

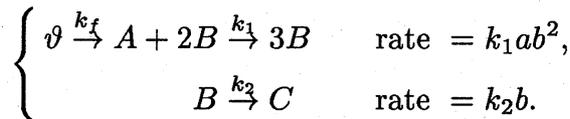
Pulses, kinks and fronts in the Gray-Scott model

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1. Introduction

The Gray-Scott model represents what is called *cubic autocatalysis* [GS1-3], and is given by the chemical reaction equations



Here k_1 , k_2 and k_f are positive rate constants. In this lecture we discuss the situation in which the reactant A is fed *continuously* into an *unstirred reactor*. The rate ϑ at which A is supplied is assumed to be positive if the concentration a of A drops below a preassigned value a_0 , and negative if it exceeds a_0 . Specifically, it is assumed that

$$\vartheta = k_f(a_0 - a).$$

The kinetics of this system leads to a pair of ordinary differential equations for the concentrations $a(t)$ and $b(t)$ of, respectively, A and B :

$$\left\{ \begin{array}{l} a' = -k_1 ab^2 + k_f(a_0 - a), \\ b' = +k_1 ab^2 - k_2 b. \end{array} \right. \quad \begin{array}{l} (1.1a) \\ (1.1b) \end{array}$$

For all values of the rate constants k_1 , k_2 and k_f the point

$$(a, b) = (a_0, 0) \quad \text{is a stable node,}$$

and if

$$\lambda \stackrel{\text{def}}{=} \frac{k_1 k_f}{k_2} a_0^2 > 4, \quad (1.2)$$

there are two additional critical points, $P_1 = (a_1, b_1)$ and $P_2 = (a_2, b_2)$, numbered so that $0 < a_2 < a_1 < a_0$. The point P_1 is a *saddle* and the point P_2 is a *spiral*, which may be stable or unstable. For $\lambda = 4$ these two points coincide.

In the absence of stirring, the different concentrations depend not only on time t , but, due to diffusion, also on the location in the reactor. Assuming a one-dimensional geometry, with spatial coordinate x , the Gray-Scott model then leads to the following system of reaction-diffusion equations for the concentration profiles $a(x, t)$ and $b(x, t)$ of, respectively, A and B :

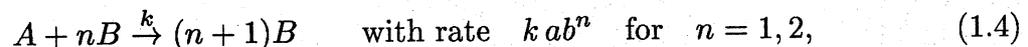
$$\left\{ \begin{array}{l} \frac{\partial a}{\partial t} = D_A \frac{\partial^2 a}{\partial x^2} - k_1 ab^2 + k_f(a_0 - a), \\ \frac{\partial b}{\partial t} = D_B \frac{\partial^2 b}{\partial x^2} + k_1 ab^2 - k_2 b. \end{array} \right. \quad \begin{array}{l} (1.3a) \\ (1.3b) \end{array}$$

Here D_A and D_B are the diffusion coefficients of the chemicals A and B .

Proposed in 1983 by Gray and Scott [GS1], the Gray-Scott model has been studied a great deal, as a simple polynomial mass-action model which has rich dynamics. For background information we refer to the papers of Horsthemke, Pearson, Röhricht, Swinney and Vastano [P,RH,VP1,VP2], in which bifurcation phenomena and Turing patterns are discussed, and to Reynolds, Pearson & Ponce-Dawson [RPP], in which self-replicating patterns are analyzed. The Gray-Scott model is related to another autocatalytic reaction, the Brusselator [NP, p. 93]. We also mention here the more recent studies by Nishiura & Ueyama [NU1,2] on self-replicating patterns and Mimura & Nagayama [MN] on the phenomenon of non-annihilation.

More analytic studies have been carried out by Merkin & Sadiq [MS], and Muratov [M]. In papers by Doelman, Kaper & Zegeling [DKZ], Doelman, Gardner & Kaper [DGK] and Doelman, Eckhaus & Kaper [DEK], singular perturbation methods were used to study the existence and stability of pulses under the assumption that $D_B/D_A \ll 1$ and $k_f/D_A \ll k_2/D_B$.

We also mention the related work of Billingham & Needham [BN1-3] and Foquant & Gallay [FG]. They discuss the existence and stability of travelling waves in the *closed* system of chemical reactions



in the absence of feeding of the chemical A and degeneration of the catalyst B .

In this lecture we discuss stationary *Pulses* and *Kinks* and their stability. Specifically we shall obtain explicit expressions for such solutions if

$$\frac{k_f}{D_A} = \frac{k_2}{D_B}, \quad (1.5)$$

Regarding stability we find that if the diffusion coefficients are equal:

$$D_A = D_B, \quad (1.6)$$

the pulses constructed above are unstable and the kinks are stable.

In this lecture we present results obtained in collaborations with J.K. Hale (Georgia Tech) and W.C. Troy (Pittsburgh) [HP1,2] and with Th. Gallay (Paris Sud) [GP].

2. Dynamics

The reaction diffusion equations (1.3) can be simplified by introducing the dimensionless variables

$$u = \frac{a}{a_0}, \quad v = \frac{b}{a_0}, \quad \tilde{x} = \sqrt{\frac{k_1 a_0^2}{D_A}} x, \quad \tilde{t} = k_1 a_0^2 t, \quad (2.1)$$

and the dimensionless constants

$$A = \frac{k_f}{k_1 a_0^2}, \quad B = \frac{k_2}{k_1 a_0^2} \quad \text{and} \quad d = \frac{D_B}{D_A}. \quad (2.2)$$

When we drop then drop the tildes again, we obtain the system of equations,

$$\begin{cases} u_t = u_{xx} - uv^2 + A(1 - u) \\ v_t = dv_{xx} + uv^2 - Bv \end{cases} \quad x \in \mathbf{R}, \quad t > 0. \quad (2.3a)$$

$$(2.3b)$$

We assume that initially the concentration profiles $a(x, 0)$ and $b(x, 0)$ are given, and we set

$$u(x, 0) = u_0(x) \quad \text{and} \quad v(x, 0) = v_0(x) \quad \text{for} \quad x \in \mathbf{R}, \quad (2.3c)$$

where, in view of the definition of u and v , the initial data u_0 and v_0 are assumed to be nonnegative functions.

We make the following observations: Let (u, v) be a solution of the system (2.3) in the strip $S_T = \{(x, t) : x \in \mathbf{R}, 0 \leq t < T\}$. Then

$$(1) \quad u(x, t) \geq 0 \quad \text{for} \quad (x, t) \in S_T.$$

This follows immediately because $u = 0$ is a sub-solution of equation (2.3a).

$$(2) \quad v(x, t) \geq 0 \quad \text{for} \quad (x, t) \in S_T,$$

because $v = 0$ is a solution of equation (2.3b).

$$(3) \quad u(x, t) \leq 1 \quad \text{for} \quad (x, t) \in S_T,$$

because $u = 1$ is a super-solution of equation (2.3a).

There exists a constant $M > 0$ which depends on the initial data u_0 and v_0 , such that

$$(4) \quad v(x, t) \leq M \quad \text{for} \quad (x, t) \in S_T.$$

The proof of this upper bound is more delicate and uses ideas of Collet & Xin [CX] (see [GP]).

3. Stationary solutions

For stationary solutions of (2.3) we can further reduce the number of parameters by introducing new independent and dependent variables:

$$\tilde{x} = Bx, \quad \tilde{u}(\tilde{x}) = u(x), \quad \tilde{v}(\tilde{x}) = \frac{1}{B}v(x) \quad (3.1)$$

and the constants

$$\lambda = \frac{A}{B^2} \quad \text{and} \quad \gamma = Bd. \quad (3.2)$$

The constant λ in (3.2) is the same as the one defined in (1.2). These scalings yield a system of equations which involves only two parameters: λ and γ :

$$\begin{cases} u'' = uv^2 - \lambda(1-u), & (3.3a) \\ \gamma v'' = v - uv^2. & (3.3b) \end{cases}$$

If $\lambda < 4$ the only constant solution is $P_0 = (1, 0)$ and if $\lambda > 4$ the constant solutions are P_0 , as well as P_1 and P_2 .

In [HPT1] it was shown that it is possible to obtain *explicit* pulse and kink type solutions of Problem (2.3) if

$$\lambda\gamma = 1 \quad \text{and} \quad \lambda > 4 \quad (\text{or } 0 < \gamma < \frac{1}{4}). \quad (3.4)$$

This range of λ values coincides with the range of values for which the null-clines along which u'' and v'' vanish intersect. That is, if we write

$$K = \{(u, v) : u'' = 0\} \quad \text{and} \quad L = \{(u, v) : v'' = 0\}, \quad (3.5)$$

then $K \cap L \neq \emptyset$ if and only if $\lambda > 4$ (see Fig. 1).

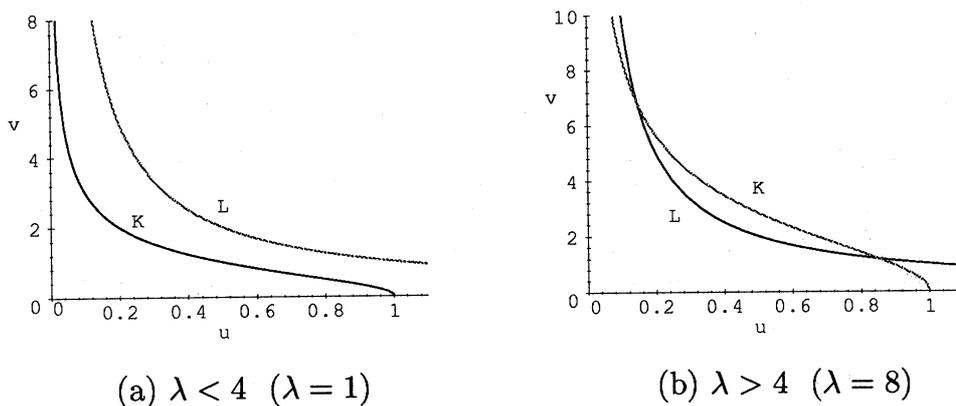


Fig. 1. Null-clines

In [DKZ], [DGK] and [DEK] the existence of solutions is investigated under the assumption that d is small and that $\lambda\gamma \ll 1$. Thus, Figure 1a describes the relative position of the null-clines in these papers. In this paper, the null-clines intersect and Figure 1b applies.

We establish the existence of the following pulses:

Theorem 3.1. Let λ and γ satisfy (3.4), and $0 < \gamma < \frac{2}{9}$, then the pair of functions $u(x)$ and $v(x)$ given by

$$u(x) = 1 - \frac{3\gamma}{1 + Q \cosh(x/\sqrt{\gamma})}, \quad v(x) = \frac{3}{1 + Q \cosh(x/\sqrt{\gamma})}, \quad (3.6)$$

in which $Q = \sqrt{1 - \frac{9\gamma}{2}}$, is a homoclinic solution of Problem (3.3).

Theorem 3.2. Let λ and γ satisfy (3.4), and $\frac{2}{9} < \gamma < \frac{1}{4}$, then the pair of functions $u(x)$ and $v(x)$ given by

$$u(x) = \frac{1 - \omega}{2} + \frac{a\gamma}{1 + b \cosh(cx)}, \quad v(x) = \frac{1 + \omega}{2\gamma} - \frac{a}{1 + b \cosh(cx)}, \quad (3.7a)$$

in which

$$a = \frac{3\omega(1 + \omega)}{\gamma(1 + 3\omega)}, \quad b = \frac{\sqrt{1 - 3\omega}}{1 + 3\omega}, \quad c = \frac{\sqrt{\omega(1 + \omega)}}{\gamma\sqrt{2}}, \quad \omega = \sqrt{1 - 4\gamma}, \quad (3.7b)$$

is a homoclinic solution of Problem (3.3).

In Figures 2a and 2b we give graphs of u and v corresponding to Parts (a) and (b) of Theorem 3.1 for the specific values $\gamma = 0.15$ and $\gamma = 0.23$. The corresponding (v, v') phase planes are given in Figures 4a and 4c.

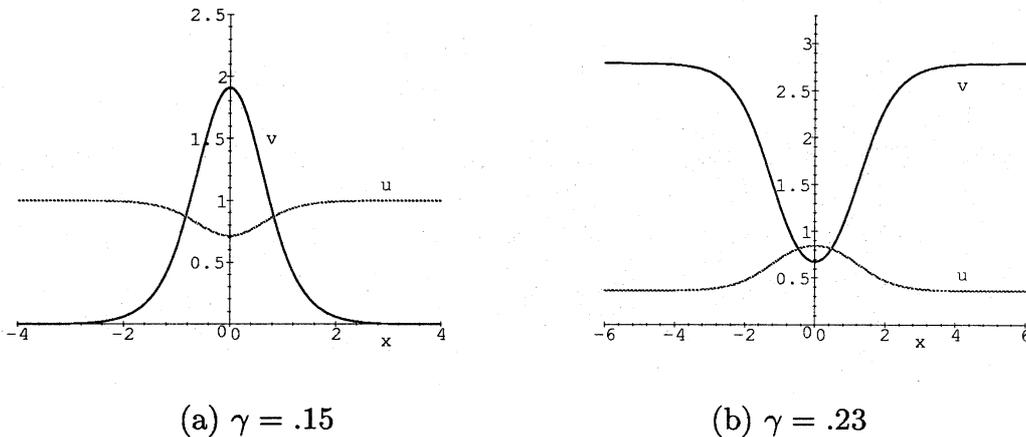


Fig. 2. Homoclinic orbits

For $\gamma = \frac{2}{9}$ we have a kink:

Theorem 3.3. Let λ and γ satisfy (3.4), and let $\gamma = \frac{2}{9}$. Then the pair of functions $u(x)$ and $v(x)$ given by

$$u(x) = \frac{1}{3} \left\{ 2 - \tanh\left(\frac{3x}{2\sqrt{2}}\right) \right\}, \quad v(x) = \frac{3}{2} \left\{ 1 + \tanh\left(\frac{3x}{2\sqrt{2}}\right) \right\}, \quad (3.8)$$

is a heteroclinic solution of Problem (3.3).

In Figure 3 we give graphs of u and v for $\gamma = \frac{2}{9}$. The corresponding (v, v') phase plane is given in Figure 4b.

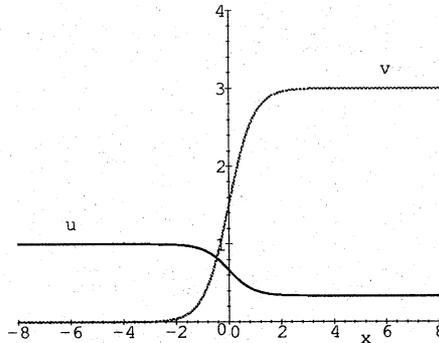


Fig. 3. The heteroclinic orbit for $\gamma = \frac{2}{9}$

The proof of Theorems 3.1, 3.2 and 3.3 is based on the following simple observation: when we add equations (3.3a) and (3.3b) we eliminate the nonlinear term and we obtain the linear equation

$$u'' + \gamma v'' = \lambda(u - 1) + v = \lambda(u + \gamma v - 1) + v(1 - \lambda\gamma). \quad (3.9)$$

When we now set $p = u + \gamma v - 1$, then (3.9) becomes

$$p'' - \lambda p = v(1 - \lambda\gamma). \quad (3.10)$$

Observe that for homoclinic orbits to $P_0 = (1, 0)$ we have

$$(u(x), v(x)) \rightarrow (1, 0) \quad \text{as } x \rightarrow \pm\infty. \quad (3.11)$$

This implies that

$$p(x) \rightarrow 0 \quad \text{as } x \rightarrow \pm\infty. \quad (3.12)$$

If $\lambda\gamma = 1$, it then follows from (3.10) that $p(x) = 0$ for all $x \in \mathbf{R}$, and hence, that

$$u(x) = 1 - \gamma v(x) \quad \text{for } x \in \mathbf{R}. \quad (3.13)$$

When we now use (3.13) to eliminate u from equation (3.3b), we obtain the autonomous second order equation

$$v'' = f(v, \gamma) \stackrel{\text{def}}{=} \frac{1}{\gamma} v(1 - v + \gamma v^2). \quad (3.14)$$

This equation can be analysed by means of phase plane methods. In Figure 4 we show the phase plane for different values of γ .

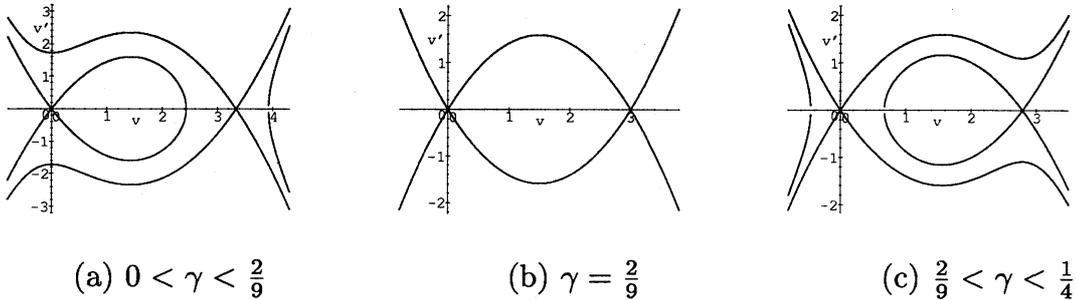


Fig. 4. The phase plane

The proofs of Theorems 3.1-3 can now be given by elementary computations.

In addition to the homoclinic and heteroclinic orbits we obtain a family of *periodic solutions*:

For every $\gamma \in (0, \frac{1}{4})$ Problem (3.3) has a one-parameter family of periodic orbits when $\lambda\gamma = 1$.

These periodic orbits accumulate on one of the homoclinic orbits, or the heteroclinic orbits, when their periods tend to infinity [VF].

4. General properties of pulses

Let (u, v) be a pulse type solution of (3.3) such that

$$(u(x), v(x)) \rightarrow (1, 0) \quad \text{as } x \rightarrow \pm\infty. \quad (4.1)$$

Then we can make the following observations.

(a) We begin with an upper bound for u :

$$u(x) < 1 \quad \text{for } x \in \mathbf{R}. \quad (4.2)$$

Proof. We write equation (3.3a) as

$$u'' - v^2 u = -\lambda(1 - u) \quad \text{on } \mathbf{R}. \quad (4.2)$$

Suppose that $\max_{\mathbf{R}} u > 1$. Then u attains its maximum at a point $x_0 \in \mathbf{R}$. Plainly, at x_0 the left hand side of (4.2) is negative, and the right hand side is positive; a contradiction. Therefore $u \leq 1$ on \mathbf{R} , so that

$$u'' - v^2 u \geq 0 \quad \text{on } \mathbf{R}. \quad (4.3)$$

Thus, by the strong maximum principle, $u < 1$ on \mathbf{R} .

(b) Property (a) enables us to prove that

$$v(x) > 0 \quad \text{for } x \in \mathbf{R}. \quad (4.4)$$

Proof. We write equation (3.3b) as

$$\gamma v'' - v = -uv^2 \leq 0 \quad \text{on } \mathbf{R}, \quad (4.5)$$

and we see that (4.4) holds by the strong maximum principle.

(c) We have

$$\lambda\gamma \leq 1 \quad (\geq 1) \quad \implies \quad u + \gamma v < 1 \quad (> 1). \quad (4.6)$$

This is an immediate consequence of Property (b), equation (3.7) and the strong maximum principle.

(d) *In the region $\lambda\gamma < 1$ there can only exist homoclinic orbits to $(u, v) = (1, 0)$ if $\gamma < \frac{1}{4}$.*

Proof. Plainly, the maximum of v is attained at an interior point; let us denote it by x_0 . Then $v''(x_0) \leq 0$. This means that

$$v > \frac{1}{u} \quad \text{at } x_0. \quad (4.7a)$$

Because, by Property (c),

$$v < \frac{1}{\gamma}(1 - u) \quad \text{at } x_0, \quad (4.7b)$$

The conditions (4.7a) and (4.7b) can only be reconciled if $\gamma < \frac{1}{4}$.

5. Continuation

The branch of exact solutions $\Sigma = \{(\lambda, \gamma) : 0 < \gamma < \frac{1}{4}\}$ can be taken as a starting point of a continuation to values of (λ, γ) in the neighbourhood of Σ . This has been done in [HPT1], both for the homoclinic and the heteroclinic orbits.

Below we give an outline of the argument for the heteroclinic orbits. It uses the Implicit Function theorem and is an application Lin's method [L]. We start from the explicit kink at

$$(\lambda, \gamma) = (\lambda_0, \gamma_0) \quad \text{where } \lambda_0 = \frac{9}{2}, \quad \gamma_0 = \frac{2}{9}. \quad (5.1)$$

We denote this kink by

$$v(x) = v_0(x), \quad u(x) = 1 - \gamma v_0(x), \quad (5.2)$$

where v_0 is given in Theorem 3.3.

We first reformulate the problem. We introduce a small parameter ε and small perturbations of λ_0 , γ_0 , $p = 0$ and v_0 :

$$\lambda\gamma = 1 + \varepsilon, \quad p = \varepsilon r, \quad v = v_0 + w. \quad (5.3)$$

When we substitute these expressions into the equations for p and v we obtain for r and w the system

$$\begin{cases} -r'' + \frac{1+\varepsilon}{\gamma}r = v_0 + w & (5.4a) \\ -w'' + q_0(x)w = h(\varepsilon r, w, \gamma). & (5.4b) \end{cases}$$

Here

$$q_0 = f_v(0, v_0, \gamma_0) = \frac{1}{\gamma_0}(1 - 2v_0 + 3\gamma_0 v_0^2) \rightarrow \frac{1}{\gamma_0} \quad \text{as } x \rightarrow \pm\infty. \quad (5.5)$$

We shall prove the following theorem:

Theorem 5.1. (a) *There exists a smooth arc*

$$\mathcal{C} = \{(\lambda(\varepsilon), \gamma(\varepsilon)) : |\varepsilon| < \varepsilon_0\}, \quad (\varepsilon_0 > 0)$$

of heteroclinic orbits $(u(\varepsilon), v(\varepsilon))$ of Problem (3.3) such that

$$(\lambda(\varepsilon), \gamma(\varepsilon)) \rightarrow (\lambda_0, \gamma_0) \quad \text{and} \quad (u(\varepsilon), v(\varepsilon)) \rightarrow (u_0, v_0) \quad \text{as } \varepsilon \rightarrow 0,$$

(b) *The arc \mathcal{C} intersects the curve $\{\lambda\gamma = 1\}$ under an angle given by*

$$\left. \frac{d\lambda}{d\gamma} \right|_{\mathcal{C}}(\lambda_0, \gamma_0) = \frac{10 - \pi^2}{\pi^2 - 7} \cdot \frac{\lambda_0}{\gamma_0} = 0.920165 \dots \quad (5.6)$$

Here the convergence is in the space of bounded continuous functions on \mathbf{R} .

We proceed in a series of steps.

Step 1. We choose an element w in the set $C_B(\mathbf{R})$ of continuous functions on \mathbf{R} which are uniformly bounded. With this function w we can solve equation (5.4a) uniquely; we denote its solution by

$$r = H(\gamma, \varepsilon)(v_0 + w), \quad \text{so that } r_0 = H(\gamma_0, 0)(v_0). \quad (5.7)$$

We put this solution into the second equation (5.4b). This yields an equation of the form

$$-y'' + q_0(x)y = g(x) \quad \text{on } \mathbf{R}, \quad (5.8)$$

in which $q_0(x)$ has been defined in (5.5). Before we can solve this equation, we need to inspect the eigenvalue problem

$$-y'' + q_0(x)y = \kappa y \quad \text{on } \mathbf{R}. \quad (5.9)$$

Step 2. Equation (5.9) has a zero eigenvalue with corresponding eigenfunction $v'_0(x)$, so that if y is a solution of equation (5.8), then so is $y + tv'_0$ for any $t \in \mathbf{R}$. We therefore split the space $C_B(\mathbf{R})$:

$$C_B(\mathbf{R}) = Y_0 \oplus Y_1, \quad (5.10a)$$

where

$$Y_0 = \{tv'_0 : t \in \mathbf{R}\} \quad \text{and} \quad Y_1 = \{y \in C_B : (y, v'_0) = 0\}. \quad (5.10b)$$

It is well known that if $g \in Y_1$, then there exists a unique solution $y \in Y_1$ of the equation (5.8).

Step 3. We define the projection operators

$$P : C_B \rightarrow Y_0 \quad \text{and} \quad 1 - P : C_B \rightarrow Y_1, \quad (5.11)$$

and solve the equation

$$-y'' + q_0(x)y = (I - P)h(\varepsilon H(\gamma, \varepsilon)(v_0 + w), w, \gamma) \quad \text{on } \mathbf{R}. \quad (5.12)$$

We denote the unique solution in Y_1 by

$$y \stackrel{\text{def}}{=} \mathcal{T}(w, \gamma, \varepsilon) \in Y_1. \quad (5.13)$$

Step 4. We prove that for

$$|\gamma - \gamma_0| + |\varepsilon| < \nu,$$

where ν is a small number, the operator \mathcal{T} in equation (5.13) has a fixed point $w^*(\gamma, \varepsilon)$. This solution will be a solution of the *original* problem if

$$Ph(\varepsilon H(\gamma, \varepsilon)(v_0 + w^*), w^*, \gamma) = 0, \quad (5.14)$$

or, in view of the definition of the projection P ,

$$\mathcal{G}(\gamma, \varepsilon) \stackrel{\text{def}}{=} \int_{\mathbf{R}} h(\varepsilon H(\gamma, \varepsilon)(v_0 + w^*), w^*, \gamma) v'_0 dx = 0. \quad (5.15)$$

Because \mathcal{G} is differentiable near $(\gamma_0, 0)$ we have

$$\mathcal{G}_\gamma(\gamma_0, 0)\gamma'(\varepsilon) + \mathcal{G}_\varepsilon(\gamma_0, 0) = 0. \quad (5.16)$$

Since

$$\mathcal{G}_\gamma(\gamma_0, 0) = -\frac{3^4}{4\gamma_0} \quad \text{and} \quad \mathcal{G}_\varepsilon(\gamma_0, 0) = \frac{1}{\gamma_0} \int_{\mathbf{R}} v_0^2 v_0' r_0 \, dx,$$

we conclude that

$$\gamma'(0) = \frac{4}{3^4} \int_{\mathbf{R}} v_0^2 v_0' r_0 \, dx = \frac{\pi^2 - 7}{3} \gamma_0.$$

This yields the desired expression:

$$\left. \frac{d\lambda}{d\gamma} \right|_c(\lambda_0, \gamma_0) = \frac{10 - \pi^2}{\pi^2 - 7} \cdot \frac{\lambda_0}{\gamma_0} = 0.920165 \dots \quad (5.17)$$

In Figure 5a we show the computed graph of \mathcal{C} , extended away from the point (λ_0, γ_0) ; a blowup of the branch is shown in Figure 5b. The computations were made with AUTO97 [Do].

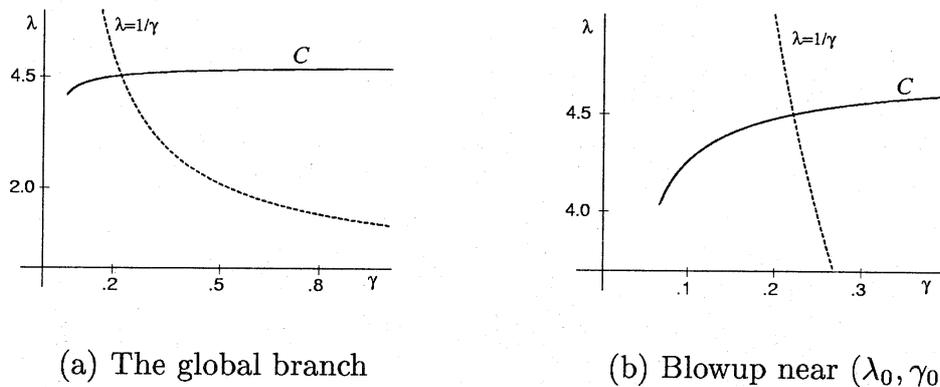


Fig. 5. The branch \mathcal{C} of heteroclinic orbits

We conclude with a few remarks about the stability of the pulses and kinks which we constructed. When the two diffusion coefficients D_A and D_B are equal, it is still possible to decouple the two equations, and so analyse the spectrum around the solutions on the branch $\{\lambda\gamma = 1 : \lambda > 4\}$, using well known results about the second order equation (3.14). It turns out that the spectrum of the kink lies entirely in the negative half plane, implying local stability [He], and that the spectrum of the pulses has eigenvalues with both positive and negative real part, implying instability [HPT2].

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