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Numerical computation of heteroclinic orbits

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Abstract: We give a numerical method for the computation of heteroclinic orbits connecting two saddle points in $\mathbb{R}^2$. These can be computed to very high period due to an integral phase condition and an adaptive discretization. We can also compute entire *branches* (one-dimensional continua) of such orbits. The method can be extended to compute an invariant manifold that connects two fixed points in $\mathbb{R}^n$. As an example we compute branches of traveling wave front solutions to the Huxley equation. Using weighted Sobolev spaces and the general theory of approximation of nonlinear problems we show that the errors in the approximate wave speed and in the approximate wave front decay exponentially with the period.

Keywords: Heteroclinic orbits, traveling waves, numerical computation and continuation, weighted Sobolev spaces, approximation of nonlinear problems.

1. Introduction

The problem of finding traveling wave front solutions of constant speed to nonlinear parabolic partial differential equations is equivalent to the problem of finding trajectories that connect two fixed points of an associated system of ordinary differential equations. Such a trajectory is an example of a *heteroclinic orbit*, i.e. an orbit with several fixed points on it. The period of such orbits is necessarily infinite.

In this paper we give an accurate, robust, and systematic method for computing entire families of orbits connecting two saddle points. In a forthcoming paper [8] we shall consider, more generally, the computation of manifolds connecting two fixed points in $\mathbb{R}^n$.

Calculations using the numerical methods described here are easily carried out with existing continuation software. The method is essentially very straightforward, but its particular formulation of the problem of computing the heteroclinic connection makes it very powerful. Orbits of

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high period can be computed effectively, and more importantly, entire branches of such orbits can be computed very efficiently. This is due to the use of adaptive mesh selection [19] and the use of a phase condition that keeps the wave front at the same location.

In our applications we use the software package AUTO. This package incorporates algorithms for the numerical bifurcation analysis of differential equations. The first reference to the package is in [6]. The most complete description of AUTO is given in [7], which contains an overview of the algorithms, a large number of illustrative applications, and a user manual with detailed examples of actual use of the software.

Traveling wave solutions to nonlinear parabolic equations arise in numerous problems of physical interest, for example, in chemical-biochemical systems [1,3,9,16,17,18], flame propogation [4,21], etc.. We next review briefly some numerical results. In Miura [16], solitary waves for the Fitz–Hugh–Nagumo (FHN) equations were calculated by a variant of the Crank–Nicolson scheme, where the interval $-\infty < x < \infty$ was replaced by a finite interval with an adaptive outgoing wave boundary condition, and the "wave integrals" were used to determine the wave speed and to measure the closeness of the computed solutions to the exact solitary wave solution. Another method used in [16] was to solve a boundary value problem (in a moving coordinate system) on a finite interval with boundary conditions chosen as in Lentini and Keller [15]. A similar method was used in Hassard [10] to calculate traveling wave solutions to the Hodgkin-Huxley equations by using higher order approximations of the stable and unstable manifolds. Recently Keller and his students developed efficient methods to approximate systems of ODE and PDE on infinite domains by the problems with appropriate boundary conditions on finite domains (see e.g. Lentini and Keller [15] and Hagstrom and Keller [12,13] and the references there). In particular, in [13] appropriate boundary conditions were derived to calculate traveling waves by solving the original parabolic PDE.

The numerical method proposed here is based on ideas similar to those in [15] and is a generalization of the methods in [16] and [10]. In the derivation of error estimates, we use weighted Banach spaces, combining an approach in Babuška [2] and the general theory of approximation of nonlinear problems in Keller [14] and in Descloux and Rappaz [5]. The numerical method is described in Section 2. Section 3 contains applications. An error analysis is given in Section 4.

2. Numerical method

The algorithm is based upon the following equations:

$$u'(t) = Tf(u(t), \lambda), \quad 0 \leqslant t \leqslant 1, \quad T \text{ "large"}, \quad \lambda \equiv (\lambda_1, \lambda_2), \tag{2.1}$$

$$\text{(a)}\ f(w_0, \lambda) = 0 \qquad \text{(b)}\ f(w_1, \lambda) = 0, \tag{2.2}$$

$$\text{(a)}\ f_u(w_0, \lambda)v_0 = \mu_0 v_0, \qquad \text{(b)}\ f_u(w_1, \lambda)v_1 = \mu_1 v_1, \quad f_u \equiv D_1 f, \tag{2.3}$$

$$\text{(a)}\ \langle v_0, v_0 \rangle = 1, \qquad \text{(b)}\ \langle v_1, v_1 \rangle = 1, \tag{2.4}$$

$$\int_0^1 \langle f(u, \lambda) - f(\hat{u}, \hat{\lambda}), f_u(u, \lambda) f(u, \lambda) \rangle \, dt = 0, \tag{2.5}$$

$$\text{(a)}\ u(0) = w_0 + \epsilon_0 v_0, \qquad \text{(b)}\ u(1) = w_1 + \epsilon_1 v_1. \tag{2.6}$$

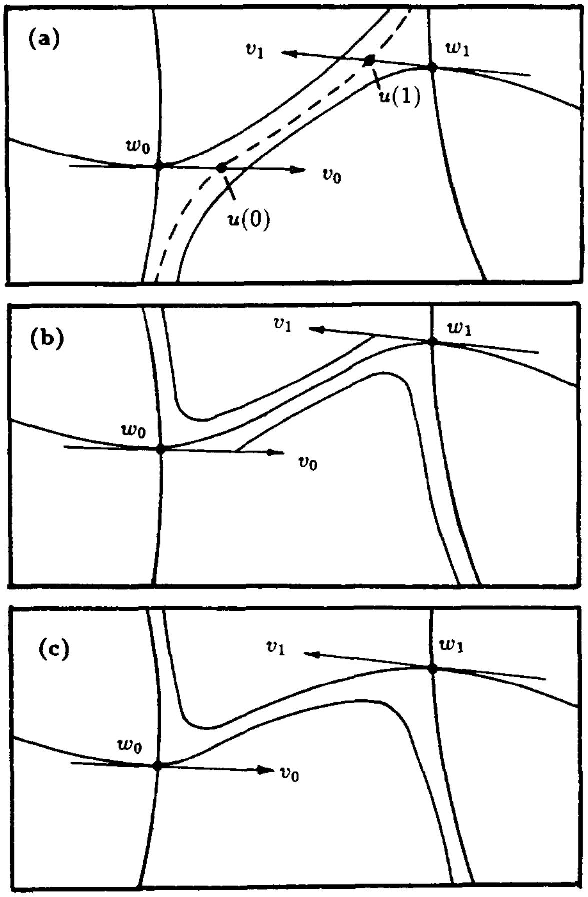

Fig. 1. Geometric interpretation of equations (2.1)–(2.5). Consider λ_2 as fixed here. For $\lambda_1 = \lambda_1^*$ we assume the existence of the heteroclinic connection in (b). Generically, perturbation of λ_1 will produce either (a) or (c), depending on the sign of the perturbation. If ϵ_0 and ϵ_1 are sufficiently small, then there exists a λ_1 close to λ_1^* for which the equations (2.1)–(2.4) (and (2.6)) can be satisfied (Here in case (a)). Furthermore, the radii ϵ_0 and ϵ_1 can be chosen such that the period of the orbit equals a given large value T, and such that the phase condition (2.5) is satisfied.

Above $\langle \cdot, \cdot \rangle$ is the ℓ^2 inner product in $\mathbb{R}^2$, the corresponding norm will be denoted by $\|\cdot\|$. Equation (2.1) is the differential equation, with $u(\cdot)$, $f(\cdot, \cdot) \in \mathbb{R}^2$. Note that the time variable t has been scaled so that it varies from 0 to 1. The actual period T therefore appears explicitly in (2.1). There are two problem parameters, viz., λ_1 and λ_2, and we want to compute entire *branches* (one-parameter continua) of approximate heteroclinic orbits. Equation (2.2) defines two fixed points, w_0 and w_1, of the vector field. These are assumed to be saddle points. Thus the Jacobian matrix $f_u(w_0, \lambda)$ has one positive and one negative eigenvalue and the same holds for $f_u(w_1, \lambda)$. For definiteness let the eigenvalue μ_0 of $f_u(w_1, \lambda)$ as defined by (2.3a) be negative and let the eigenvalue μ_1 of $f_u(w_0, \lambda)$ defined in (2.3b) be positive. The corresponding eigenvectors are called v_0 and v_1, respectively. We have v_0, v_1, w_0, $w_1 \in \mathbb{R}^2$. Equation (2.6a) then requires that the starting point $u(0)$ of the orbit $u(t)$ lie on the line $\ell(\epsilon) \equiv w_0 + \epsilon v_0$ and at distance ϵ_0 from the fixed point w_0 (see Fig. 1). Note that $\ell(\epsilon)$ passes through w_0 and that it has the direction of the eigenvector v_0. Equation (2.6b) imposes the corresponding requirement on the endpoint $u(1)$ at w_1. Thus the equations (2.6) require the points $u(1)$ and $u(0)$ to lie on the linear approximation of the stable and unstable manifold at w_1 and w_0, respectively. Finally (2.5) represents a phase condition. Its significance will be discussed below.

The unknowns w_0 and w_1 can be eliminated entirely from (2.1)–(2.5) by using (2.6). Then (2.1)–(2.5) consist of two coupled differential equations with eleven side conditions, of which (2.5) is an integral constraint. Since we are interested in an entire branch of orbits, a formal count shows that we should have ten scalar variables in addition to the vector function variable $u(t) \in \mathbb{R}^2$. These scalar variables are

$$\lambda_1,\ \lambda_2,\ \epsilon_0,\ \epsilon_1,\ \mu_0,\ \mu_1 \in \mathbb{R}, \qquad v_0,\ v_1 \in \mathbb{R}^2. \tag{2.7}$$

The period T is kept fixed in this continuation. For T large and ϵ_0 and ϵ_1 small, each solution on the branch represents an approximate heteroclinic connection. Example 2 illustrates such a computation. If we want to increase the period T, then we can replace one of the problem parameters, say λ_2, by T and thus use the scalar variables

$$\lambda_1,\ T,\ \epsilon_0,\ \epsilon_1,\ \mu_0,\ \mu_1 \in \mathbb{R}, \qquad v_0,\ v_1 \in \mathbb{R}^2. \tag{2.8}$$

Such a calculation is illustrated in Example 1.

A heteroclinic connection $u(t)$, $-\infty < t < \infty$, of two saddle points of $f(u(t), \lambda)$ is not uniquely defined because for any real σ, $u(t+\sigma)$ is also a connection. This is very similar to the phase shift invariance of periodic solutions. The indeterminacy persists in the truncated problem: if $u(t)$ is a heteroclinic connection then both $u(t)$ on $[0, T]$ and $u(t)$ on $[\sigma, T+\sigma]$ are truncated solutions of integration length T. We remove the indeterminacy by adding an appropriate constraint which we shall call a *phase condition* in analogy with the periodic case.

One simple way to fix the phase is to set one of the components of $u(t)$ at $t = \frac{1}{2}$ equal to some appropriate value in the time-scaled equations (2.1). However, it is easy to give examples where this phase condition fails to work. It also leads to multi-point boundary conditions although this is a much less serious disadvantage.

A better phase condition is obtained by requiring that the current heteroclinic orbit "look like" the previously computed orbit as much as possible. To be more precise, let $\hat{u}(t)$ denote the previous orbit on a branch of heteroclinic orbits. Let $\tilde{u}(t+\sigma)$ be the continuum from which the current orbit is to be selected. Since $\| u'(t) \| \to 0$ exponentially as $|t| \to \infty$, a good measure of how close $\tilde{u}$ and $\hat{u}$ are is the integral

$$D(\sigma) \equiv \int_{-\infty}^{\infty} \| \tilde{u}'(t+\sigma) - \hat{u}'(t) \|^2 \, \mathrm{d}t.$$

The necessary condition for a minimum is $\mathrm{d}D(\sigma_*)/\mathrm{d}\sigma = 0$. With $u(t) \equiv \tilde{u}(t+\sigma_*)$ this necessary condition can be written as

$$\int_{-\infty}^{\infty} \langle u'(t) - \hat{u}'(t),\ u''(t) \rangle \, \mathrm{d}t = 0. \tag{2.9}$$

We truncate this integral to the finite interval $[0, T]$ and then scale the independent variable t as before. Using $u'(t) = f(u, \lambda)$ and $u''(t) = f_u(u, \lambda) u'(t) = f_u(u, \lambda) f(u, \lambda)$ we then obtain the phase condition (2.5) of the algorithm.

Remark. Integrating by parts in (2.9) one obtains

$$\int_{-\infty}^{\infty} \langle u'(t) - \hat{u}'(t),\ \hat{u}''(t) \rangle \, \mathrm{d}t = 0. \tag{2.10}$$

Computationally, (2.9) and (2.10) (in a truncated form) lead to the same results. However, (2.10) is more convenient for the error analysis.

As in [7], the effect of the integral phase condition (2.5) is that it minimizes translation of wave fronts along a solution branch. This facilitates the adaptive mesh selection. In practice it allows much greater steps to be taken along a branch of orbits.

3. Examples

Example 1. *Computing orbits of high period.* As a simple first example we consider

$$\begin{aligned} u_1'(t) &= 1 - u_1(t)^2, \\ u_2'(t) &= u_2(t) + \lambda_1 u_1(t), \quad -\infty < t < \infty. \end{aligned} \tag{3.1}$$

We only have one problem parameter here, viz. λ_1. Indeed, in this example the objective is not to compute a two-parameter branch of heteroclinic orbits, but rather to show how large a period T we can compute, and to illustrate the effect of the phase condition (2.5). With $\lambda_1 = 0$, equation (3.1) has the following exact solution for a heteroclinic orbit connecting the saddle points $(u, v) = (-1, 0)$ and $(u, v) = (1, 0)$:

$$u_1(t) = \left(\tfrac{1}{3}e^{2t} - 1\right)/\left(\tfrac{1}{3}e^{2t} + 1\right), \qquad u_2(t) = 0, \quad -\infty < t < \infty. \tag{3.2}$$

With scaled time variable t, equation (3.1) on a finite interval $[0, T]$ becomes

$$\begin{aligned} u_1'(t) &= T\left(1 - u_1(t)^2\right), \\ u_2'(t) &= T\left(u_2(t) + \lambda_1 u_1(t)\right), \quad 0 \leqslant t \leqslant 1. \end{aligned} \tag{3.3}$$

As starting orbit for (3.3) one can use

$$u_1(t) = \frac{\tfrac{1}{3}e^{2\log(3)t} - 1}{\tfrac{1}{3}e^{2\log(3)t} + 1}, \qquad u_2(t) = 0, \quad 0 \leqslant t \leqslant 1, \quad T = \log(3),$$

so that $u(0) = -\frac{1}{2}$ and $u(1) = \frac{1}{2}$. Continuation with AUTO, using the scalar variables (2.8), gives a branch of orbits of increasing period T. Some computed orbits are shown in Fig. 2. Note that the phase condition has the effect of keeping the increasingly sharper front in the same location. This facilitates the automatic mesh adaption and allows bigger steps to be taken along the solution branch. The mesh adaption also enables the computation of very large period. In Fig. 2 the orbit with label 7 has the largest period ($T = 10\,000$). Since the time variable t has been scaled to the unit interval, this orbit looks like a step function.

Example 2. *The Huxley equation.* We apply the algorithm of Section 2 to the problem of finding traveling wave fronts in the Huxley equation. This is the problem for which we give an error analysis in the next section. The equation is given by

$$\left.\begin{aligned} w_t &= w_{zz} + f(a, w), \quad -\infty < z < \infty,\ t > 0, \\ f(a, w) &\equiv w(1 - w)(w - a), \quad 0 < a < 1. \end{aligned}\right\} \tag{3.4}$$

We look for solutions to (3.4) of the form $w(z, t) = u(z + bt)$, where b is the wave speed. This gives the first order system

$$\left.\begin{aligned} u_1'(x) &= u_2(x), \\ u_2'(x) &= bu_2(x) - f(a, u_1(x)), \end{aligned}\right\} \tag{3.5}$$

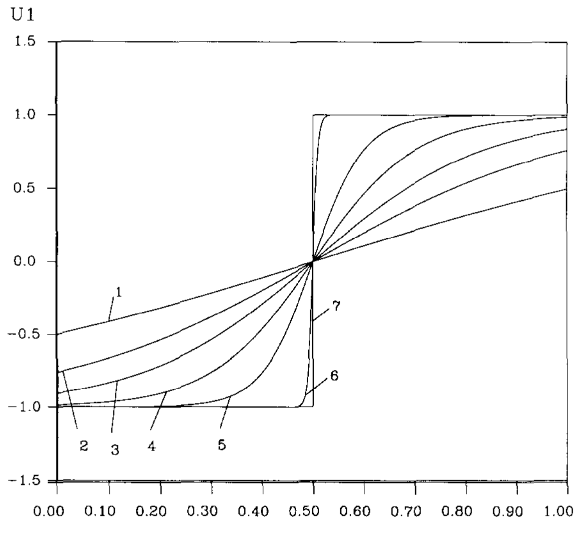

Fig. 2. Some orbits along the computed branch of solutions to (2.1)–(2.6) for problem (3.1). The scalar variables are given by (2.8). The periods of the orbits shown are (1) $T = \log(3)$ (the starting orbit), (2) $T = 2$, (3) $T = 3$, (4) $T = 5$, (5) $T = 10$, (6) $T = 100$, (7) $T = 10000$. The calculation was done using AUTO [7] with 25 mesh intervals, 4 orthogonal collocation points per mesh interval, and adaptive mesh selection.

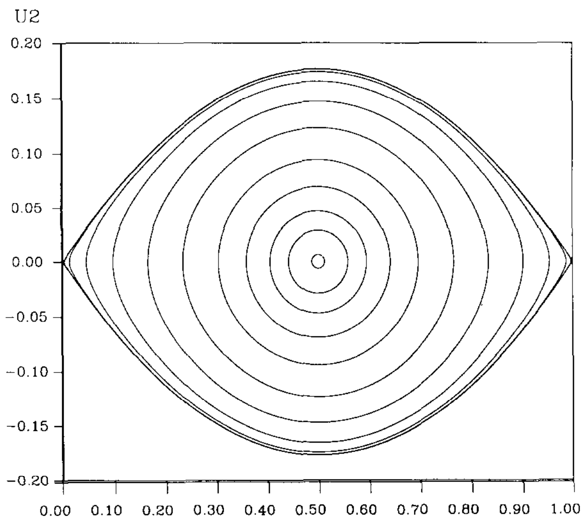

Fig. 3. Phase plane representation of (3.5) when $a = 0.5$ and $b = 0$. For this choice of parameters the solutions form a family of periodic orbits. In the limit, as the period T goes to ∞, the orbits approach a heteroclinic cycle with rest points (0, 0) and (1, 0). Each of the two (approximate) heteroclinic orbits can be continued in the scalar variables (2.7) with $\lambda_1 = a$ and $\lambda_2 = b$. The result of this continuation is shown in Fig. 4.

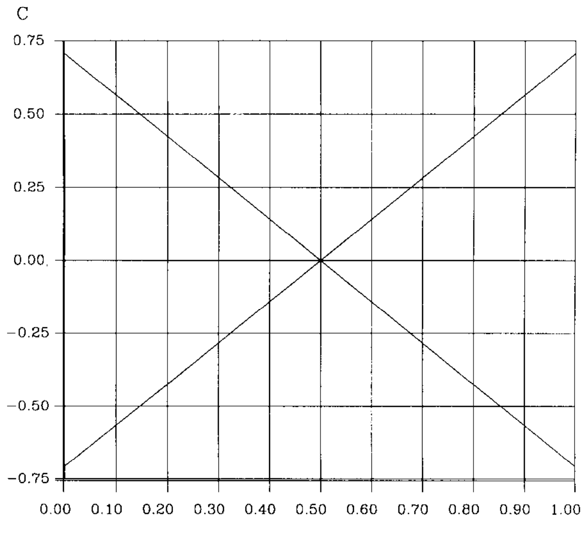

Fig. 4. The two branches of traveling wave front solutions to (3.4). Along each branch the orbits actually remain unchanged. The exact representation of the two branches is $b = \pm\sqrt{2}\,(a - \frac{1}{2})$. The calculation was done using AUTO with 50 mesh intervals, 4 orthogonal collocation points per mesh interval, and adaptive mesh selection. The (fixed) period used in this calculation was $T = 1000$.

where $x = z + bt$, and $' = \mathrm{d}/\mathrm{d}x$. If $a = 0.5$ and $b = 0$ then (3.5) has a family of periodic orbits of increasing period. Its phase portrait is shown in Fig. 3. One of the solutions is a double heteroclinic connection (in fact a heteroclinic cycle). The first of the two heteroclinic orbits has the exact representation

$$u_1(x) = \frac{\exp(\frac{1}{2}\sqrt{2}\,x)}{1 + \exp(\frac{1}{2}\sqrt{2}\,x)}, \qquad u_2(x) = u_1'(x), \quad -\infty < x < \infty. \tag{3.6}$$

The second heteroclinic connection is obtained by reflecting the phase plane representation of the first with respect to the horizontal axis $u_2 = 0$ (see Fig. 3). The two exact solutions can be used as starting points in the continuation algorithm defined by (2.1)–(2.6). The scalars are now given by (2.7). The resulting two branches are shown in Fig. 4. It happens that the orbits actually remain unchanged along the two branches. Furthermore, the branches have the analytical representation $b = \pm\sqrt{2}\,(a - \frac{1}{2})$.

4. Error analysis for the Huxley equation

In Section 2 we have formulated our algorithm for computation of branches of heteroclinic orbits in $\mathbb{R}^2$. In this section we derive error estimates. Our approach is to formulate first the problem as an operator equation in a weighted Banach space and then to apply the general theory of approximation of nonlinear problems. We use weighted Banach spaces because the linearized operator in our problem has, in general, nice spectral properties on these spaces (see

[20] and the discussion there). Our approach will be shown on a model problem, approximation of wave fronts for the Huxley equation (3.4).

In the preceding section we computed solutions to (3.4) of the form

$$w(z, t) = \tilde{u}(z + bt), \tag{4.1}$$

where b is the *wave speed*. It is well known (see e.g. [20]) that for given a there exists $\tilde{u}(x)$ which satisfies for some $b > 0$

$$\left.\begin{aligned} &\tilde{u}'' - b\tilde{u}' + f(a, \tilde{u}) = 0, \quad -\infty < x < \infty, \\ &\tilde{u}(-\infty) = 0, \qquad \tilde{u}(\infty) = 1, \end{aligned}\right\} \tag{4.2}$$

where $x = z + bt$ and $' = \mathrm{d}/\mathrm{d}x$. Let $\chi \in C^\infty(\mathbb{R})$ be such that for some $T_+ > 0$, $T_- < 0$

$$\chi(x) = \begin{cases} 1 & \text{for } x > T_+, \\ 0 & \text{for } x < T_-. \end{cases}$$

Then $u(x) = \tilde{u}(x) - \chi(x)$ satisfies

$$\left.\begin{aligned} &-u'' + bu' - f(a, u + \chi) - \chi'' + b\chi' = 0, \\ &u(-\infty) = u(\infty) = 0. \end{aligned}\right\} \tag{4.3}$$

We want to solve equation (4.3) in weighted Sobolev spaces. To determine the right weight function, we need to know the asymptotic behavior of the solutions. Let (a_0, b_0, u_0) be a solution of (4.3). We first rewrite (4.3) as a first order system, setting $u_1 \equiv u_0$,

$$\left.\begin{aligned} &u_1' = u_2, \\ &u_2' = b_0 u_2 - f(a_0, u_1 + \chi) - \chi'' + b_0\chi'. \end{aligned}\right\} \tag{4.4}$$

The linearization of (4.4) about a solution (a_0, b_0, u_0) is

$$\begin{pmatrix} v_1' \\ v_2' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -f_{u_1}(a_0, u_1(x) + \chi(x)) & b_0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}. \tag{4.5}$$

For $x \to -\infty$ the matrix in (4.5) becomes

$$\begin{pmatrix} 0 & 1 \\ a_0 & b_0 \end{pmatrix}.$$

Its eigenvalues are given by the roots of $\mu^2 - b_0\mu - a_0$. Since $\lim_{x \to -\infty} u(x) = 0$, we choose the positive eigenvalue $\mu_1 = \frac{1}{2}(b_0 + \sqrt{b_0^2 + 4a_0})$. Corresponding to this root we have a solution of the form

$$v_1 = \mathrm{e}^{\mu_1 x}, \qquad v_2 = \mu_1\, \mathrm{e}^{\mu_1 x}. \tag{4.6}$$

Similarly, for $x \to \infty$ the matrix in (4.5) becomes

$$\begin{pmatrix} 0 & 1 \\ -(-1 + a_0) & b_0 \end{pmatrix}.$$

Then equation (4.5) has a solution of the form

$$v_1 = \mathrm{e}^{\mu_1 x}, \quad v_2 = \mu_1 \mathrm{e}^{\mu_0 x}, \quad \text{where } \mu_0 = \tfrac{1}{2}\left(b_0 - \sqrt{b_0^2 + 4 - 4a_0}\right) < 0. \tag{4.7}$$

For some $\mu_0 < 0$, $\mu_1 > 0$ we next set $\mu = (\mu_0, \mu_1)^{\mathrm{T}}$,

$$w_\mu(x) = \begin{cases} \mathrm{e}^{-2\mu_1 x}, & x < 0, \\ \mathrm{e}^{-2\mu_0 x}, & x \geq 0. \end{cases} \tag{4.8}$$

Analogously to Babuška [2] we now let $H^{\ell,\mu} = H^{\ell,\mu}(\mathbb{R})$, $\ell \geqslant 0$, integer, be the Banach space of all functions u such that

$$\| u \|^2_{H^{\ell,\mu}} = \int_{-\infty}^{\infty} w_\mu(x) \sum_{k=0}^{\ell} | u^{(k)} |^2 \, dx < \infty.$$

We denote by $H^{-\ell,-\mu}$ the dual space to $H^{\ell,\mu}$, with the norm

$$\| v \|_{H^{-\ell,-\mu}} = \sup_{\| u \|_{H^{\ell,\mu}} = 1} |(u, v)|.$$

By $\langle u, v \rangle$ we shall mean the duality pairing on $H^{\ell,\mu} \times H^{-\ell,-\mu}$.

Remark 1. In the solution of equation (4.3) we employ a continuation procedure with a and b as parameters. Suppose we know the range I_a of a and the range I_b of b. Then we shall need $u \in H^{1,\mu}$ for all $a \in I_a$, all $b \in I_b$. To achieve this we can choose $\mu = (\mu_0, \mu_1)^{\mathrm{T}}$, $\mu_0 < 0$, $\mu_1 > 0$ from

$$\mu_1 = \inf_{\substack{a \in I_a \\ b \in I_b}} \frac{b + \sqrt{b^2 + 4a}}{2} - \epsilon, \qquad \mu_0 = \sup_{\substack{a \in I_a \\ b \in I_b}} \frac{b - \sqrt{b^2 + 4 - 4a}}{2} + \epsilon, \tag{4.9}$$

for some $\epsilon > 0$, small.

We next want to reformulate equation (4.3) as an operator equation in $H^{1,\mu}$. We first define the linearization

$$A(x)u = -u'' + b_0 u' - f_u(a_0, \operatorname{sign} x)u, \tag{4.10}$$

where

$$\operatorname{sign} x = \begin{cases} 1, & x > 0, \\ 0, & x \leqslant 0, \end{cases}$$

about a solution (a_0, b_0, u_0) of (4.3). We can now rewrite (4.3) as

$$\left.\begin{aligned} &Au + \sigma u + G(a, b, u) = 0, \quad \sigma \in \mathbb{R}, \\ &u(-\infty) = u(\infty) = 0, \end{aligned}\right\} \tag{4.11}$$

where G: $\mathbb{R} \times \mathbb{R} \times H^{1,\mu} \to H^{0,\mu}$ is defined by

$$G(x, a, b, u) = -f(a, u + \chi) - \chi'' + \chi' + (b - b_0)u' + f_u(a_0, \operatorname{sign} x)u - \sigma u. \tag{4.12}$$

Define on $H^{1,\mu} \times H^{-1,\mu}$ a bilinear form

$$B(u, v) = (Au + \sigma u, v) = \int_{-\infty}^{\infty} [u'v' + b_0 u'v - f_u(a_0, \operatorname{sign} x)uv + \sigma uv] \, dx. \tag{4.13}$$

Problem (4.3) (or (4.11)) admits the variational formulation: given a, $0 < a < 1$, find $(b, u) \in \mathbb{R} \times H^{1,\mu}$ from

$$B(u, v) + (G(a, b, u), v) = 0, \quad \forall v \in H^{1,-\mu}. \tag{4.14}$$

By a slight modification of the proof of Theorem 3.1 in [2], using the inequality

$$\int uv' \,\mathrm{d}x \leqslant \tfrac{1}{2}\epsilon \int u^2 \,\mathrm{d}x + \tfrac{1}{2}\epsilon \int (v')^2 \,\mathrm{d}x,$$

we have the following lemma.

Lemma 1. *For sufficiently large* $\sigma > 0$

$$| B(u, v) | \leqslant c \| u \|_{H^{1,\mu}} \| v \|_{H^{1,-\mu'}} \tag{4.15}$$

$$\sup_{\| u \|_{H^{1,\mu}} \leqslant 1} | B(u, v) | \geqslant c \| v \|_{H^{1,-\mu}}, \tag{4.16a}$$

$$\sup_{\| v \|_{H^{1,-\mu}} \leqslant 1} | B(u, v) | \geqslant c \| u \|_{H^{1,\mu}}. \tag{4.16b}$$

Lemma 2. *Let* $f \in H^{-1,\mu}$. *Then there exists a unique solution of the problem*

$$B(u, v) = \langle f, v \rangle, \quad \forall v \in H^{1,-\mu},$$

and

$$\| u \|_{H^{1,\mu}} \leqslant c \| f \|_{H^{-1,\mu}}.$$

Proof. The functional $S_f(v) = \langle f, v \rangle$, $v \in H^{1,-\mu}$ *is bounded on* $H^{1,-\mu}$:

$$\| S_f \|_{H^{1,-\mu}} \leqslant c \| f \|_{H^{-1,\mu}}.$$

Taking into account Lemma 1 and applying the Lax–Milgram Lemma [2, Theorem 4.1] proves the lemma. □

By Lemma 2 we can now define the continuous linear operator T: $H^{-1,\mu} \to H^{1,\mu}$ by

$$B(Tf, v) = \langle f, v \rangle, \quad \forall v \in H^{1,-\mu}, \quad \forall f \in H^{-1,\mu}. \tag{4.17}$$

Then an equivalent form of the problem (4.14) is: given $a, 0 < a < 1$, find $(b, u) \in \mathbb{R} \times H^{1,\mu}$ from

$$F(a, b, u) \equiv u + TG(a, b, u) = 0. \tag{4.18}$$

Let $(a_0, b_0, u_0) \in \mathbb{R} \times \mathbb{R} \times H^{1,\mu}$ be a solution of (4.18) i.e.,

$$F(a_0, b_0, u_0) = 0 \tag{4.19}$$

and define the linearized operator $H^{1,\mu} \to H^{1,\mu}$

$$\begin{aligned} \mathrm{D}_u F(a_0, b_0, u_0) &\equiv I + TG_u(a_0, b_0, u_0) \\ &= I - T\left[\sigma + f_u(a_0, u_0 + \chi) - f_u(a_0, \operatorname{sign} x)\right] \\ &\equiv I - T(\sigma + \tilde{\sigma}(\cdot)), \end{aligned} \tag{4.20}$$

where

$$\tilde{\sigma}(x) = f_u(a_0, u_0 + \chi) - f_u(a_0, \operatorname{sign} x)$$

Denote $\mathbb{R} u = \{ cu\colon\ c \in \mathbb{R} \}$.

Theorem 1. (i) $\mathrm{D}_u F(a_0, b_0, u_0) = I - T(\sigma + \tilde{\sigma}) : H^{1,\mu} \to H^{1,\mu}$ *is singular and*

$$H_1 \equiv \operatorname{Ker} \mathrm{D}_u F(a_0, b_0, u_0) = \mathbb{R} \tilde{\phi}_0,$$

$$\tilde{\phi}_0 = c(\chi' + u_0'), \qquad \| \tilde{\phi}_0 \|_{H^{1,\mu}} = 1. \tag{4.21}$$

There exists $\tilde{\phi}_0^* \in H^{-1,-\mu}$ *such that*

$$(\mathrm{D}_u F(a_0, b_0, u_0))^* \tilde{\phi}_0^* = 0, \qquad \langle \tilde{\phi}_0, \tilde{\phi}_0^* \rangle = 1. \tag{4.22}$$

(ii)
$$H_2 \equiv \mathrm{Range}(\mathrm{D}_u F(a_0, b_0, u_0)) = \{ u \in H^{1,\mu} : \langle u, \tilde{\phi}_0^* \rangle = 0 \}, \tag{4.23a}$$

$$H^{1,\mu} = H_1 + H_2. \tag{4.23b}$$

Moreover $\mathrm{D}_u F(a_0, b_0, u_0)$ *is an isomorphism of* H_2, *and consequently there exists a positive constant* c *such that*

$$\| D_u F(a_0, b_0, u_0) u \|_{H^{1,\mu}} \geqslant c \| u \|_{H^{1,\mu}}, \quad \forall u \in H_2. \tag{4.24}$$

(iii)
$$\mathrm{D}_b F(a_0, b_0, u_0) \in H_2, \tag{4.25a}$$

and consequently for $x = (b, u)$

$$\mathrm{Range}\ \mathrm{D}_x F(a_0, b_0, u_0) = H^{1,\mu}, \tag{4.25b}$$

and

$$\mathrm{Ker}\ \mathrm{D}_x F(a_0, b_0, u_0) = \mathbb{R}\phi_0, \quad \phi_0 = (0, \tilde{\phi}_0). \tag{4.26}$$

Proof. (i) It is proved in Sattinger [20] (see also Henry [11]) that $\tilde{\phi}_0$ defined by (4.21) is smooth and $\mathrm{Ker}(A - \tilde{\sigma}) = \mathbb{R}\tilde{\phi}_0$. Since $(A - \tilde{\sigma})\tilde{\phi}_0 = 0$ is equivalent to $(A + \sigma - \tilde{\sigma})\tilde{\phi}_0 = \sigma\tilde{\phi}_0$ which in turn is equivalent to $\tilde{\phi}_0 - T(\sigma + \tilde{\sigma})\tilde{\phi}_0 = 0$ by (4.17) and (4.13), then (4.21) follows from (4.20). To verify (4.22) we first define the continuous linear operator T^0: $H^{-1,-\mu} \to H^{1,-\mu}$ by

$$B(u, T^0 v) = \langle u, v \rangle, \quad \forall u \in H^{1,\mu}, \quad \forall v \in H^{-1,-\mu}. \tag{4.27}$$

Hence for $u \in H^{1,\mu}$, $v \in C_0^\infty(\mathbb{R})$ we have

$$\langle Tu, v \rangle = \langle Tu, (A + \sigma I)^* T^0 v \rangle = \langle (A + \sigma I) Tu, T^0 v \rangle = \langle u, T^0 v \rangle.$$

Thus by the density of $C_0^\infty(\mathbb{R})$ in $H^{-1,-\mu}$, $T^0 = T^*$. This implies

$$(\mathrm{D}_u F(a_0, b_0, u_0))^* = (I - T(\sigma + \tilde{\sigma}))^* = I - (\sigma + \tilde{\sigma}) T^*.$$

By Sattinger [20], $\mathrm{Ker}(A - \tilde{\sigma})^* = \mathbb{R}\tilde{\psi}_0^*$ for some $\tilde{\psi}_0^*$, in fact, $\tilde{\psi}_0^* = \mathrm{e}^{-b_0 x}\tilde{\phi}_0(x)$. Finally, taking into account that $(A - \tilde{\sigma})^* \tilde{\psi}^* = 0$ is equivalent to $\tilde{\psi}_0^* - T^*(\sigma + \tilde{\sigma})\tilde{\psi}_0^* = 0$, we arrive at (4.22) with

$$\tilde{\phi}_0^* = (T^*)^{-1} \tilde{\psi}_0^*. \tag{4.28}$$

(ii) follows from (i).

(iii) For $x = (b, u)$ we have by the definitions (4.18) and (4.12) of F and G, respectively, and (i)

$$\begin{aligned} \mathrm{D}_x F(a_0, b_0, u_0)\delta x &\equiv \mathrm{D}_b F(a_0, b_0, u_0)\delta b + \mathrm{D}_u F(a_0, b_0, u_0)\delta u \\ &= \delta b T(\chi' + u_0') + (I - T(\sigma + \tilde{\sigma}))\delta u \\ &= \frac{\delta b}{c} T\tilde{\phi}_0 + (I - T(\sigma + \tilde{\sigma}))\delta u. \end{aligned} \tag{4.29}$$

By (4.23) the condition (4.25a) is equivalent to

$$\langle \mathrm{D}_b F(a_0, b_0, u_0), \tilde{\phi}_0^* \rangle \neq 0,$$

or, using (4.28) and (4.29),

$$0 \neq \langle T\tilde{\phi}_0, \tilde{\phi}_0^* \rangle = \langle \tilde{\phi}_0, \tilde{\psi}_0^* \rangle = \int_{-\infty}^{\infty} \mathrm{e}^{-b_0 t} (\phi_0(t))^2 \, \mathrm{d}t$$

which, obviously, holds. Next, (4.25b) follows from the decomposition (4.23), and (4.26) follows from (4.29). □

Define the mapping Φ: $\mathbb{R} \times \mathbb{R} \times H^{1,\mu} \to \mathbb{R} \times H^{1,\mu}$ by

$$\Phi(a, x) = (\ell(x - x_0), F(a, x)), \quad x = (b, u), \quad x_0 = (b_0, u_0), \tag{4.30a}$$

where for $\tilde{\phi}_0$ defined by (4.21)

$$\ell(x) = \int_{-\infty}^{\infty} \left[u(t)\tilde{\phi}_0(t) + u'(t)\tilde{\phi}_0'(t)\right] \mathrm{d}t, \quad x = (b, u). \tag{4.31}$$

For any $\xi \in \mathbb{R} \times H^{1,\mu}$ we have

$$\mathrm{D}_x\Phi(a_0, x_0)\xi = (\ell(\xi), \mathrm{D}_x F(a_0, x_0)\xi). \tag{4.30b}$$

From (4.25b) and (4.26) by the Banach Theorem we deduce the following corollary.

Corollary 1. $\mathrm{D}_x\Phi(a_0, x_0)$ *is an isomorphism in* $\mathbb{R} \times H^{1,\mu}$.

Remark. In the derivation of error estimates we use the phase condition in the form

$$\ell(x - x_0) \equiv \int_{-\infty}^{\infty} [(\tilde{u} - \tilde{u}_0)\tilde{u}_0' + (\tilde{u}' - \tilde{u}_0')\tilde{u}_0''] \mathrm{d}t = 0, \tag{4.31'}$$

which differs from the condition (2.9) (or (2.10)) used in actual computations. In the notation of this section (2.10) takes the form

$$\int_{-\infty}^{\infty} [(\tilde{u}' - \tilde{u}_0')\tilde{u}_0'' + (\tilde{u}'' - \tilde{u}_0'')\tilde{u}_0'''] \mathrm{d}t = 0.$$

Computations indicate that this condition leads to more accurate results than (4.31′). One can justify the use of (2.10) instead of (4.31′) by assuming additional regularity of the solution.

Our numerical method (2.1)–(2.6) essentially consists in replacing for large $|t|$ the differential operator (4.2) or (4.11) by a limiting linearized differential operator with constant coefficients. We set

$$G_T(t, a, b, u) = \begin{cases} [-f_u(a, 1) - \sigma + f_u(a_0, 1)]u + (b - b_0)u', & t > T_+ \\ G(t, a, b, u), & T_- \leqslant t \leqslant T_+, \\ [-f_u(a, 0) - \sigma + f_u(a_0, 0)]u + (b - b_0)u', & t < T_-, \end{cases} \tag{4.32}$$

where G is defined by (4.12). Then (4.2) or (4.11) is approximated by

$$\left.\begin{aligned} &Au + \sigma u + G_T(a, b, u) = 0, \\ &u(-\infty) = u(\infty) = 0, \end{aligned}\right\} \tag{4.33}$$

and (4.18) is approximated by

$$F_T(a, b, u) \equiv u + TG_T(a, b, u) = 0. \tag{4.34}$$

We also define an approximation Φ_T: $\mathbb{R} \times \mathbb{R} \times H^{1,\mu} \to \mathbb{R} \times H^{1,\mu}$ to Φ by

$$\Phi_T(a, x) = (\ell_T(x - x_0), F_T(a, x)), \quad x = (b, u), \quad x_0 = (b_0, u_0), \tag{4.35}$$

where

$$\ell_T(x) = \int_{T_-}^{T_+} \left[u(t)\tilde{\phi}_0(t) + u'(t)\tilde{\phi}_0'(t)\right] \mathrm{d}t, \quad x = (b, u). \tag{4.36}$$

To establish existence, uniqueness and error estimates for the approximate problem, we shall use a simplified version of the implicit function theorem in Descloux and Rappaz [5] and in Keller [14].

Theorem 2. *Let E_1 and E_2 be two real Banach spaces and let $I \subset \mathbb{R}$ and $D \subset E_1$ be open subsets of $\mathbb{R}$ and E_1, respectively. Let Φ, $\Phi_n : I \times D \to E_2$ be a C^1 mapping and a family of mappings, respectively, that satisfy*

(i) $\Phi(a_0, x_0) = 0$, $(a_0, x_0) \in I \times D$;

(ii) $D_x\Phi(a_0, x_0)$ *is an isomorphism of* E_1 *onto* E_2;

(iii) *For an open subset* $\Lambda \subset I$

$$\lim_{n \to \infty} \sup_{a \in \Lambda} \| D_x\Phi(a, x_0) - D_x\Phi_n(a, x_0) \| = 0;$$

(iv) $$\lim_{n \to \infty} \sup_{a \in \Lambda} \| \Phi(a, x) - \Phi_n(a, x) \| = 0, \quad \forall x \in D.$$

Then the problem

$$\Phi(a, x) = 0$$

has a unique C^1 solution branch $\{(x(a), a) : a \in \Lambda\}$ that contains (a_0, x_0), moreover, there exists n so that for all $n \geqslant N$ the problem

$$\Phi_n(a, x_n) = 0$$

has a unique C^1 solution branch $\{(x_n(a), a) : a \in \Lambda\}$ and

$$\| x(a) - x_n(a) \| \leqslant C \| \Phi_n(x(a), a) \|,$$

where C is a positive constant independent of n.

Theorem 2 requires a consistency condition (a pointwise convergence) and a stability condition. These conditions are given by the following lemma.

Lemma 3. *Let $x = (b, u) \in I_b \times H^{1,\mu}$, $a \in I_a$ for some finite intervals I_a, $I_b \subset \mathbb{R}$, see* (4.9). *Then we have*

$$\| \Phi(a, x) - \Phi_T(a, x) \|_{H^{1,\mu}} \leqslant c\epsilon(u, T_-, T_+)(e^{T_-\mu_0} + e^{T_+\mu_1}), \tag{4.37}$$

where $\mu_0 < 0$ and $\mu_1 > 0$ are as in (4.9), *c does not depend on a, b, T_-, T_+, and $\epsilon(u, T_-, T_+) \to 0$ as $T_+ \to \infty$, $T_- \to -\infty$;*

$$\| D_x\Phi(a, x_0) - D_x\Phi_T(a, x_0) \|_{L(R \times H^{1,\mu})} \leqslant c(e^{T_-\mu_0} + e^{T_+\mu_1}) \tag{4.38}$$

uniformly in $a \in I_a$.

Proof. From the definitions (4.18) and (4.34) of F and F_T, respectively, we have

$$F(a, x) - F_T(a, x) = T(G(a, x) - G_T(a, x)).$$

Using that $T: H^{0,\mu} \to H^{1,\mu}$, defined by (4.17), is bounded and the definition (4.32) of G_T,

$$\| F(a, x) - F_T(a, x) \|_{H^{1,\mu}} \leqslant \| T \| \, \| G(a, x) - G_T(a, x) \|_{H^{0,\mu}((-\infty, T_-] \cup [T_+, \infty))} \tag{4.39}$$

By the definitions (4.12) and (4.32) of G and G_T

$$\begin{aligned}\| G(a, x) - G_T(a, x) \|_{H^{0,\mu}[T_+,\infty)} &= \| f(a, u+1) - f_u(a, 1)u \|_{H^{0,\mu}[T_+,\infty)} \\ &\leqslant \tfrac{1}{2}\sup | f_{uu}(a, v) | \, \| u^2 \|_{H^{0,\mu}[T_+,\infty)} \leqslant c \sup_{t \geqslant T_+} | u(t) | \, \| u \|_{H^{0,\mu}[T_+,\infty)}. \quad \square \end{aligned} \tag{4.40}$$

Remark. Here, with some abuse of notation, we have assumed that $| f_{uu} |$ is bounded uniformly in a, v. What we actually mean by this is the following. We show below, without using $| f_{uu} | \leqslant c$, that the solution of the exact problem is bounded. Hence, without changing the solution we can modify f for large $|v|$, $|a|$ so that $| f_{uu} | \leqslant c$ holds.

Using the definition (4.8) of w_μ, for $t \geqslant T_+$ we have

$$\begin{aligned}| u(t) | &= \left| \int_t^\infty u'(s) \, \mathrm{d}s \right| \leqslant \int_t^\infty \mathrm{e}^{\mu_1 s} \, \mathrm{e}^{-\mu_1 s} | u'(s) | \, \mathrm{d}s \\ &\leqslant \left[\int_t^\infty \mathrm{e}^{2\mu_1 s} \, \mathrm{d}s \int_t^\infty \mathrm{e}^{-2\mu_1 s} (u')^2 \, \mathrm{d}s \right]^{1/2} \leqslant c \, \mathrm{e}^{\mu_1 T_+} \| u \|_{H^{1,\mu}[T_+,\infty)}. \end{aligned}$$

Substituting the above into (4.40), gives

$$\| G(a, x) - G_T(a, x) \|_{H^{0,\mu}[T_+,\infty)} \leqslant c \, \mathrm{e}^{\mu_1 T_+} \| u \|^2_{H^{1,\mu}[T_+,\infty)} \tag{4.41a}$$

Similarly,

$$\| G(a, x) - G_T(a, x) \|_{H^{0,\mu}(-\infty,T_-]} \leqslant c \, \mathrm{e}^{\mu_0 T_-} \| u \|^2_{H^{1,\mu}(-\infty,T_-]}. \tag{4.41b}$$

By the definitions (4.31), (4.36) and (4.21) of ℓ, ℓ_T and $\tilde{\phi}_0$, respectively, for $\xi = (b, u) \in I_b \times H^{1,\mu}$,

$$| \ell(\xi) - \ell_T(\xi) | = \left| \int_{t \notin [T_-,T_+]} (u u_0' + u' u_0'') \, \mathrm{d}t \right|.$$

Combining this with the estimates of the type

$$\begin{aligned}\left| \int_{T_+}^\infty u u_0' \, \mathrm{d}t \right| &= \left| \int_{T_+}^\infty \mathrm{e}^{2\mu_1 t} \, \mathrm{e}^{-2\mu_1 t} u u_0' \, \mathrm{d}t \right| \\ &\leqslant \mathrm{e}^{2\mu_1 T_+} \left| \int_{T_+}^\infty \mathrm{e}^{-2\mu_1 t} u u_0' \, \mathrm{d}t \right| \leqslant \mathrm{e}^{2\mu_1 T_+} \| u \|_{H^{0,\mu}} \| u_0 \|_{H^{1,\mu'}} \end{aligned}$$

we arrive at

$$| \ell(\xi) - \ell_T(\xi) | \leqslant c(\mathrm{e}^{2\mu_0 T_-} + \mathrm{e}^{2\mu_1 T_+}). \tag{4.42}$$

Now (4.37) follows from (4.41), (4.42) and the definitions (4.30a) and (4.35) of Φ and Φ_T, respectively.

Similarly, (4.38) follows from (4.42) and the estimates for any $v \in H^{1,\mu}$ of the type:

$$\| (D_u F(a, x_0) - D_u F_T(a, x_0)) v \|_{H^{1,\mu}}$$
$$\leqslant \| T \| \, \| (D_u G(a, x) - D_u G_T(a, x)) v \|_{H^{0,\mu}((-\infty, T_-] \cup [T_+, \infty))},$$
$$\| (D_u G(a, x_0) - D_u G_T(a, x_0)) v \|_{H^{0,\mu}[T_+, \infty)}$$
$$= \| (f_u(a, u_0 + 1) - f_u(a, 1)) v \|_{H^{0,\mu}[T_+, \infty)}$$
$$\leqslant c \| u_0 v \|_{H^{0,\mu}[T_+ \infty)} \leqslant c \, e^{\mu_1 T_+} \| v \|_{H^{1,\mu'}}$$
$$\| D_b F(a, b, u) - D_b F_T(a, b, u) \|_{H^{1,\mu}}$$
$$= \| T \, D_b(G(a, b, u) - G_T(a, b, u)) \|_{H^{1,\mu}} = 0.$$

From Lemma 3 and Theorem 2 we have the next theorem.

Theorem 3. *Let* $x = (b, u) \in [0, \infty) \times H^{1,\mu}$ *and* $x_0 = (b_0, u_0)$, *where* $(a_0, x_0) \in (0, 1) \times [0, \infty) \times H^{1,\mu}$ *is a solution of* (4.3) *or* (4.11), *or* ((4.14), *or* (4.18)).

((i) *Then there exist positive constants* T_+^0, $-T_-^0$, $\bar{a}_0$, α, K *and two unique maps* $x(a)$, $x_T(a) \in \mathbb{R} \times H^{1,\mu}$, $|a - a_0| < \bar{a}_0$ *satisfying, respectively, the conditions*

$$\Phi(a, x(a)) = 0, \quad \| x(a) - x_0 \|_{\mathbb{R} \times H^{1,\mu}} < \alpha \quad \text{for } |a - a_0| < \bar{a}_0, \tag{4.43}$$

$$\Phi_T(a, x_T(a)) = 0, \quad \| x_T(a) - x_0 \|_{\mathbb{R} \times H^{1,\mu}} < \alpha,$$
$$\text{for } |a - a_0| < \bar{a}_0, \quad T_+ > T_+^0, \quad T_- < T_-^0. \tag{4.44}$$

(ii) *Moreover,* $x(a_0) = x_0$, *and for* $T_+ > T_+^0$, $T_- < T_-^0$, $|a - a_0| < \bar{a}_0$

$$|b(a) - b_T(a)| + \| u(a) - u_T(a) \|_{H^{1,\mu}}$$
$$\leqslant K \epsilon(u(a), T_+, T_-)(e^{T_- \mu_0} + e^{T_+ \mu_1}), \tag{4.45}$$

where $\epsilon(u(a), T_+, T_-) \to 0$ *as* $T_- \to -\infty$, $T_+ \to \infty$, *and* $\mu_0 > 0$ *and* $\mu_1 < 0$ *are as in* (4.9).

Remark. The results of Theorem 3 apply to a branch (calculated in Section 3) which has the analytical representation

$$b = \begin{cases} -\sqrt{2}(a - 1/2), & 0 < a \leqslant \frac{1}{2}, \\ \sqrt{2}(a - 1/2), & \frac{1}{2} < a < 1. \end{cases}$$

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