Numerical methods for the travelling wave solutions in reaction-diffusion equations

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Abstract

In this work we consider how shooting and relaxation methods can be used to investigate propagating waves solutions of PDEs. Particular attention is paid to overcoming some of the numerical difficulties. The linear stability of these solutions are analyzed by using the Evans function approach. As an illustration, we shall apply the above methods to an autocatalytic reaction involving two diffusing chemicals in one spatial dimension. Prospects of further work are also discussed.

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Contents

1 Introduction

Many physical, chemical and biological phenomena such as combustion waves, optical solitons, chemical reactions, propagation of dominant genes and nerve pulses etc. are modelled by nonlinear Partial Differential Equations (PDEs) exhibiting travelling wave solutions [1, 2, 3, 4, 5].

Steady propagating solutions in the form of a pulse or front travelling without change of form and speed are of special interest. In this case the governing PDEs can be reduced to a system of Ordinary Differential Equations(ODEs) by introducing a moving coordinate frame. The form of the front(pulse) is then given by the solution of the system of ODEs, which usually can be found only numerically as a solution of a two-point boundary value problem (BVP).

This BVP can be stated in the following form: we want to find

the solution of N coupled first-order ODEs, satisfying n_1 boundary conditions at the starting point x_1, and $n_2 = N - n_1$ boundary conditions at the final point x_2. Once the problem is formulated in the form of a two-point BVP, methods for numerical integration such as *shooting* and *relaxation* [6] can be employed to find the form of the steady propagating front(pulse). In section 3 we illustrate the application of these methods to the example of an autocatalytic reaction involving two chemical species in one spatial dimension. Following the work in [7] we obtain major properties of travelling front solution such as the dependence of the speed of the propagating front on the parameters of the system.

Steady propagating solutions can lose stability as we change parameters of the system. For example, in [7, 8] it was shown that the travelling fronts lost their stability in an oscillatory manner and appears to exhibit a period doubling route to chaos. To investigate the travelling front stability, the corresponding linear stability problem was solved using the Nyquist technique via an Evans function [9]. In section 4 we introduce the definition of the Evans function and describe its relation to the linear stability problem.

In this case, however, the conventional algorithm for a calculating the Evans function introduced in [9] encounters serious obstacles due to the necessity of numerical tracing of two solutions with different rates of exponential growth or decay. In section 5 we show how this difficulty was overcome by using the compound matrix method [11, 12, 13, 14, 15, 16].

2   Statement of problem

Let us consider an autocatalytic reaction involving two chemicals (the autocatalyst $u(x,t)$, and the reactant $v(x,t)$) in one spatial

dimension. In non-dimensional coordinates, the equations governing this process can be found in [7] and are

$$u_t = u_{xx} + vf(u), \quad v_t = \tau v_{xx} - vf(u), \tag{1}$$

where τ is the inverse of the Lewis number (the ratio of the diffusion rates of the two chemicals) and the reactant rate is

$$f(u) = \begin{cases} u^m, & u \geq 0, \\ 0, & u < 0, \end{cases} \tag{2}$$

where m is the reaction order. We assume the following boundary conditions:

$$\begin{aligned} u(x,t) &\to 1, \ v(x,t) \to 0 \ \text{ as } \ x \to -\infty, \\ u(x,t) &\to 0, \ v(x,t) \to 1 \ \text{ as } \ x \to +\infty. \end{aligned} \tag{3}$$

Solution of (1) with (3) are sought by assuming the form $u(x,t) = U(x - ct)$ and $v(x,t) = V(x - ct)$ of a front travelling with speed c. After substitution of this solution into (1) it is easy to obtain

$$U_{\xi\xi} + U^m V = -cU_\xi, \quad \tau V_{\xi\xi} - U^m V = -cV_\xi, \tag{4}$$

and the boundary conditions

$$\begin{aligned} U(\xi) &\to 1, \ V(\xi) \to 0 \ \text{ as } \ \xi \to -\infty, \\ U(\xi) &\to 0, \ V(\xi) \to 1 \ \text{ as } \ \xi \to +\infty, \end{aligned} \tag{5}$$

where $\xi = x - ct$ is a coordinate in the moving frame. It can be shown (see [7] for details) that (4) has a unique solution if and only if c is greater than a minimum value $c_\star(m, \tau)$. All fronts travelling with speed $c > c_\star$ decay algebraically as $\xi \to +\infty$. On the contrary, the front with $c = c_\star$ decays exponentially as $\xi \to +\infty$. In the discussion that follows, we will only be interested in the latter case. System (4) has two fixed points: S_1 of $U = 1$, $V = 0$; and S_2 of $U = 0$, $V = 1$. Equations obtained through linearization of (4) near S_1

have only one exponentially unstable solution $(U - 1, V) \sim \mathbf{q}e^{h\xi}$, where $\mathbf{q} = (-1, h(h + c))$ and $h = (-c + \sqrt{c^2 + 4\tau})/2\tau$. Any solution $U(\xi)$, $V(\xi)$ of (4) tending to S_1 as $\xi \to -\infty$ approaches S_1 as $\mathbf{q}e^{h(\xi - \xi_0)}$, where ξ_0 depends on initial conditions. Similarly, linear analysis of (4) near S_2 shows that any solution of (4) satisfying the right boundary conditions can be approximated for $\xi \to +\infty$ as $(U, V - 1) = (k_1 e^{-c(\xi - \xi_0)}, \ k_2 e^{-c(\xi - \xi_0)/\tau})$ where k_1 and k_2 are constants. The travelling front solution of (1) corresponds to the solution of (4) connecting two fixed points and satisfying the given asymptotic behavior.

3 Travelling front solution

It is convenient to rewrite (4) as the system of first-order ODEs

$$\dot{y}_i = f_i(\mathbf{y}, \xi), \tag{6}$$

where $i = 1, \ldots, 4$, $y_1 = U$, $y_2 = U_\xi$, $y_3 = V$, $y_4 = V_\xi$, and $f_1 = y_2$, $f_2 = -f(y_1)y_3 - cy_2$, $f_3 = y_4$, $f_4 = (f(y_1)y_3 - cy_4)/\tau$. As a first step we will find an approximate solution of (6) using a *shooting* method [6]. Numerically we integrate (6) from $\xi = -\ell_1$ to $\xi = \ell_2$, where ℓ_1 and ℓ_2 are considered to be sufficiently large. We used the fourth order Runge-Kutta method of integration. On the left boundary we define initial conditions, which satisfy the asymptotic behavior for $\xi \to -\infty$ given above, as

$$\mathbf{y} = (1 - e^{-h\ell_1}, \ -he^{-h\ell_1}, \ h(h + c)e^{-h\ell_1}, \ h^2(h + c)e^{-h\ell_1})^T, \tag{7}$$

where T stands for the transpose. Note that due to the translational symmetry of (1) we can take the initial conditions at any point lying on the unstable manifold of S_1. Linear analysis of (6) shows that (7) approximates it near S_1, where ℓ_1 can be considered as a parameter

characterizing the distance between S_1 and point on the unstable manifold. Furthermore, the approximation (7) holds if $h\ell_1 \gg 1$.

On the right boundary we cannot prescribe the value of any component of the vector $\mathbf{y}$; except to say that it must satisfy definite asymptotic behavior for large ξ. For this reason we use the Cauchy boundary conditions

$$B_1 = cy_1 + y_2 = 0, \quad B_2 = cy_3 + \tau y_4 = 0, \tag{8}$$

where $\mathbf{y}$ is taken at $\xi = \ell_2$. By assuming that c is the free parameter, we make a guess for the value of c and integrate (6) with initial conditions (7). We consider the discrepancy of one of the conditions on the right boundary (B_1, for instance). Then, by using Newton-Raphson method the root of equation $B_1(c) = 0$ can be found with desired accuracy. We exploit another condition $B_2(c) = 0$ to check the accuracy of the method.

We can now make use of the solution obtained from the *shooting* as a guess for a more accurate scheme—the *relaxation*. In contrast to the *shooting* method described previously, the *relaxation* scheme improves the guess solution on every mesh point. The system of N ODEs given by (6) is replaced by finite-difference equations(FDE) on M mesh points. We use a second-order FDE relating values at two points k and $k-1$

$$\mathbf{y}_k - \mathbf{y}_{k-1} = (\xi_k - \xi_{k-1})\mathbf{f}[(\mathbf{y}_k - \mathbf{y}_{k-1})/2]. \tag{9}$$

Higher order formulas are discussed in [17]. Now we have a system of equations for $M \times N$ variables, which can be solved using a multi-dimensional Newton's method (see [6] for details). In our case we have the system of four ODEs (6) with c as a free parameter which also has to be found. This problem is reducible to standard boundary value problem [6]. We introduce new variable $y_5 \equiv c$ and another differential equation $\dot{y}_5 = 0$. Now we have five equations. We

take three boundary conditions from (7) on the left boundary and two Cauchy conditions (8) on the right boundary. The relaxation method is then used to calculate the solution of the problem (4–5). Results obtained for $\tau = 0.1$ and $m = 2,\ 13$ are shown in Figure 1.

As we increase m for fixed τ the autocatalyst u front becomes flatter and the interval of the integration $(-\ell_1, \ell_2)$ has to be increased. In contrast, the front of reactant v steepens and we must decrease the step of integration near the point of the maximal slope. This imposes additional difficulties if we want to investigate properties of the travelling front solution such as speed c as a function of the parameters τ and m. The best way to overcome this obstacle is to introduce the tangential transformation $\xi = \arctan(\theta)$ which maps the infinite interval $\xi \in (-\infty, \infty)$ onto $\theta \in (-\pi/2, \pi/2)$. Then we modify the equations (4) and introduce the uniform mesh on $(-\pi/2, \pi/2)$. Figure 2 shows the speed of the front solution as a function of parameter m for fixed values of τ. For every point on the parameter plane (m, τ) under consideration, we use the *shooting* method as a prediction and then correct the results with the *relaxation* method outlined above.

Neither the *shooting* nor the *relaxation* scheme allows us to analyze the stability of steady propagating solutions. In the next section a linear stability problem of (1) is considered.

4   **Stability analysis**

As a first step in the analysis of travelling wave stability we linearize (1) around the front solution

$$u(\xi, t) = U(\xi - ct) + \varphi(\xi - ct, t), \quad v(\xi, t) = V(\xi - ct) + \chi(\xi - ct, t),$$
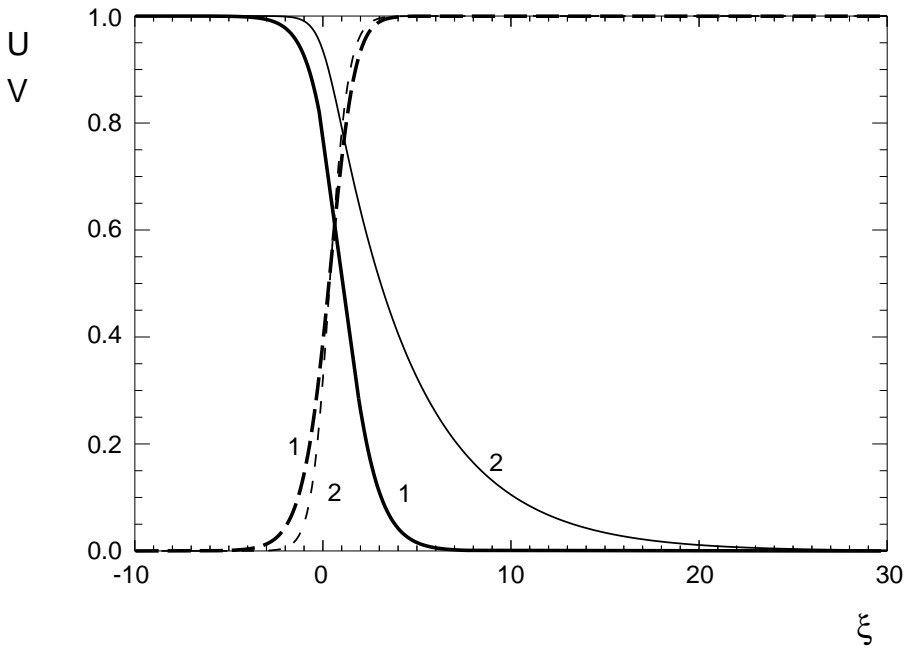$$(10)$$

FIGURE 1: Solutions of (4) obtained by *relaxation* method for parameters $\tau = 0.1$ and $m = 2$ (curves 1), $m = 13$ (curves 2). Solid curves correspond to $U(\xi)$ and dashed to $V(\xi)$
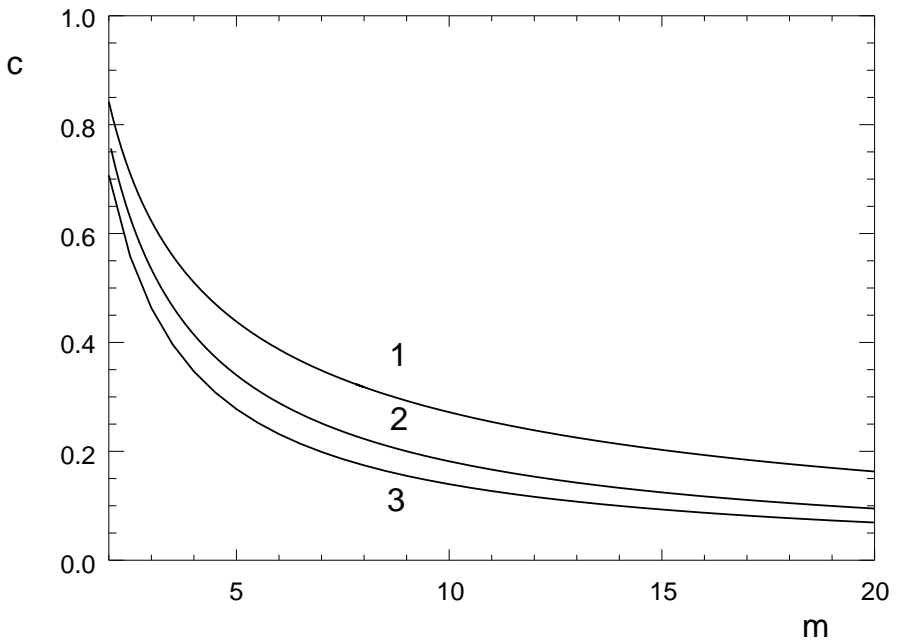
FIGURE 2: Dependence of front speed c on parameter m for $\tau = 0.1$ (curve 1), 0.5 (curve 2), 1 (curve 3).

where φ and χ are linear perturbation terms. After substituting (10) into (1), it is straightforward to derive

$$\begin{pmatrix} \partial\varphi/\partial t \\ \partial\chi/\partial t \end{pmatrix} = \hat{L} \begin{pmatrix} \varphi \\ \chi \end{pmatrix}, \tag{11}$$

where

$$\hat{L} = \begin{pmatrix} \partial_\xi^2 + mVU^{m-1} + c\partial_\xi & U^m \\ -mVU^{m-1} & \tau\partial_\xi^2 - U^m + c\partial_\xi \end{pmatrix}. \tag{12}$$

The stability of the travelling front is then defined from the spectra of $\hat{L}$. It is straightforward to show that the essential spectra of this operator always lies in the left half plane and therefore the discrete spectra is solely responsible for the transition to instability. We seek the solution of (11) of the form

$$\varphi(\xi, t) = \varphi(\xi)e^{\lambda t}, \quad \chi(\xi, t) = \chi(\xi)e^{\lambda t}, \tag{13}$$

where λ is a spectral parameter. If the operator $\hat{L}$ has points of discrete spectra with $\Re(\lambda) > 0$ then the travelling front solution of (1) is unstable. Substituting (13) into (11) and introducing a vector with the components $z_1 = \varphi$, $z_2 = \varphi_\xi$, $z_3 = \chi$, $z_4 = \chi_\xi$ we obtain the system of ODEs in the form

$$\dot{\mathbf{z}} = \mathbf{A}\mathbf{z}, \tag{14}$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \lambda - mVU^{m-1} & -c & -U^m & 0 \\ 0 & 0 & 0 & 1 \\ \frac{m}{\tau}VU^{m-1} & 0 & \frac{\lambda+U^m}{\tau} & -\frac{c}{\tau} \end{pmatrix}. \tag{15}$$

Using the fact that $U \to 1$, $V \to 0$ as $\xi \to -\infty$ and $U \to 0$, $V \to 1$ as $\xi \to +\infty$ it is easy to obtain the limit matrices $\mathbf{A}^{\pm}(\lambda) =$

$\lim_{\xi \to \pm\infty} \mathbf{A}(\xi, \lambda)$. The eigenvalues of $\mathbf{A}^+$ and $\mathbf{A}^-$ are

$$
\mu_{1,2}^-(\lambda) = \frac{-c \mp \sqrt{c^2 + 4\lambda}}{2}, \qquad \mu_{1,2}^+ = \mu_{1,2}^-,
$$

$$
\mu_{3,4}^-(\lambda) = \frac{-c \mp \sqrt{c^2 + 4\tau(\lambda + 1)}}{2\tau}, \quad \mu_{3,4}^+(\lambda) = \mu_{3,4}^-(\lambda - 1),
$$

(16)

with corresponding eigenvectors denoted by $\zeta_i^\pm$ which will be considered as normalized. The limit matrix $\mathbf{A}^-$ has two eigenvalues μ_2^- and μ_4^- with positive real parts. Let us represent the 2-dimensional space of solutions of equation (14) bounded at $\xi = -\infty$ as

$$
Z^- = \sum_{i=2,4} \alpha_i z_i^-(\xi, \lambda),
$$

(17)

where α_i are constant coefficients and $z_i^-(\xi, \lambda) = (z_{i1}^-, z_{i2}^-, z_{i3}^-, z_{i4}^-)^T$ are the solutions of (14) satisfying

$$
\lim_{\xi \to \infty} \exp(-\mu_i^- \xi) z_i^-(\xi, \lambda) = \zeta_i^-, \quad i = 2, 4.
$$

(18)

Similarly limit matrix $\mathbf{A}^+$ has two eigenvalues μ_1^+ and μ_3^+ with negative real part and we introduce a space of solutions bounded at $\xi = +\infty$

$$
Z^+ = \sum_{i=1,3} \beta_i z_i^+(\xi, \lambda),
$$

(19)

where β_i are constants and

$$
\lim_{\xi \to \infty} \exp(-\mu_i^+ \xi) z_i^+(\xi, \lambda) = \zeta_i^+, \quad i = 1, 3.
$$

(20)

If λ is a point of discrete spectra then equation (14) has a solution bounded both at $\xi = \pm\infty$ and we require the following matching conditions at $\xi = 0$ to be satisfied

$$
\sum_{i=2,4} \alpha_i z_i^-(0, \lambda) = \sum_{i=1,3} \beta_i z_i^+(0, \lambda).
$$

(21)

The last equation is algebraic for the four coefficients $\alpha_{2,4}$ and $\beta_{1,3}$ if $z_{2,4}^-(0, \lambda)$ and $z_{1,3}^+(0, \lambda)$ are known. It has a nontrivial solution if

$$D(\lambda) = 0 \,, \tag{22}$$

where

$$D(\lambda) = \begin{vmatrix} z_{21}^-(0,\lambda) & z_{41}^-(0,\lambda) & z_{11}^+(0,\lambda) & z_{31}^+(0,\lambda) \\ z_{22}^-(0,\lambda) & z_{42}^-(0,\lambda) & z_{12}^+(0,\lambda) & z_{32}^+(0,\lambda) \\ z_{23}^-(0,\lambda) & z_{43}^-(0,\lambda) & z_{13}^+(0,\lambda) & z_{33}^+(0,\lambda) \\ z_{24}^-(0,\lambda) & z_{44}^-(0,\lambda) & z_{14}^+(0,\lambda) & z_{34}^+(0,\lambda) \end{vmatrix}. \tag{23}$$

We will refer to $D(\lambda)$ as the Evans function. Similar definitions of the Evans function are given in [7, 9]. Now according to the method introduced in [9] we should take one of the vectors $\zeta_{2,4}^-$ as the initial conditions at $\xi = -\ell_1$ and integrate (14) until $\xi = \ell_2$, where $\ell_{1,2}$ are sufficiently large. A special technique of integration is introduced to avoid exponential divergence of the solution. Then we represent the solution at $\xi = \ell_2$ as a superposition of two solutions $z_{2,4}$ unbounded as $\xi \to +\infty$ and satisfying $\lim_{\xi\to\infty} \exp(-\mu_i^+ x) z_i = \zeta_i^+$, $i = 2, 4$. This procedure gives us four coefficients (two for each value of initial conditions ζ_2^- or ζ_4^-) which are sometimes called *transmission* coefficients. A determinant can then be constructed using these coefficients and the Evans function can be defined then via this determinant(see [7] for details). A more precise definition based on the solutions of the problem adjoint to (14) can be found in [10].

However, the method of the Evans function calculation briefly outlined above has difficulties for the problem presented here. The main difficulty is that it can be applied only to a class of rather specific systems which have one dimensional space of solutions bounded (or unbounded) at both $\xi = +\infty$ or $-\infty$. This is not the case in our problem where we have the example of a stiff system (see [12] for definition). There are two coefficients $\mu_{2,4}^\pm$, one is always bigger

than the other (except in some special case when they are equal for some value of λ). We are not able to trace the solution which corresponds to the lower coefficient of exponential growth numerically, because another solution is always excited due to the errors of numerical integration if we use a standard integration method like the fourth order Runge-Kutta, which is not appropriate to treat the stiff systems. This is the reason why we can manage to calculate only one *transmission* coefficient between solutions with maximal exponential growth at $\xi = \pm\infty$. This, however, is not sufficient for investigating the stability of the travelling front.

A way to overcome this difficulty was proposed in [12, 13]. The authors introduced an alternative definition of the Evans function which numerically implies using the *compound* matrix method [14, 15, 16]. We shall now proceed to describe this method.

5   Compound matrix method

Let z_2 and z_4 be two solutions of (14) bounded at $\xi = -\infty$. Consider the 4×2 solution matrix

$$\mathbf{\Phi}(\xi) = \left(\begin{array}{cccc} z_{21} & z_{22} & z_{23} & z_{24} \\ z_{41} & z_{42} & z_{43} & z_{44} \end{array} \right)^T. \tag{24}$$

We arrange the 2×2 minors of $\mathbf{\Phi}$ to a vector with the components

$$\begin{array}{ll} \phi_1 = z_{21}z_{42} - z_{41}z_{22} \,, & \phi_4 = z_{22}z_{43} - z_{42}z_{23} \,, \\ \phi_2 = z_{21}z_{43} - z_{41}z_{23} \,, & \phi_5 = z_{22}z_{44} - z_{42}z_{24} \,, \\ \phi_3 = z_{21}z_{44} - z_{41}z_{24} \,, & \phi_6 = z_{23}z_{44} - z_{43}z_{24} \,. \end{array} \tag{25}$$

We call ϕ the second compound of $\mathbf{\Phi}$ and it satisfies the equation

$$\dot{\phi} = \mathbf{B}\phi \,, \tag{26}$$

where $\mathbf{B}$ is a 6×6 matrix those elements are found from the spectral problem for operator L (12) (see [14, 15] for details). It can be shown that the eigenvalues $s_i^{\pm}$ of $\mathbf{B}$ in the limits $\xi = \pm\infty$ are

$$s_1^{\pm} = \mu_1^{\pm} + \mu_2^{\pm}, \quad s_4^{\pm} = \mu_2^{\pm} + \mu_3^{\pm},$$

$$s_2^{\pm} = \mu_1^{\pm} + \mu_3^{\pm}, \quad s_5^{\pm} = \mu_2^{\pm} + \mu_4^{\pm}, \tag{27}$$

$$s_3^{\pm} = \mu_1^{\pm} + \mu_4^{\pm}, \quad s_6^{\pm} = \mu_3^{\pm} + \mu_4^{\pm}.$$

See that the two-dimensional space of solutions of (14) bounded at $\xi = -\infty$ degenerates to one solution $\phi^-(\xi)$ of the equation (26) with the largest rate of exponential decay s_5^- as $\xi \to -\infty$. Similarly, the two-dimensional space of solutions of (14) bounded at $\xi = +\infty$ degenerates to the solution $\phi^+(x)$ of the equation (26) with the largest rate of exponential decay s_3^+ as $\xi \to +\infty$. In this case localized solutions of (26) and corresponding values of λ can be found using the method introduced in [9]. After numerical integration of (26) from $\xi = \ell^-$ to $\xi = 0$ with appropriate initial conditions we can find the approximation of the solutions of (14) exponentially decaying as $\xi \to -\infty$ by inversion of the system (25). In the same way integration of (26) from $\xi = \ell^+$ to $\xi = 0$ gives us the solutions of (14) exponentially decaying as $\xi \to +\infty$. Then we define the Evan's function via 4×4 determinant (23). However it is much easier to express this determinant in terms of $\phi^{\pm}$

$$D(\lambda) = (\phi^-(0) \cdot \Sigma \phi^+(0)), \tag{28}$$

where $(\cdot)$ denotes scalar product of two vectors and

$$\Sigma = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{29}$$

The problem of stability of the travelling front of (1) reduces to the search for zeros of the Evans function (28) located in the right half plane. Zeros of $D(\lambda)$ can be calculated using argument principle. The number of zeros in the right half plane equals to the number of times the image of the imaginary axis under $D(it)$, $t \in R$ winds around the origin. Pictures of $D(it)$, $t \in R$ are called Nyquist plots. Figure 3 shows Nyquist plots for $\tau = 0.1$ and $m = 8.2$, 8.35, 8.6. For $m = 8.2$ the curve does not encircle the origin, hence the travelling front is stable. Transition to instability occurs for $m = 8.35$, when two complex conjugate eigenvalues cross the imaginary axes and the curve passes through the origin three times. The front is clearly unstable for $m = 8.6$ when the curve encircles the origin two times and therefore there are two points of discrete spectra in right half plane.

6   Conclusions

In this work we have investigated propagation of travelling front solutions on the example of an autocatalytic reaction involving two diffusing chemicals in one spatial dimension using two methods: shooting and relaxation. Both methods were successful in obtaining solutions.

The Evans function method was employed to examine the linear stability problem. It was shown that the compound matrix method significantly expands the applicability of the Evans function approach. Although in this work we found simple numerical criteria for the transition to instability for steady propagating solutions, we believe that an advanced Evans function method would provide more detailed information such as the location and the number of points of discrete spectra and the corresponding modes for
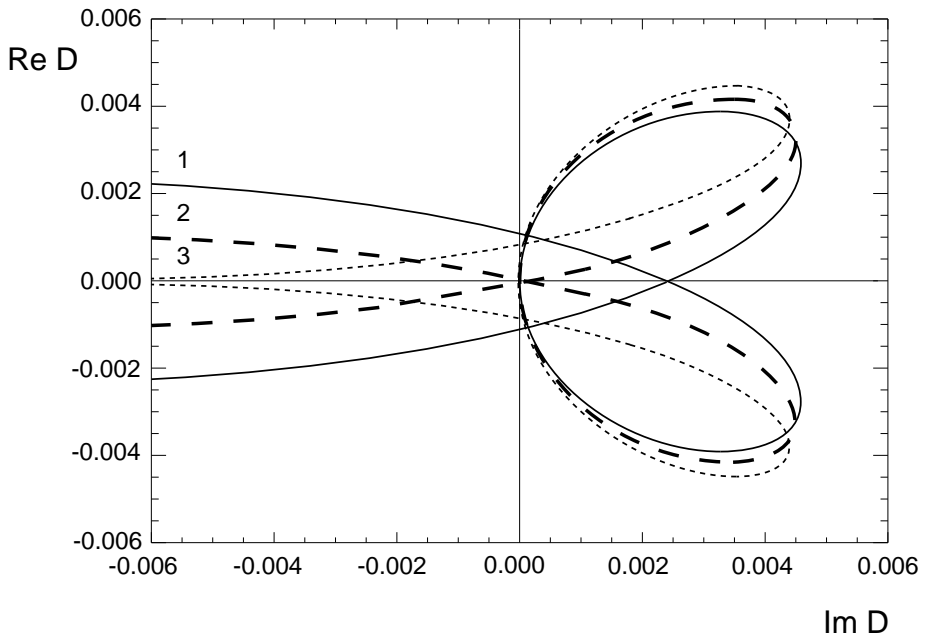
FIGURE 3: Transition to instability. The image of the imaginary axis $D(it)$ near the origin for $t = 0.1$ and for $m = 8.2$ (curve 1), 8.35 (curve 2), 8.6 (curve 3).

the linearized stability problem.

We are currently in the process of applying these methods to a similar system with Arrhenius kinetics which describes the propagation of combustion waves.

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