.219$, $\tilde{B}$ becomes negative and no solution of the eigenvalue problem exists. However, for $\tilde{v} \geqslant \tilde{v}^*$, the unstable manifold of the point (0, 1, 0) becomes asymptotic to the $\tilde{A}$-axis. From our knowledge of the solutions of equation (15a, b) and the behaviour of the full system of equations (27a, b, c) we deduce that for $\tilde{v} > \tilde{v}^*$, the unstable manifold of the point (0, 1, 0) strictly enters the 'nodal' region of the $\tilde{A}$-axis, while when $\tilde{v} = \tilde{v}^*$ the unstable manifold of the point (0, 1, 0) lies in the 'stable manifold' of the $\tilde{A}$-axis. From equation (42a, b, c) we can deduce the following two types of asymptotic behaviour as $z \to \infty$.

For

$$\tilde{v} > \tilde{v}^*, \quad \tilde{A} \sim \tilde{v}z, \quad \tilde{B} \sim 2/z^2, \quad \tilde{W} \sim -4/z^3, \qquad (43a)$$

$$\tilde{v} = \tilde{v}^*, \quad \tilde{A} \sim \tilde{v}z, \quad \tilde{B} \sim e^{-\tilde{v}z}, \quad \tilde{W} \sim -\tilde{v}\, e^{-\tilde{v}z}, \quad \text{as} \quad z \to \infty. \qquad (43b)$$

Since $\alpha = D\tilde{A} \sim D\tilde{v}z$ as $z \to \infty$, the approximation becomes non-uniform when $z = O(D^{-1})$ in both cases. Thus we need to introduce a new region with $z \gg 1$ to complete the solution. When $\tilde{v} > \tilde{v}^*$, $\tilde{A} = O(D^{-1})$, $\tilde{B} = O(D^2)$, $\tilde{W} = O(D^3)$ as $z \to \infty$, which suggests that we introduce the scaled variables $\theta = Dz$, $\hat{A} = D\tilde{A}$, $\hat{B} = D^{-2}\tilde{B}$, $\hat{W} = D^{-3}\tilde{W}$. We define region II to be that in which $\hat{A}, \hat{B}, \hat{W} = O(1)$. On writing equation (27) in terms of the new variables, the leading order solution in region II, which matches with the solution in region I, is readily obtained as

$$\hat{A} = 1 - e^{-\tilde{v}\theta}, \quad \hat{B} = \tilde{v}^2(\tilde{v}\theta - e^{-\tilde{v}\theta} - 1)^{-1}, \qquad (44a, b)$$

$$\hat{W} = -\tilde{v}^3(1 - e^{-\tilde{v}\theta})(\tilde{v}\theta + e^{-\tilde{v}\theta} - 1)^{-2}. \qquad (44c)$$

Although $\hat{B} \to 0$ and $\tilde{W} \to 0$, and both are uniform approximations as $\theta \to \infty$, a calculation of further terms shows that a non-uniformity arises in the asymptotic expansion of $\hat{A}$ at $O(D^2)$ as $\theta \to \infty$. This is due to a term of $O(D^2\tilde{v}/\theta)$ which is larger than terms of $O(e^{-\tilde{v}\theta})$ for sufficiently large θ. Thus a third region with $\theta \gg 1$, which we label region IIa, is required to complete the asymptotic solution for α. In region IIa we simply find that $\alpha = \hat{A} \sim 1-(D^2\tilde{v}/\theta)+\dots$, as $\theta \to \infty$, and $\alpha \to 1$ as $\theta \to \infty$ through algebraically small terms in θ. When $\tilde{v} = \tilde{v}^*$, the leading order approximation for $\tilde{B}$ and $\tilde{W}$ given by(43b) remain uniform as $z \to \infty$, while region II is again required for $\hat{A}$. However, in this case, approximation (44a) remains uniform as $\theta \to \infty$ and region IIa is not required. We have now constructed an asymptotic solution of the eigenvalue problem which exists for all $\tilde{v} \geqslant \tilde{v}^*$, and hence $v_2^*(D) \sim \tilde{v}^* D$, as $D \to 0^+$. This result is consistent with the numerically calculated values of $v_2^*(D)$ plotted in figure 6.

The permanent form travelling wave solutions of the full system (27) with $D = 0.001$, shown in figure 7(a, b), display some of the features of the asymptotic solution for $0 < D \ll 1$. The concentration, α, exhibits a slow exponential decay to unity given by (44a). In figure 7b, where $v > v_2^*$, the predicted algebraic decay in region IIa cannot be seen, since this region begins only when $z \gg D^{-1} = 1000$. The concentration β, given by (43), exhibits rapid exponential decay in figure 7a, where $v = v_2^*$, and slower algebraic decay in figure 7b, where $v > v_2^*$.

$D \gg 1$. Our numerical calculation of $v_2^*(D)$ suggests that $v_2^*(D)$ is of $O(\surd D)$ for $D \gg 1$, so that it is again convenient to use the scaled variables (23) in terms of which equation (27) becomes

$$D^{-1}\hat{\alpha}_{\hat{z}} = \hat{v}(1-\hat{\alpha}-\hat{\beta})-\hat{w}, \quad \hat{\beta}_{\hat{z}} = \hat{w}, \quad \hat{w}_{\hat{z}} = -(\hat{\alpha}\hat{\beta}^2+\hat{v}\hat{w}). \qquad (45a, b, c)$$

Equation (45a) indicates that, for $D \gg 1$, $\hat{\alpha}$ changes rapidly, except where $\hat{w} \sim \hat{v}(1-\hat{\alpha}-\hat{\beta})$ which forms a centre manifold for the system (45).The two equilibrium points at (0, 1, 0) and (1, 0, 0) lie in the centre manifold and thus, at leading order, the integral path which connects these two points and represents the travelling wave solution lies entirely within the centre manifold. To analyse the behaviour of the travelling wave solution we put $\hat{w} = \hat{v}(1-\hat{\alpha}-\hat{\beta})$ and substitute into equations (45) to obtain, at leading order, as $D \to \infty$,

$$\hat{\alpha}_{\hat{z}} = \hat{\alpha}\hat{\beta}^2/\hat{v}, \quad \hat{\beta}_{\hat{z}} = \hat{v}(1-\hat{\alpha}-\hat{\beta}). \qquad (46a, b)$$

This second-order system has just two finite equilibrium points in the $(\hat{\alpha}, \hat{\beta})$ phase plane at (1, 0) and (0, 1). The point (0, 1) is a saddle and the only integral path which satisfies condition (13b) as $\hat{z} \to -\infty$ is the unstable manifold of (0, 1) in $\hat{\alpha} > 0$, which we label S_1. The point (1, 0) is a saddle-node and we label its stable manifold S_0. We thus seek conditions under which S_1 enters the saddle-node at (1, 0). This may be achieved by considering the function $g_\infty(\hat{v})$. In the $(\hat{\alpha}, \hat{\beta})$ phase plane, the projections of line segments L_1 and L_2 on to the centre manifold $\hat{w} = \hat{v}(1-\hat{\alpha}-\hat{\beta})$ are

$$\hat{L}_1 = \{(\hat{\alpha}, \hat{\beta}): \hat{\alpha}+\hat{\beta} = 1,\ \hat{\alpha} > 0,\ \hat{\beta} > 0\},\ \hat{L}_2 = \{(\hat{\alpha}, 1): 0 \leqslant \hat{\alpha} \leqslant 1\}. \qquad (47a, b)$$

Thus if S_0 intersects the line segment $\hat{L}_1$ at the point $(1-\bar{\hat{\beta}}, \bar{\hat{\beta}})$, then $g_\infty(\hat{v}) = \bar{\hat{\beta}}$, while if S_0 intersects the line segment $\hat{L}_2$ at the point $(\hat{\alpha}, 1)$, then $g_\infty(\hat{v}) = 1+\hat{\alpha}$. We now state two lemmas which concern the function $g_\infty(\hat{v})$.

Lemma 4.7. *The function $g_\infty(\hat{v})$ is single-valued for $\hat{v} > 0$.*

Lemma 4.8. *The function $g_\infty(\hat{v})$ is monotone increasing for $\hat{v} > 0$.*

The proofs of these two lemmas are straightforward, following the ideas in Billingham & Needham (1990), and will not be given here.

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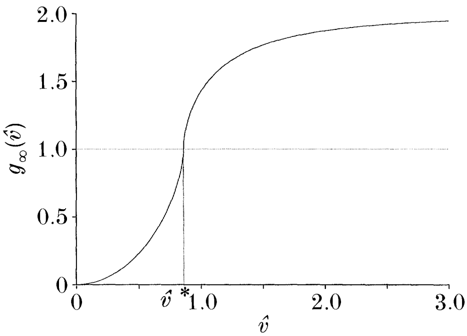

Figure 8. A graph of the function $g_\infty(\hat{v})$.

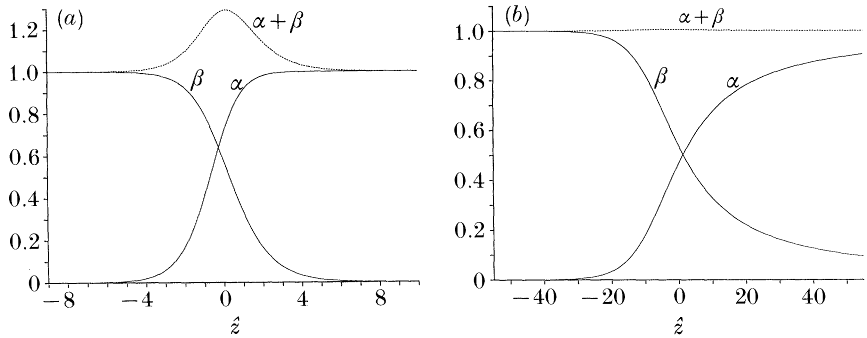

Figure 9. Graphs of the travelling wave solutions of equation (46), when: (a) $\hat{v} = \hat{v}^* \approx 0.862$; (b) $\hat{v} = 5$.

Our analysis of the function $g(v, D)$ shows that $g_\infty(\hat{v}) \to 0$ as $\hat{v} \to 0^+$, and $g_\infty(\hat{v}) \to 2$ as $\hat{v} \to \infty$. Together with Proposition 4.5 and Lemmas 4.7 and 4.8, this leads to the following result.

Proposition 4.9. *A unique, permanent form, travelling wave solution of equations* (46*a*, *b*) *exists if and only if* $\hat{v} \geqslant \hat{v}^*$, *where* $\hat{v}^*$ *is the single, positive solution of* $g_\infty(\hat{v}) = 1$.

A graph of $g_\infty(\hat{v})$ against $\hat{v}$ is illustrated in figure 8. This graph was obtained by using a fourth-order Runge–Kutta method to numerically integrate equations (46*a*, *b*) with $\hat{z}$ decreasing and initial conditions $\hat{\alpha} = 1$, $\hat{\beta} = 10^{-6}$. The integration was continued into the region $\hat{\beta} > 0$ until the point $(\hat{\alpha}, \hat{\beta})$ crossed either of the line segments $\hat{L}_1$ and $\hat{L}_2$ after which $g_\infty(\hat{v})$ was calculated accordingly. A refined numerical integration gives $\hat{v}^* \approx 0.862$. We have now shown that $v_2^*(D) \sim \hat{v}^* \sqrt{D}$ as $D \to \infty$. Finally, we obtain an asymptotic solution of equation (46*a*, *b*) as $\hat{v} \to \infty$. Once again it is convenient to make the change of variable, $\bar{z} = \hat{z}/\hat{v}$. The leading order form of equation (46*a*, *b*) can then be integrated directly to obtain the implicit solution which satisfies (13*a*, *b*)

$$\ln\left(\frac{\hat{\alpha}_0}{1-\hat{\alpha}_0}\right) + \frac{1}{1-\hat{\alpha}_0} = \bar{z}, \quad \ln\left(\frac{1-\hat{\beta}_0}{\hat{\beta}_0}\right) + \frac{1}{\hat{\beta}_0} = \bar{z}, \tag{48}$$

where $\hat{\alpha}(\bar{z}) = \hat{\alpha}_0(\bar{z}) + O(\hat{v}^{-2})$, $\hat{\beta}(\bar{z}) = \hat{\beta}_0(\bar{z}) + O(\hat{v}^{-2})$. Permanent form travelling wave solutions of equations (46) are illustrated in figure 9, for $\hat{v} = \hat{v}^*$, and $\hat{v} = 5$. These indicate that the asymptotic solution given implicitly by (48) is attained for moderate values of $\hat{v}$. Once more we can conclude that the width of the wavefront is of $O(\hat{v})$ and hence, for $D \gg 1$, the width of the wavefront of permanent form travelling wave solutions of equation (27) is of $O(v)$.

5. Asymptotic properties of the permanent form travelling wave solution

For a given $v \geqslant v_n^*(D)$, under both quadratic and cubic autocatalysis, the solution of the eigenvalue problem (12) and (13 a, b) leaves the unstable equilibrium point (0, 1, 0) along the unstable manifold, S_1. From expression (17 c),

$$\alpha(z) \sim \lambda_3(D\lambda_3+v)\,\mathrm{e}^{\lambda_3 z}, \quad \beta(z) \sim 1-\mathrm{e}^{\lambda_3 z}, \quad \text{as} \quad z \to -\infty. \tag{49}$$

Thus in both cases ($n = 1, 2$), the concentrations α and β decay exponentially to their final values of zero and unity, respectively, as $z \to -\infty$.

For quadratic autocatalysis, $n = 1$, the solution of the eigenvalue problem enters the stable node at (1, 0, 0). By linearizing equation (16) about the point (1, 0, 0), the asymptotic behaviour of the solution as $z \to \infty$ is readily determined. We find that this depends upon the eigenvalues μ_1, μ_2 and μ_3 of the equilibrium point(1, 0, 0) given by (18 a, b, c). However, the important feature is that α and β decay exponentially to their final values of unity and zero, respectively, as $z \to \infty$, for all $v \geqslant v_1^*(D) = 2\surd D$.

For cubic autocatalysis $n = 2$, the solution of the eigenvalue problem enters the saddle-node at the point (1, 0, 0) as $z \to \infty$. We have shown in §4 that, for $v = v_2^*(D)$, the integral path which represents the solution of the eigenvalue problem lies in the stable manifold of the point (1, 0, 0), while, for $v > v_2^*(D)$, this integral path enters the point (1, 0, 0) along the centre manifold. From the equations (30) and (32) of the stable manifold and centre manifold, respectively, the following asymptotic behaviour can be deduced:

$$\left.\begin{aligned} &v > v_2^*(D), \quad \alpha \sim 1-v/z, \quad \beta \sim v/z, \\ &v = v_2^*(D), \quad \alpha \sim 1-\mathrm{e}^{-v/z}, \quad \beta \sim \mathrm{e}^{-vz/D}, \quad \text{as} \quad z \to \infty. \end{aligned}\right\} \tag{50}$$

Hence the concentrations α and β decay exponentially to their final values of unity and zero, respectively, in the minimum speed travelling wave solution, but only decay algebraically in all faster travelling wave solutions, as $z \to \infty$.

6. Discussion

In this paper we have established that a minimum propagation speed, $v_n^*(D)$, exists for permanent form travelling wave solutions of equation (6 a, b) under both quadratic autocatalysis, $n = 1$, and cubic autocatalysis, $n = 2$. Each one of these solutions represents a travelling wave which could develop from the initial value problem (6) and (7) in the long time. In the case of quadratic autocatalysis with equal diffusion rates, $D = 1$, it has been shown by Larson (1978) that the travelling wave which develops in the long time depends upon the behaviour of the initial concentration of the autocatalyst, $\beta(x, 0)$, as $x \to \infty$. In a later paper it will be shown that this conclusion extends to the case $D > 0$. In particular, we find that

$$\left.\begin{aligned} &\beta(x,0) \leqslant A\,\mathrm{e}^{-x/\surd D}, \quad \text{as} \quad x \to \infty \Rightarrow v = v_1^* = 2\surd D, \\ &\beta(x,0) \sim A\,\mathrm{e}^{-\sigma x}, \quad 0 < \sigma < 1/\surd D, \quad \text{as} \quad x \to \infty \Rightarrow v = D\sigma + \sigma^{-1} > v_1^*, \\ &\beta(x,0) > \mathrm{e}^{-\sigma x}, \quad \forall \sigma > 0, \quad \text{as} \quad x \to \infty \Rightarrow \text{no travelling wave develops,} \end{aligned}\right\} \tag{51}$$

where A is an arbitrary constant. Thus from localized initial conditions (i.e. $\beta(x,0)$ has compact support), the minimum speed wave will always develop. However, for initial conditions with linear exponential decay the speed of the travelling wave depends upon the size of the exponent, while for initial conditions which decay more slowly than any linear exponential no travelling wave will develop in the long time. Thus the minimum speed wave is structurally unstable to any disturbance which decays more slowly than $e^{-x/\sqrt{D}}$ as $x \to \infty$.

However, in the case of cubic autocatalysis there is a fundamental difference. Only the minimum speed wave has exponential decay of β as $z \to \infty$, all faster waves having weaker algebraic decay as $z \to \infty$. This suggests that the faster travelling waves may be generated by initial conditions with decay of $O(1/x)$ as $x \to \infty$, a situation which does not lead to a travelling wave in the quadratic case. This possibility is being considered by one of the authors at present and we tentatively conjecture the following version of (51) for the cubic case:

$$\left.\begin{aligned} \beta(x,0) \leqslant v_2^*/x, \quad \text{as} \quad x \to \infty \Rightarrow v = v_2^*, \\ \beta(x,0) \sim \sigma/x, \quad \sigma > v_2^*, \quad \text{as} \quad x \to \infty \Rightarrow v = \sigma, \\ \beta(x,0) \geqslant \sigma/x, \quad \forall \sigma > 0, \quad \text{as} \quad x \to \infty \Rightarrow \text{no travelling wave develops.} \end{aligned}\right\} \tag{52}$$

This suggests that the minimum speed wave will be structurally unstable only to disturbances that decay more slowly than v_2^*/x as $x \to \infty$, making it more robust than that of the quadratic case. These results indicate that, in a chemical system for which quadratic or cubic autocatalysis is a good model, it may be possible to observe wavefronts which propagate with higher speeds than the minimum if the initial concentration of B does not decay too rapidly away from the initial reaction zone. However, these faster wavefronts are more likely to be observed in quadratic autocatalytic systems since an initial concentration of the autocatalyst with exponential decay will be easier to achieve, in practice, than the slower algebraic decay needed to generate a fast wave in cubic autocatalysis. In particular, when the autocatalyst, B, diffuses at a much slower rate than the reactant, A, so that $0 < D \ll 1$, (51) shows that even a rapid exponential decay of B as $x \to \infty$ can lead to a wave which propagates faster than the minimum speed.

When the autocatalyst, B, is immobilized, so that $D = 0$, the minimum propagation speed is zero under both quadratic and cubic autocatalysis. This suggests that initial concentrations, $\beta(x,0)$, with compact support will not generate travelling waves in the initial value problem (6) and (7). This is reasonable, on physical grounds, since if B is initially localized in the region $|x| \leqslant \lambda$, say, then it cannot diffuse out of this region and thus no wavefront can propagate away. The initial value problem with $D = 0$ and the implications for the case $0 < D \ll 1$ are currently being studied by one of the authors.

Since localized initial concentrations of B produce travelling waves which propagate at the minimum speed, it is of interest to consider the form of $v_n^*(D)$. Firstly we note that $v_2^*(D) < v_1^*(D)$ for $D > 0$, so that the minimum speed wave propagates more slowly under cubic autocatalysis than under quadratic autocatalysis. We can explain this by considering the rate of reaction ahead of the front in both cases. The reaction rate is of $O(\alpha\beta)$ under quadratic autocatalysis and of $O(\alpha\beta^2)$ under cubic autocatalysis, so that the reaction generally proceeds more slowly ahead of the wavefront, where $0 < \beta \ll 1$, in cubic autocatalysis than in quadratic autocatalysis. This means that the autocatalyst, B, is produced more slowly and thus the wave cannot propagate as rapidly under cubic autocatalysis. Now consider the dimensional form of the minimum propagation speed, $v_n^*(D)$. Although we do not have an analytical expression for $v_2^*(D)$, we can deduce from the asymptotic expressions obtains in §4 that the dimensional minimum propagation speed, V_2^*, satisfies

$$V_2^*(D_A, D_B, k_2, a_0) \sim \tilde{v}^* D_B (k_2 a_0^2 / D_A)^{\frac{1}{2}}, \quad \text{when} \quad D_B \ll D_A, \tag{53a}$$

$$V_2^*(D_A, D_B, k_2, a_0) \sim \hat{v}^* (D_B k_2 a_0^2)^{\frac{1}{2}}, \quad \text{when} \quad D_B \gg D_A. \tag{53b}$$

Thus, when $D_B \gg D_A$, the rate of diffusion of the reactant, A, does not influence the minimum propagation speed at leading order. In general, when D_A and D_B are of the same order, both diffusion rates influence the minimum propagation speed. From Proposition 3.3, the dimensional minimum propagation speed, V_1^*, for quadratic autocatalysis is

$$V_1^*(D_A, D_B, k_1, a_0) = 2(D_B k_1 a_0)^{\frac{1}{2}}, \tag{54}$$

which is independent of D_A. This is an unexpected result which is hard to account for on physical grounds. Note that although D_A does not influence the minimum propagation speed, it still determines the form of the minimum speed travelling wave solution via the parameter D.

Further insight can be gained by studying the permanent form travelling wave solutions of equation ($12a, b, c$) for $n > 0$. A preliminary numerical investigation for various $n > 1$ suggests that a minimum propagation speed exists with $v_n^* \to 0$ as $n \to \infty$, $v_n^*(D) = O(\sqrt{D})$ for $D \gg 1$ and $v_n^*(D) \sim k(n) D$ for $0 < D \ll 1$, where $k(n) \to \infty$ as $n \to 1^+$. It is also easy to see that Propositions 2.1 and 2.4 still hold and that $v_n^*(D) < 2\sqrt{D}$. The permanent form travelling wave solutions have a similar form to those studied here for $n = 2$. However, when $0 < n < 1$, the behaviour of the system of equation (12) is very different. Indeed, it is not clear that travelling wave solutions will exist with $0 < n < 1$. Equation ($12a, b, c$) have proved much harder to integrate numerically when $0 < n < 1$ which supports our non-existence conjecture. These preliminary results indicate that $n = 1$ is a bifurcation point of the system of equation (12). We note that when the reaction scheme $A + nB \to (n+1)B$ was studied in a well-stirred open system by D'Anna *et al.* (1986) it was found that, in the context of singularity theory, the behaviour of the system is equivalent for all $n > 1$ and that this behaviour changes dramatically when $n = 1$. This is in line with the behaviour of the system studied in this paper for $n \geq 1$.

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