Analysis of Newton's Method to Compute

Travelling Waves in Discrete Media

H. J. Hupkes ^{a,*}, S. M. Verduyn Lunel ^a

^aMathematical Insitute of the University of Leiden

Abstract

We present a variant of Newton's Method for computing travelling wave solutions to scalar bistable lattice differential equations. We prove that the method converges to a solution, obtain existence and uniqueness of solutions to such equations with a small second order term and study the limiting behaviour of such solutions as this second order term tends to zero. The robustness of the algorithm will be discussed using numerical examples. These results will also be used to illustrate phenomena like propagation failure, which are encountered when studying lattice differential equations. We finish by discussing the broad application range of the method and illustrate that higher dimensional systems exhibit richer behaviour than their scalar counterparts.

Key words: Computation of Travelling waves, Functional differential equations, Newton's Method, Bistable lattice differential equations, Numerical computation, Ising Model, Discrete Media, Myelinated Nerve Fibers.

1 Introduction

The main purpose of this paper is to analyze a numerical method to solve families of scalar bistable differential difference equations of the form

$$-\gamma \phi''(\xi) - c\phi'(\xi) = F(\phi(\xi), \phi(\xi + r_1), \dots, \phi(\xi + r_N), \rho).$$
 (1.1)

*Corresponding author:

H.J. Hupkes

Mathematisch Instituut Universiteit Leiden P.O. Box 9512 2300 RA Leiden tel. +31715277120

Email address: hhupkes@math.leidenuniv.nl (H. J. Hupkes).

Here $\gamma \geq 0$ is a fixed parameter, c is an unknown wavespeed, ρ can be thought of as a detuning parameter and the diagonal function $-F(x,\ldots,x,\rho)$ is an N-shaped function which depends C^1 smoothly on ρ . The numbers r_i are shifts which may have either sign.

The algorithm we discuss consists of a combination of a Newton-type method with parameter continuation techniques and is based upon ideas proposed in [1, 2, 16]. Our main contribution here is to give a detailed analysis of the method. In particular, we shall show that the algorithm converges to a solution of (1.1) and use numerical examples to discuss some of the issues involved when solving (1.1). In addition, we shall obtain existence and uniqueness of connecting solutions to (1.1) and prove that these solutions depend C^1 -smoothly on the detuning parameter ρ . These results extend earlier results obtained by Mallet-Paret in [28], where the $\gamma = 0$ case was treated. To relate this interesting and widely studied case to the numerically feasible situation where $\gamma > 0$, we shall also prove that a sequence of solutions to (1.1) with γ tending to zero converges to a solution with $\gamma = 0$.

Equation (1.1) arises naturally when studying travelling wave solutions to so-called lattice differential equations, which are infinite systems of ordinary differential equations indexed by points on a spatial lattice. As an example we mention the infinite system

$$\dot{u}_{i,j} = \alpha(L_D u)_{i,j} - f(u_{i,j}, \rho), \quad (i,j) \in \mathbb{Z}^2, \quad \alpha \in \mathbb{R}, \tag{1.2}$$

on the lattice \mathbb{Z}^2 . Here $f: \mathbb{R} \times (-1,1) \to \mathbb{R}$ typically is a bistable nonlinearity of the form

$$f(u,\rho) = (u-\rho)(u^2 - 1) \tag{1.3}$$

for some parameter $-1 < \rho < 1$ and L_D is a discrete Laplacian, which is often given by

$$(L_D u)_{i,j} = (\Delta^+ u)_{i,j} \equiv u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}.$$
(1.4)

The lattice differential equation (1.2) with $\alpha = h^{-2}$ arises when one discretizes the two dimensional reaction diffusion equation,

$$u_t = \Delta u - f(u, \rho), \tag{1.5}$$

on a rectangular lattice with spacing h. In the analysis of the PDE (1.5), travelling wave solutions of the form $u(x,t) = \phi(k \cdot x - ct)$ have played a crucial role and thus have been studied extensively, starting with the classic work by Fife and McLeod [18]. The unit vector k indicates the propagation

direction of the wave and c is the unknown wavespeed which has to be determined along with the waveprofile ϕ . Following this approach, we can also study travelling wave solutions to equation (1.2). Substituting the travelling wave ansatz $u_{i,j}(t) = \phi(ik_1 + jk_2 - ct)$ into (1.2), we arrive at a forward-backward differential difference equation of the form

$$-c\phi'(\xi) = \alpha(\phi(\xi + k_1) + \phi(\xi - k_1) + \phi(\xi + k_2) + \phi(\xi - k_2) - 4\phi(\xi)) - f(\phi(\xi), \rho), \tag{1.6}$$

which is a special case of (1.1) with $\gamma = 0$. In [10] results are given concerning the asymptotic stability of travelling wave solutions to (1.2), showing that it is indeed worth while to study this class of solutions.

It is by now well known that away from the continuous limit, i.e., for small positive values of α , the dynamical behaviour of (1.2) is quite different than that of its continuous counterpart (1.5). A feature which is immediately visible from (1.6) is the presence of lattice anisotropy, which means that the wavespeed c of a travelling wave solution to (1.2) depends on the vector of propagation through the lattice k. This is illustrated in Figure 1, where we set $k = (\cos \theta, \sin \theta)$ and give a plot of the wavespeed $c(\theta)$ for travelling wave solutions to the system

$$\dot{u}_{i,j} = (L_D u)_{i,j} - 10(u_{i,j}^2 - 1)(u_{i,j} - \rho), \quad (i,j) \in \mathbb{Z}^2, \tag{1.7}$$

which satisfy the limits

$$\lim_{\xi \to \pm \infty} \phi(\xi) = \pm 1. \tag{1.8}$$

The results, which can also be found in [16], were obtained with the numerical method discussed in this paper by adding a small term $-\gamma\phi''(\xi)$ to the left hand of (1.6), where $\gamma=10^{-5}$. The polar plots clearly reveal the anisotropy of the lattice for small values of the detuning parameter ρ . After substituting the travelling wave ansatz into the PDE (1.5), it is clear that this feature of lattice anisotropy vanishes in the continuous limit. Another interesting example of a property which distinguishes lattice differential equations from their continuous counterparts, is the phenomenon of propagation failure. In the discrete case (1.6), a nontrivial interval of the detuning parameter ρ can exist in which the wavespeed satisfies c=0. This means the waveform $\phi(\xi)$ does not propagate and thus the solution $u_{i,j}(t) = \phi(ik_1 + jk_2 - ct) = \phi(ik_1 + jk_2)$ to (1.2) remains constant in time. This behaviour does not occur for the reaction diffusion equation (1.5). This phenomenon has been

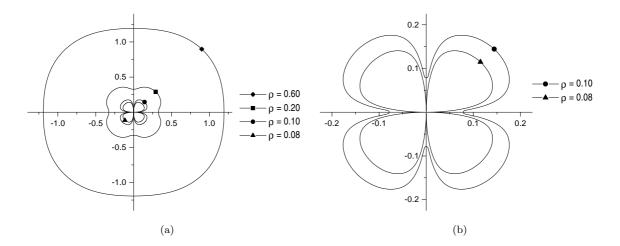


Fig. 1: A plot of the wavespeed $c(\theta)$ as a function of the propagation angle θ of travelling waves solutions to (1.7). Figure (b) is just a magnification of (a) to illustrate the behaviour for small values of the wavespeed c in greater detail.

studied extensively in [7], where one replaces the cubic nonlinearity f by an idealized nonlinearity to obtain explicit solutions to (1.6). For each propagation angle θ , the quantity $\rho^*(\theta)$ is defined to be the supremum of values $\rho > 0$ for which the wavespeed satisfies $c(\rho, \theta) = 0$. It is proven that this critical value $\rho^*(\theta)$ typically satisfies $\rho^* > 0$, depends continuously on θ when $\tan \theta$ is irrational and is discontinuous when $\tan \theta$ is rational or infinite. Numerical investigations in [16] and the present work suggest that the phenomenon of propagation failure is not just an artifact of the idealized nonlinearity f, but also occurs in the case of a cubic nonlinearity. This has recently been confirmed by Mallet-Paret in [29].

The ability to incorporate nonlocal interactions into a model together with the relatively rich structure of lattice differential equations present a strong motivation for the study of such systems. At present, models involving lattice differential equations can be found in many scientific disciplines, including chemical reaction theory [17, 25], image processing and pattern recognition [11], material science [4, 6] and biology [5, 23]. Early papers on the subject by Chi, Bell and Hassard [9] and by Keener [24] were followed by many others which developed the basic theory; see, for example, [7, 10, 19, 21, 22, 26, 28, 30, 35, 36, 38]. As a particular example we mention here the work of Bates [3], who analyzed a model which incorporates infinite range interactions. The early work by Chi, Bell and

Hassard [9] already contained computations of solutions to lattice differential equations and Elmer and Van Vleck have performed extensive calculations on equations of the form (1.1) in [13, 14, 15, 16]. In their early works [13, 14], the nonlinearity f was replaced by an idealized nonlinearity, but this restriction was lifted in [16], where a larger class of bistable functions f is considered. At present, they are pursuing a collocation approach to solve a class of functional differential equations which includes the family (1.1) [1]. We note here that when applying the methods in [1, 16] to (1.1), one essentially performs a series of Newton iterations of the same type as those studied in this paper, which means that the theory developed here can be directly applied to this situation. Our results should thus be seen as a first step towards establishing a general theoretical background for the numerical analysis of (1.1).

Notice that (1.6) contains no second derivative term, in contrast to the family (1.1) where γ may be strictly positive. As we have seen above while discussing the phenomenon of propagation failure, very interesting features of lattice differential equations arise when $\gamma=0$ and the wavespeed c satisfies $c\approx 0$. Unfortunately, the possible lack of continuity properties of the solutions in this regime makes it extremely difficult to numerically solve (1.1) directly, as all known methods would require handling singularly perturbed boundary value problems. However, setting $\gamma>0$ in (1.1) has a smoothening effect on solutions, ensuring every solution to be at least twice differentiable. This allows the successfull application of numerical techniques to solve (1.1) even as $c\to 0$, but immediately raises the question if the rich behaviour in the limit $\gamma, c\to 0$ can still be uncovered. In this paper we give rigorous theoretical and numerical evidence that this is indeed the case. In particular, we prove in Theorem 3.10 that solutions to (1.1) with increasingly small γ converge to a solution with $\gamma=0$. We strengthen the argument in Sections 5 and 6 by discussing a number of numerical examples which clearly exhibit the phenomenon of propagation failure. These examples also illustrate the important fact that the convergence proved in Theorem 3.10 already occurs at numerically feasible values of γ .

In addition to the technical reasons mentioned above, there is also a physical reason to introduce a second order term in (1.1). Such a term arises naturally if we consider systems which have local as well as nonlocal interactions and it allows us to perform continuation from systems with a continuous Laplacian to systems with a discrete Laplacian. As an example in solid-state physics, we mention

the Frenkel-Kontorova type equations discussed in [33, 34].

The numerical method discussed in this paper combines the merits of both the strategies employed in [1, 16]. In particular, we remark here that the direct collocation technique employed in [1] is numerically robuster than the method used in [16], but also requires significantly more computer time and storage space to execute a Newton iteration step. In Section 4 we show that away from the continuous limit, i.e., for small values of α in (1.6), the approach in [16] can be expected to work best. In Section 5 this information is combined with our continuation techniques to give a more thorough investigation into the phenomenon of propagation failure than previously possible. On the other hand, in Section 6.2 we numerically solve a two dimensional periodic diffusion problem, which requires the robustness of the direct collocation technique along with our path following strategies.

This paper is organized as follows. In Section 2 we recall the general Fredholm theory developed in [27] for linear functional equations of mixed type and apply it to scalar second order equations. In Section 3, we set out to establish existence and uniqueness of solutions to (1.1). We introduce the operator $\mathcal{G}: W_0^{2,\infty} \times \mathbb{R} \times V \to L^{\infty}$ associated with (1.1) and given by

$$\mathcal{G}(\phi, c, \rho)(\xi) = -\gamma \phi''(\xi) - c\phi'(\xi) - F(\phi(\xi), \phi(\xi + r_1), \dots, \phi(\xi + r_N), \rho). \tag{1.9}$$

Solutions to (1.1) correspond to zeroes of \mathcal{G} . In the first part of Section 3, Theorem 2.5 is used to prove that the Frechet derivative $D_{1,2}\mathcal{G}$ of \mathcal{G} , evaluated at a solution (ϕ, c) to (1.1) at some parameter ρ_0 , is, in fact, an isomorphism from $W_0^{2,\infty} \times \mathbb{R}$ to L^{∞} (Proposition 3.7). This allows us to make a smooth local continuation $(\phi(\rho), c(\rho))$ of solutions around $\rho = \rho_0$. In the second part of Section 3, we establish the uniqueness of solutions and prove Theorem 3.10. This enables us to turn the local continuation from the first part into a global continuation. In order to obtain the existence of solutions, we solve an explicit equation of the form (1.1) and use a homotopy of systems to extend this solution to an arbitrary family (1.1).

Having developed the underlying theory, we discuss the algorithm in Section 4 and we prove its convergence to a solution of (1.1). The algorithm is a modified Newton iteration, which uses the inverse of a linear operator $D_{1,2}\mathcal{F}$ that is closely related to the operator $D_{1,2}\mathcal{G}$, but with a relaxation on the shifted terms. Our analysis of the method relies heavily on the isomorphism result in Proposition 3.7, which can be extended to the operator $D_{1,2}\mathcal{F}$. In Section 5 we use our algorithm to calculate solutions to a specific family (1.1). The results are used to illustrate some of the technical difficulties involved in the application of our method. Considerable attention is devoted to the phenomenon of propagation failure and the issue of approaching the solutions in the singular perturbation limit $\gamma \to 0$ and $c \to 0$.

Finally, in the last section, we address some issues connected to a possible generalization of the theory developed in this paper. In particular, the numerical method can handle a broader class of equations than those analyzed here. We illustrate this by numerically computing solutions to a differential difference equation that arises when studying Ising models, which are very important for applications in the material sciences [4]. In addition, we discuss higher dimensional systems of the form (1.1) and show numerically that here the uniqueness of solutions breaks down, indicating that higher dimensional systems have a richer structure than their one dimensional counterparts. In future work this will be analyzed in a more theoretical setting.

2 Linear Functional Differential Equations of Mixed Type

In this section we apply the results obtained in [27] to second order scalar linear functional differential equations of mixed type

$$-\gamma x''(\xi) - cx'(\xi) = \sum_{j=0}^{N} A_j(\xi)x(\xi + r_j) + h(\xi).$$
 (2.1)

Here x, A_j and h represent real valued functions and the parameter γ is assumed to satisfy $\gamma \neq 0$ throughout this section. In the homogeneous case we have h = 0 and (2.1) reduces to

$$-\gamma x''(\xi) - cx'(\xi) = \sum_{j=0}^{N} A_j(\xi) x(\xi + r_j).$$
 (2.2)

Linear equations of the form (2.1) arise when one considers the linearization of (1.1) around a particular solution $\phi(\xi)$. In order to investigate the nonlinear equation (1.1) it will turn out to be crucial to understand the properties of the associated linear differential difference equation. Results in this direction will be given in this section, after we have introduced the terminology we shall need.

Throughout this section we will assume that the coefficients $A_j: J \to \mathbb{R}$ are measurable and uniformly bounded on some (usually infinite) interval J and that the inhomogeneity $h: J \to \mathbb{R}$ is locally integrable. The quantities r_j , the so-called shifts, can have either sign. As a technical

restriction we shall assume $r_0 = 0$ and $r_i \neq r_j$ whenever $i \neq j$. For convenience we demand that $N \geq 1$. It should be noted that in this case this is not a restriction on (2.1), as we can always take any coefficient A_j to vanish identically on J.

Following the standard notation for differential difference equations as introduced in [27], we define the quantities

$$r_{\min} = \min \{ r_j \mid j = 0 \dots N \},$$

 $r_{\max} = \max \{ r_j \mid j = 0 \dots N \}$ (2.3)

and observe that $r_{\min} \leq 0 \leq r_{\max}$ and $r_{\min} < r_{\max}$. We also define the state $x_{\xi} \in C([r_{\min}, r_{\max}], \mathbb{R})$ of a solution by $x_{\xi}(\theta) = x(\xi + \theta)$ for $\theta \in [r_{\min}, r_{\max}]$. This allows us to rewrite (2.1) as

$$-\gamma x''(\xi) - cx'(\xi) = L(\xi)x_{\xi} + h(\xi). \tag{2.4}$$

Here $L(\xi)$, for almost every $\xi \in J$, denotes the bounded linear functional

$$L(\xi)\phi = \sum_{j=0}^{N} A_j(\xi)\phi(r_j), \quad \phi \in C([r_{\min}, r_{\max}], \mathbb{R})$$
(2.5)

from $C([r_{\min}, r_{\max}], \mathbb{R})$ into \mathbb{R} . When the function h is absent, we have the homogeneous system

$$-\gamma x''(\xi) - cx'(\xi) = L(\xi)x_{\xi}. \tag{2.6}$$

A special case of (2.5) occurs when all the matrix functions $A_j(\xi)$ are constants, giving rise to the constant coefficient operator

$$L_0(\phi) = \sum_{j=0}^{N} A_{j,0}\phi(r_j)$$
 (2.7)

and the homogeneous constant coefficient system

$$-\gamma x''(\xi) - cx'(\xi) = L_0 x_{\xi}. \tag{2.8}$$

Definition 2.1. A solution to equation (2.4) on an interval J is a continuously differentiable function $x: J^{\#} \to \mathbb{R}$, defined on the larger interval

$$J^{\#} = \{ \xi + \theta \mid \xi \in J \text{ and } \theta \in [r_{\min}, r_{\max}] \},$$
 (2.9)

such that both x and x' are absolutely continuous on J and x satisfies (2.4) for almost every $\xi \in J$.

From now on we shall assume $J = \mathbb{R}$, unless explicitly stated otherwise. We will be particularly interested in the spaces

$$W^{1,\infty} = \{ f \in L^{\infty} \mid f \text{ is absolutely continuous and } f' \in L^{\infty} \},$$

$$W^{2,\infty} = \{ f \in L^{\infty} \mid f \text{ is absolutely continuous and } f' \in W^{1,\infty} \},$$

$$(2.10)$$

where we have used the shorthand $L^{\infty} = L^{\infty}(\mathbb{R}, \mathbb{R})$.

Associated to the homogeneous equation (2.6) we have the bounded linear operator $\Lambda_{c,\gamma,L}$: $W^{2,\infty} \to L^{\infty}$ defined by

$$(\Lambda_{c,\gamma,L}x)(\xi) = -\gamma x''(\xi) - cx'(\xi) - L(\xi)x_{\xi}. \tag{2.11}$$

The adjoint equation of (2.6) is given by

$$-\gamma y''(\xi) + cy'(\xi) = -L^*(\xi)y_{\xi}, \tag{2.12}$$

in which

$$L^*(\xi)\phi = -\sum_{j=0}^{N} A_j(\xi - r_j)\phi(-r_j), \quad \phi \in C([-r_{\text{max}}, -r_{\text{min}}], \mathbb{R}).$$
 (2.13)

The corresponding adjoint operator $\Lambda_{c,\gamma,L}^*:W^{2,\infty}\to L^\infty$ is defined by

$$(\Lambda_{c,\gamma,L}^* y)(\xi) = -\gamma y''(\xi) + cy'(\xi) + L^*(\xi)y_{\xi}$$
(2.14)

and one can indeed easily verify that for test functions x and y we have $(x, \Lambda_{c,\gamma,L}y) = (\Lambda_{c,\gamma,L}^*x, y)$, where (,) denotes the standard inner product $(x,y) = \int_{-\infty}^{\infty} x(\xi)y(\xi)d\xi$.

Associated to the constant coefficient system (2.8) is the characteristic equation, given by

$$\Delta_{c,\gamma,L_0}(s) = 0, (2.15)$$

where Δ_{c,γ,L_0} , called the characteristic function, is given by

$$\Delta_{c,\gamma,L_0}(s) = -\gamma s^2 - cs - \sum_{j=0}^{N} A_{j,0} e^{sr_j}.$$
(2.16)

We recall that a number $\lambda \in \mathbb{C}$ is an eigenvalue of the constant coefficient system (2.8) if and only if it satisfies the characteristic equation, i.e., $\Delta_{c,\gamma,L_0}(\lambda) = 0$. Elementary solutions $y(\xi)$ of the constant coefficient system (2.8) corresponding to the eigenvector λ can be written as $y(\xi) = \operatorname{Re} e^{\lambda \xi} p(\xi)$, for some complex polynomial p. We will also refer to these solutions as eigensolutions.

Definition 2.2. The constant coefficient system (2.8) is called hyperbolic in case $\Delta_{c,\gamma,L_0}(i\eta) \neq 0$ for all $\eta \in \mathbb{R}$, i.e., there are no eigenvalues on the imaginary axis.

We shall often write the operator $L(\xi)$ in (2.5) as a sum

$$L(\xi) = L_0 + M(\xi) \tag{2.17}$$

of a constant coefficient operator L_0 and a perturbation operator $M(\xi): C([r_{\min}, r_{\max}], \mathbb{R}) \to \mathbb{R}$ and we will be specially interested in cases where $M(\xi)$ vanishes as $\xi \to \pm \infty$.

Definition 2.3. The system (2.6) (or more simply L) is asymptotically autonomous at $\pm \infty$ if there exist L_0 and M as in (2.17), for which

$$\lim_{\xi \to \pm \infty} ||M(\xi)|| = 0. \tag{2.18}$$

In this case (2.8) is called the limiting equation at $\pm \infty$. If in addition this limiting equation is hyperbolic, then we say that (2.6) is asymptotically hyperbolic at $\pm \infty$. If (2.6) is asymptotically autonomous or hyperbolic at both $\pm \infty$, then we simply drop the suffix "at $\pm \infty$ ".

We are now ready to state the main theorem of this section which establishes useful properties of the operator $\Lambda_{c,\gamma,L}$. In addition, two important propositions concerning the asymptotic behaviour of solutions to (2.4) are included. These results can be seen as extensions of the main results from [27] to second order scalar systems and are derived in [20] by embedding the second order equation (2.1) into a first order two-dimensional system which is covered by the results in [27].

Theorem 2.1 (The Fredholm Alternative). Assume the homogeneous equation (2.6) is asymptotically hyperbolic. Then the operator $\Lambda_{c,\gamma,L}$ from $W^{2,\infty}$ to L^{∞} is a Fredholm operator and its range $\mathcal{R}(\Lambda_{c,\gamma,L}) \subseteq L^{\infty}$ is given by

$$\mathcal{R}(\Lambda_{c,\gamma,L}) = \left\{ h \in L^{\infty} \mid \int_{-\infty}^{\infty} y(\xi)h(\xi)d\xi = 0 \text{ for all } y \in \mathcal{K}(\Lambda_{c,\gamma,L}^*) \right\}.$$
 (2.19)

In particular,

$$\dim \mathcal{K}(\Lambda_{c,\gamma,L}^*) = \operatorname{codim} \mathcal{R}(\Lambda_{c,\gamma,L}), \quad \dim \mathcal{K}(\Lambda_{c,\gamma,L}) = \operatorname{codim} \mathcal{R}(\Lambda_{c,\gamma,L}^*), \quad \operatorname{ind}(\Lambda_{c,\gamma,L}) = -\operatorname{ind}(\Lambda_{c,\gamma,L}^*),$$
(2.20)

where ind denotes the Fredholm index. Furthermore, the Fredholm index of $\Lambda_{c,\gamma,L}$ depends only on the limiting operators L_{\pm} , namely the limits of $L(\xi)$ as $\xi \to \pm \infty$. Finally, if L_{ρ} for $-1 \le \rho \le 1$ is a continuously varying one-parameter family of hyperbolic constant coefficient operators (2.7) with $L_{\pm 1} = L_{\pm}$, then $\operatorname{ind}(\Lambda_{c,\gamma,L}) = 0$.

The next proposition will turn out to be extremely useful when obtaining asymptotic estimates on solutions to (1.1). It enables us to turn the detailed information about the eigenvalues of (2.6) which we shall obtain for our class of differential difference equations into very precise statements concerning the decay rate of the solutions. However, this result does not rule out the existence of solutions which decay superexponentially, as defined below.

Definition 2.4. Let $x: J \to \mathbb{R}$ be a continuous function on the interval $J = [\tau, \infty)$ for some $\tau \in \mathbb{R}$. Then we say x decays superexponentially or has superexponential decay at $+\infty$ if

$$\lim_{\xi \to \infty} e^{b\xi} x(\xi) = 0 \tag{2.21}$$

for every $b \in \mathbb{R}$. We define superexponential decay at $-\infty$ analogously. We will drop the distinction "at $\pm \infty$ " if this is clear from the context.

Proposition 2.2. Let $x: J^{\#} \to \mathbb{R}$ be a solution to equation (2.6) on the interval $J = [\tau, \infty)$ for some $\tau \in \mathbb{R}$. Assume that x does not decay superexponentially and that (2.6) is asymptotically autonomous at $+\infty$, with L written as in (2.17). Also assume for some real number a and some positive number k > 0, that

$$x(\xi) = O(e^{-a\xi}), \quad x'(\xi) = O(e^{-a\xi}), \quad ||M(\xi)|| = O(e^{-k\xi}), \quad \xi \to \infty.$$
 (2.22)

Then there exist $b \ge a$ and $\epsilon > 0$ such that

$$x(\xi) = y(\xi) + O(e^{-(b+\epsilon)\xi}), \quad \xi \to \infty,$$

$$x'(\xi) = y'(\xi) + O(e^{-(b+\epsilon)\xi}), \quad \xi \to \infty,$$
(2.23)

where y is a nontrivial eigensolution of the limiting equation (2.8) corresponding to the nonempty set of eigenvalues with $\operatorname{Re} \lambda = -b$.

In light of Proposition 2.2, the following lemma will be useful when studying the asymptotic behaviour of solutions to the linear homogeneous equation (2.6).

Lemma 2.3. Consider a real-valued function $x: [\tau, \infty) \to \mathbb{R}$ of the form

$$x(\xi) = y(\xi) + O(e^{-(b+\epsilon)\xi}), \quad \xi \to \infty, \tag{2.24}$$

for some $b \in \mathbb{R}$ and $\epsilon > 0$, where y is a nontrivial solution of the constant coefficient system (2.8) with $\gamma \neq 0$, given by a finite sum of eigensolutions corresponding to a set Λ of eigenvalues λ , all of which satisfy $\operatorname{Re} \lambda = -b$. If $\operatorname{Im} \lambda \neq 0$ for all $\lambda \in \Lambda$, then there exist arbitrarily large ξ for which $x(\xi) > 0$ and arbitrarily large ξ for which $x(\xi) < 0$. On the other hand, if $\Lambda = \{-b\}$, then $x(\xi) \neq 0$ for all large ξ . The analogous result for $\xi \to -\infty$ also holds.

The next proposition shows that solutions to (2.6) which are in $W^{2,\infty}$ decay exponentially. Note that it is not required here that the coefficients $A_i(\xi)$ approach their limits exponentially fast.

Proposition 2.4. Assume that equation (2.4) is asymptotically hyperbolic at $+\infty$. Then there exist positive quantities K, K' and a such that for all pairs of functions $x \in W^{2,\infty}$ and $h \in L^{\infty}$ which satisfy $\Lambda_L x = h$, the estimate

$$\left(x(\xi)^{2} + x'(\xi)^{2}\right)^{\frac{1}{2}} \leq Ke^{-a\xi} \left(\left\|x\right\|_{L^{\infty}}^{2} + \left\|x'\right\|_{L^{\infty}}^{2}\right)^{\frac{1}{2}} + K'\left\|h\right\|_{L^{\infty}}$$
(2.25)

holds for all $\xi \geq 0$.

Due to the conditions we impose on our nonlinear equation (1.1), the linear equations (2.1) encountered in the sequel often satisfy the following conditions.

Assumption 2.1. The parameter γ satisfies $\gamma > 0$ and the function $h: J \to \mathbb{R}$ is a continuous function satisfying $h(\xi) \geq 0$ for all $\xi \in J$. In addition, for every $0 \leq j \leq N$, the function $A_j(\xi)$ is continuous on J and there exist constants α_j , β_j such that

$$\alpha_j \le A_j(\xi) \le \beta_j, \quad \xi \in J. \tag{2.26}$$

In addition, we have $\alpha_j > 0$ for $1 \leq j \leq N$.

The final theorem of this section concerns homogeneous equations (2.2) that satisfy the above conditions and will be the main ingredient for establishing the results in the next section. The proof is deferred to Appendix A, where the necessary machinery is developed.

Theorem 2.5. Consider the homogeneous linear equation (2.2) and suppose that Assumption (2.1) is satisfied. Assume that equation (2.2) is asymptotically autonomous and that in addition the limiting equations are approached at an exponential rate, so

$$|A_i(\xi) - A_{i\pm}| = O(e^{-k|\xi|}), \quad \xi \to \pm \infty, \quad j = 0 \dots N$$
 (2.27)

for some k > 0. Also assume that each of the sums $A_{\Sigma_{\pm}}$ given below, of the limiting coefficients at $\pm \infty$, is negative, namely

$$A_{\Sigma_{\pm}} = \sum_{j=0}^{N} A_{j\pm} < 0. \tag{2.28}$$

Finally, assume that there exists a nontrivial solution $x = p(\xi) \in W^{2,\infty}$ to (2.2) which satisfies $p(\xi) \geq 0$ for all $\xi \in \mathbb{R}$. Then equation (2.2) is asymptotically hyperbolic and the associated operator $\Lambda_{c,\gamma,L} \colon W^{2,\infty} \to L^{\infty}$ is a Fredholm operator. In addition, we have

$$\dim \mathcal{K}(\Lambda_{c,\gamma,L}) = \dim \mathcal{K}(\Lambda_{c,\gamma,L}^*) = \operatorname{codim} \mathcal{R}(\Lambda_{c,\gamma,L}) = 1, \quad \operatorname{ind}(\Lambda_{c,\gamma,L}) = 0. \tag{2.29}$$

The element $p \in \mathcal{K}(\Lambda_{c,\gamma,L})$ is strictly positive,

$$p(\xi) > 0, \quad \xi \in \mathbb{R} \tag{2.30}$$

and there exists an element $p^* \in \mathcal{K}(\Lambda_{c,\gamma,L}^*)$ which is strictly positive,

$$p^*(\xi) > 0, \quad \xi \in \mathbb{R}. \tag{2.31}$$

3 Global Structure

In this section we study the family of autonomous differential difference equations introduced in the introduction,

$$-cx'(\xi) - \gamma x''(\xi) = F(x(\xi + r_0), x(\xi + r_1), x(\xi + r_2), \dots, x(\xi + r_N), \rho), \tag{3.1}$$

in which $\gamma > 0$. As in the previous section, we demand that $r_0 = 0$, $r_i \neq r_j$ if $i \neq j$ and $r_i \neq 0$ for $i = 1 \dots N$, where $N \geq 1$. Here we take $\rho \in \overline{V}$ to be a parameter, where V is an open subset of \mathbb{R} . We shall prove existence and uniqueness of solutions to (3.1) under certain conditions and establish the C^1 -dependence of the solutions on the parameter ρ .

We start out by making precise the requirements given in the introduction and give a list of conditions on the function F which we will assume to hold throughout this section.

- **(b1)** The nonlinearity $F: \mathbb{R}^{N+1} \times \overline{V} \to \mathbb{R}$ is C^1 -smooth in \mathbb{R}^{N+1} and \overline{V} .
- (b2) The derivative $D_1F: \mathbb{R}^{N+1} \times \overline{V} \to \mathbb{R}^{N+1}$ with respect to the first argument $v \in \mathbb{R}^{N+1}$ is locally Lipschitz in v.
- **(b3)** For each $\rho \in \overline{V}$ and for j = 1, ..., N, we have, writing $v = (v_0, v_1, ..., v_N) \in \mathbb{R}^{N+1}$, that either

$$\frac{\partial F(v,\rho)}{\partial v_j} \equiv 0, \quad \text{or} \quad \frac{\partial F(v,\rho)}{\partial v_j} > 0,$$
 (3.2)

that is, either F is totally independent of v_j or is strictly increasing in v_j . Furthermore, for each $\rho \in \overline{V}$ there is at least one j, satisfying $1 \leq j \leq N$, for which the nonlinearity F is not totally independent of v_j .

(b4) Let $\Phi : \mathbb{R} \times \overline{V} \to \mathbb{R}$ be defined as

$$\Phi(\phi, \rho) = F(\phi, \phi, \dots, \phi, \rho). \tag{3.3}$$

Then for some quantity $q = q(\rho) \in [-1, 1]$ we have that

$$\Phi(-1, \rho) = \Phi(q(\rho), \rho) = \Phi(1, \rho) = 0,
\Phi(\phi, \rho) > 0, \quad \phi \in (-\infty, -1) \cup (q, 1),
\Phi(\phi, \rho) < 0, \quad \phi \in (-1, q) \cup (1, \infty).$$
(3.4)

In case $\rho \in V$ we demand $q(\rho) \in (-1,1)$.

(b5) We have for $q = q(\rho)$ that

$$D_1\Phi(-1,\rho) < 0 \text{ if } q \neq -1,$$

 $D_1\Phi(q,\rho) > 0 \text{ if } q \in (-1,1),$
 $D_1\Phi(1,\rho) < 0 \text{ if } q \neq 1,$

$$(3.5)$$

with D_1 denoting the derivative with respect to the first argument $x \in \mathbb{R}$.

Condition (b3) allows us to consider families in which the shifts r_j may vary with ρ , by adding extra shifts r_j which do not affect the value of F for certain values of ρ .

In (3.1) the wavespeed c is an unknown parameter. From the above conditions we see that equation (3.1) has exactly three constant equilibrium solutions, namely $x = \pm 1$ and $x = q(\rho)$. We will be interested in solutions to (3.1) joining the two equilibrium points ± 1 . As (3.1) is autonomous, we see that all translates of a solution $x(\xi)$ to (3.1) are also solutions. We can use this freedom to demand that x(0) = 0. It will turn out that after this normalization the solution to (3.1) is unique. We thus seek our solutions in the space

$$W_0^{2,\infty} = \left\{ x \in W^{2,\infty} \mid x(0) = 0 \right\}. \tag{3.6}$$

It will be useful to introduce the operator $\mathcal{G}: W_0^{2,\infty} \times \mathbb{R} \times V \to L^{\infty}$ defined by

$$\mathcal{G}(\phi, c, \rho)(\xi) = -\gamma \phi''(\xi) - c\phi'(\xi) - F(\phi(\xi + r_0), \phi(\xi + r_1), \dots, \phi(\xi + r_N), \rho). \tag{3.7}$$

We are now ready to define the concept of a connecting solution to (3.1).

Definition 3.1. Given $\rho \in V$, a connecting solution to the nonlinear autonomous differential difference equation (3.1) is a pair $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ that satisfies (3.1) and joins the two equilibrium solutions ± 1 , i.e., for which the limits

$$\lim_{\xi \to \pm \infty} \phi(\xi) = \pm 1 \tag{3.8}$$

Please note that we will continue to use the term "solution" to indicate a function $x \in W^{2,\infty}$ satisfying the equation (3.1), but not necessarily joining the two equilibria ± 1 and not necessarily having x(0) = 0.

We are now in a position to state the main theorem of this section.

Theorem 3.1. Consider a family of autonomous differential difference equations (3.1) that satisfies the conditions (b1) through (b5). There exist C^1 -smooth functions $c: V \to \mathbb{R}$ and $P: V \to W_0^{2,\infty}$ such that for all $\rho_0 \in V$, the pair $(P(\rho_0), c(\rho_0))$ is a connecting solution to equation (3.1). Moreover, these are the only connecting solutions to (3.1).

Before proceeding with the proof of the main theorem, let us consider the differential difference equation (3.1) with fixed parameters c, γ and ρ . If x_1 and x_2 are two bounded solutions of this

equation (3.1), then the difference $y(\xi) = x_1(\xi) - x_2(\xi)$ satisfies the linear homogeneous equation (2.6) with coefficients given by

$$A_j(\xi) = \int_0^1 \frac{\partial F(u,\rho)}{\partial u_j} \bigg|_{u=t\pi(x_1,\xi)+(1-t)\pi(x_2,\xi)} dt. \tag{3.9}$$

Here π is the state projection

$$\pi(\phi,\xi) = \left(\phi(\xi + r_0), \dots, \phi(\xi + r_N)\right) \in \mathbb{R}^{N+1}.$$
(3.10)

This can easily be seen by using the formula

$$F(v,\rho) - F(w,\rho) = \int_0^1 \frac{dF(tv + (1-t)w,\rho)}{dt} dt = \sum_{j=0}^N \left(\int_0^1 \frac{\partial F(tv + (1-t)w,\rho)}{\partial u_j} dt \right) (v_j - w_j).$$
(3.11)

Similarly, suppose that $x : \mathbb{R} \to \mathbb{R}$ is any solution to (3.1) for some $\rho \in \overline{V}$. Then $x'(\xi)$ is a solution of the linearization around x, that is, the linear equation (2.6) with coefficients

$$A_j(\xi) = \left. \frac{\partial F(u, \rho)}{\partial u_j} \right|_{u=\pi(x,\xi)}.$$
 (3.12)

The linearization around the three equilibrium solutions $x = \pm 1$ and $x = q(\rho)$ are constant coefficient equations given by (2.8). We shall write L_+ , L_- and L_{\diamond} for the associated linear operators (2.7) and shall refer to the corresponding constant coefficients as

$$A_{j\pm}(\rho) = \frac{\partial F(u,\rho)}{\partial u_j} \Big|_{u=\kappa(\pm 1)},$$

$$A_{j\diamond}(\rho) = \frac{\partial F(u,\rho)}{\partial u_j} \Big|_{u=\kappa(q(\rho))},$$
(3.13)

where κ is the diagonal map $\kappa(x)=(x,\ldots,x)\in\mathbb{R}^{N+1}$. Writing $A_{\Sigma\pm}=\sum_{j=0}^N A_{j\pm}$, we have the identity

$$A_{\Sigma \pm} = D_1 \Phi(\pm 1, \rho). \tag{3.14}$$

Note that when $\rho \in V$, condition (b5) in combination with Lemma A.4 implies that the linearization of (3.1) around $x = \pm 1$ is asymptotically hyperbolic at $\pm \infty$.

The proof of Theorem 3.1 will be given in two parts. First we shall concentrate on the existence of functions $P(\rho)$ and $c(\rho)$ as in the statement of Theorem 3.1 in a small neighbourhood of the detuning parameter ρ_0 , given a connecting solution (P_0, c_0) for $\rho = \rho_0$. After we have established the existence of this local continuation in Proposition 3.2, we show that it can be extended to all $\rho \in V$ and thus prove the existence and uniqueness claims in the statement of Theorem 3.1.

Proposition 3.2. Let $(P_0, c_0) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (3.1) for some $\rho_0 \in V$ and for some $c_0 \in \mathbb{R}$. Then for each ρ near ρ_0 there exists an unique $(P, c) = (P(\rho), c(\rho)) \in W_0^{2,\infty} \times \mathbb{R}$, that depends C^1 -smoothly on ρ , for which $\mathcal{G}(P(\rho), c(\rho), \rho) = 0$, with $c(\rho_0) = c_0$ and $P(\rho_0) = P_0$. This function $P(\rho)$ satisfies the boundary conditions $\lim_{\xi \to \pm \infty} P(\rho)(\xi) = \pm 1$ and thus $(P(\rho), c(\rho))$ is a connecting solution to (3.1).

Our approach to proving the result above will be to invoke the implicit function theorem on the operator \mathcal{G} defined by (3.7). Consequently, in Proposition 3.7 we study the Frechet derivative of \mathcal{G} , which is given by

$$D_{1,2}\mathcal{G}(P_0, c_0, \rho_0)(\psi, b)(\xi) = -bP_0'(\xi) + (\Lambda_{c_0, \gamma, L}\psi)(\xi), \tag{3.15}$$

where $\Lambda_{c_0,\gamma,L}$ is the linear operator associated to the linearization of (3.1) around the solution P_0 . We shall establish that Theorem 2.5 applies to the operator $\Lambda_{c_0,\gamma,L}$ and that the derivative P'_0 is strictly positive (Lemma 3.6). In particular, this means that $P'_0 \notin \mathcal{R}(\Lambda_{c_0,\gamma,L})$ and $\mathcal{K}(\Lambda_{c_0,\gamma,L}) \cap W_0^{2,\infty} = \emptyset$. From this it is easy to see that $D_{1,2}\mathcal{G}$ is an isomorphism from $W_0^{2,\infty} \times \mathbb{R}$ onto L^{∞} , which legitimizes the use of the implicit function theorem.

We shall need the following technical lemma to prove that solutions to (3.1) which are close to connecting solutions in the $W^{2,\infty}$ norm are in fact also connecting solutions. The proof of this result closely follows the corresponding argument for $\gamma = 0$ and we therefore refer to [20] for the details.

Lemma 3.3. Let $x : \mathbb{R} \to \mathbb{R}$ be a solution to (3.1) for some $\rho \in \overline{V}$ and $c \in \mathbb{R}$. Define

$$\mu_{-} = \inf_{\xi \in \mathbb{R}} x(\xi), \quad \mu_{+} = \sup_{\xi \in \mathbb{R}} x(\xi), \tag{3.16}$$

and assume that both μ_{\pm} are finite. Then

$$\mu_{-} \in [-1, q(\rho)] \cup \{1\}, \quad \mu_{+} \in \{-1\} \cup [q(\rho), 1].$$
 (3.17)

The same conclusion (3.17) holds for

$$\mu_{-} = \lim_{\xi \to \infty} \inf x(\xi), \quad \mu_{+} = \lim_{\xi \to \infty} \sup x(\xi)$$
(3.18)

and similarly for the \liminf and \limsup at $-\infty$.

Corollary 3.4. If $(P,c) \in W_0^{2,\infty} \times \mathbb{R}$ is a connecting solution to (3.1), then

$$-1 < P(\xi) < 1, \quad \xi \in \mathbb{R}.$$
 (3.19)

Proof. Lemma 3.3 implies that $-1 \le P(\xi) \le 1$ for all $\xi \in \mathbb{R}$. The strict inequalities now follow from an application of Lemma A.8.

Lemma 3.5. Let $(P_0, c_0) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (3.1). Then for some quantities $C_{\pm} > 0$ and $\epsilon > 0$ we have that

$$P_0(\xi) = \begin{cases} -1 + C_- e^{\lambda_-^u \xi} + O(e^{(\lambda_-^u + \epsilon)\xi}), & \xi \to -\infty, \\ 1 - C_+ e^{\lambda_+^s \xi} + O(e^{(\lambda_+^s - \epsilon)\xi}), & \xi \to \infty, \end{cases}$$
(3.20)

where $\lambda_{-}^{u} \in (0, \infty)$ is the unique positive eigenvalue of the linearization of (3.1) about x = -1 and $\lambda_{+}^{s} \in (-\infty, 0)$ is the unique negative eigenvalue of the linearization about x = 1. The formulae for $P'(\xi)$ obtained by formally differentiating (3.20) also hold.

Proof. We consider only the limit $\xi \to \infty$, as the proofs of the results for $\xi \to -\infty$ are similar. Defining $y(\xi) = 1 - P(\xi)$, we see that y satisfies the linear equation (2.2) with coefficients $A_j(\xi)$ given by (3.9) with $x_1 = 1$ and $x_2 = P$. Note that $\lim_{\xi \to \infty} A_j(\xi) = A_{j+}(\rho)$, thus this linear equation is asymptotically hyperbolic. Proposition 2.4 now implies that $y(\xi)$ decays exponentially. Using the expression (3.9) together with the Lipschitz condition (b2) on the derivative of F, it follows that the coefficients $A_j(\xi)$ approach their limits exponentially fast. One can now proceed as in the proof of Theorem 2.5 to establish the claim.

Lemma 3.6. If $(P,c) \in W_0^{2,\infty} \times \mathbb{R}$ is a connecting solution to (3.1), then $P'(\xi) > 0$ for all $\xi \in \mathbb{R}$.

Proof. We note that it is sufficient to prove that $P'(\xi) \geq 0$ for all $\xi \in \mathbb{R}$, since Corollary A.7 then immediately implies the strict positivity $P'(\xi) > 0$.

By (3.20) we see that there exists $\tau > 0$ such that $P'(\xi) > 0$ whenever $|\xi| \ge \tau$ and such that $P(-\tau) < P(\xi) < P(\tau)$ whenever $|\xi| < \tau$. From this we have $P(\xi + k) > P(\xi)$ for all $\xi \in \mathbb{R}$, provided that $k \ge 2\tau$. Now suppose that $P'(\xi) < 0$ for some ξ and set

$$k_0 = \inf\{k > 0 \mid P(\xi + k) > P(\xi) \text{ for all } \xi \in \mathbb{R}\}.$$
 (3.21)

Certainly $k_0 > 0$. Also, $k_0 \le 2\tau$ and $P(\xi + k_0) \ge P(\xi)$ for all $\xi \in \mathbb{R}$. If $0 < k < k_0$ then $P(\xi + k) \le P(\xi)$ for some ξ , where necessarily $|\xi| \le \tau$. Therefore, there exists some ξ_0 , with $|\xi_0| \le \tau$, for which $P(\xi_0 + k_0) = P(\xi_0)$. We can now define $x_1(\xi) = P(\xi + k_0)$ and $x_2(\xi) = P(\xi)$. Because $x_1(\xi) \ge x_2(\xi)$

for all $\xi \in \mathbb{R}$ and $x_1(\xi_0) = x_2(\xi_0)$, Lemma A.8 implies that $P(\xi + k_0) = P(\xi)$ for all $\xi \in \mathbb{R}$. This is a contradiction, because $P'(\xi) > 0$ for all large $|\xi|$.

Proposition 3.7. Let $(P_0, c_0) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (3.1) for some $\rho_0 \in V$ and for some $c_0 \in \mathbb{R}$. Consider the linearization (2.2) of equation (3.1) about P_0 and let $\Lambda_{c_0,\gamma,L}$ denote the associated linear operator from $W^{2,\infty}$ to L^{∞} . Then the derivative of \mathcal{G} ,

$$D_{1,2}\mathcal{G}(P_0, c_0, \rho_0) : W_0^{2,\infty} \times \mathbb{R} \to L^{\infty},$$
 (3.22)

at the solution (P_0, c_0) , with respect to the first two arguments, is given by

$$D_{1,2}\mathcal{G}(P_0, c_0, \rho_0)(\psi, b)(\xi) = -bP_0'(\xi) + (\Lambda_{c_0, \gamma, L}\psi)(\xi)$$
(3.23)

and is an isomorphism from $W_0^{2,\infty} \times \mathbb{R}$ onto L^{∞} .

Proof. The fact that \mathcal{G} is C^1 -Frechet differentiable follows from the fact that F is a C^1 -function and the explicit formula (3.23) follows by direct differentiation of (3.7). The operator $\Lambda_{c_0,\gamma,L}$ can be easily seen to satisfy all the conditions of Theorem 2.5. In particular, $x(\xi) = P'_0(\xi)$ satisfies the linear equation (2.2), which by Lemma 3.6 gives the strictly positive $p = P'_0 \in \mathcal{K}_{c_0,\gamma,L}$ in the statement of Theorem 2.5. Thus, by Theorem 2.5, the kernel $\mathcal{K}_{c_0,\gamma,L}$ of $\Lambda_{c_0,\gamma,L}$ is precisely the one-dimensional span of P'_0 . The strict positivity $P'_0(0) > 0$ implies that $P'_0 \notin W_0^{2,\infty}$, hence $\mathcal{K}(\Lambda_{c_0,\gamma,L}) \cap W_0^{2,\infty} = \emptyset$. In addition, the presence of the strictly positive $p^* \in \mathcal{K}(\Lambda_{c_0,\gamma,L}^*)$ guarantees $P'_0 \notin \mathcal{R}(\Lambda_{c_0,\gamma,L})$ by Theorem 2.1, which establishes the claim.

Proof of Proposition 3.2. The local continuation follows from the implicit function theorem, together with Lemma 3.7. The limit at $+\infty$ follows from the observation that the quantity $\mu_{-}(\rho)$ in (3.18) for $P(\rho)$ varies continuously with ρ , together with $\mu_{-}(\rho_{0}) = 1$ and the identity (3.17). The limit at $-\infty$ follows similarly.

We now set out to give the proof of Theorem 3.1. Lemma 3.8 establishes the uniqueness claim in Theorem 3.1. Theorem 3.10 will allow us to extend the local continuation in Proposition 3.2 to a global continuation for all $\rho \in V$, by proving that limits of connecting solutions are connecting solutions to the limiting differential difference equation. This means that once we have established

the existence of a connecting solution to (3.1) for one value of the detuning parameter, $\rho_0 \in V$, we know that (3.1) has a connecting solution for all values $\rho \in V$. This is why we give an explicit solution to a prototype differential difference equation in Lemma 3.11. By constructing a new family (3.1), which mixes the original differential difference equation and the prototype system, we can combine Theorem 3.10 and Proposition 3.2 to establish the existence of a connecting solution to our original family (3.1) at one value of the detuning parameter ρ , as required.

We merely state the following lemma and refer to [20] for the complete proof, which closely follows the corresponding argument for the $\gamma = 0$ case.

Lemma 3.8. For each $\rho \in V$ there exists at most one value $c \in \mathbb{R}$ such that equation (3.1) possesses a monotone increasing solution $x = P(\xi)$, satisfying the boundary conditions

$$\lim_{\xi \to \pm \infty} x(\xi) = \pm 1. \tag{3.24}$$

For each $c \in \mathbb{R}$ and $\rho \in V$ there exists at most one solution $x = P(\xi)$ of (3.1), up to translation, satisfying the boundary conditions (3.24).

The following result, concerning the linearization around the (unstable) equilibrium $q(\rho)$, will prove to be useful in establishing the boundary conditions $x(\pm \infty) = \pm 1$ for limits of connecting solutions x_n .

Lemma 3.9. For every $\rho \in V$, $\gamma \in \mathbb{R}_{\geq 0}$ and $c \in \mathbb{R}$ there do not exist two monotone increasing solutions $x_{\pm} : \mathbb{R} \to \mathbb{R}$ of equation (3.1) such that

$$\lim_{\xi \to -\infty} x_{-}(\xi) = -1, \quad \lim_{\xi \to \infty} x_{-}(\xi) = q(\rho),$$

$$\lim_{\xi \to -\infty} x_{+}(\xi) = q(\rho), \quad \lim_{\xi \to \infty} x_{+}(\xi) = 1.$$
(3.25)

Proof. The case where $\gamma=0$ was considered in [28, Lemma 7.1], so we will assume $\gamma>0$. First notice that

$$\Delta_{c \sim L_{c}(\rho)}(0) = -A_{\Sigma \diamond}(\rho) = -D_{1}\Phi(q(\rho), \rho) < 0, \tag{3.26}$$

which by Lemma A.5 implies that there do not simultaneously exist eigenvalues $\lambda_{\diamond}^{u} < 0 < \lambda_{\diamond}^{s}$ for the constant coefficient system L_{\diamond} defined in (3.13).

Now assume that there exist monotone increasing x_{-} and x_{+} satisfying conditions (3.25). Consider $y(\xi) = q(\rho) - x_{-}(\xi)$, which is a monotone decreasing function on the real line, satisfying (2.2)

with coefficients given by (3.9), with $x_1 = q(\rho)$ and $x_2 = x_-(\xi)$. This linear equation satisfies all the assumptions of Lemma A.1 and thus reasoning as in the proof of this lemma we see that for all $\xi \in \mathbb{R}$,

$$y'(\xi) \ge -By(\xi) \tag{3.27}$$

for some B>0. Now take any sequence $\xi_n\to\infty$, and let $z_n(\xi)=y(\xi+\xi_n)/y(\xi_n)$. Then each z_n also satisfies $z_n'(\xi)\geq -Bz_n(\xi)$ on $\mathbb R$. As $z_n(0)=1$, we conclude that the sequence of functions z_n is uniformly bounded and equicontinuous on each compact interval and so without loss we have that $z_n(\xi)\to z(\xi)$ uniformly on compact intervals. From the differential equation (3.1) we see that we can use the uniform bound on z_n' to obtain a uniform bound on $z_n''(\xi)$, thus concluding that also $z_n'(\xi)$ is equicontinuous on each compact interval. One now easily sees that z satisfies the autonomous limiting constant coefficient equation associated to L_{\diamond} . Moreover, $-Bz(\xi)\leq z'(\xi)\leq 0$ for all $\xi\in\mathbb{R}$, with z(0)=1, so $z(\xi)>0$ and z does not decay faster than exponentially. We may now apply Proposition 2.2 to the solution z. We conclude that $z(\xi)=w(\xi)+O(e^{-(b+\epsilon)\xi})$ as $\xi\to\infty$, where w is a nontrivial sum of eigensolutions corresponding to a set of eigenvalues with $\mathrm{Re}\,\lambda=-b\leq 0$. The positivity of z, together with Lemma 2.3, implies that the linearization about $x=q(\rho)$ possesses a nonpositive eigenvalue $\lambda_{\diamond}^s\leq 0$. Since $\Delta_{c,\gamma,L_{\diamond}(\rho)}(0)<0$ we have $\lambda_{\diamond}^s<0$. We can use similar reasoning applied to $x_+(\xi)$ to conclude that the linearization about $x=q(\rho)$ must also possess a positive eigenvalue $\lambda_{\diamond}^u>0$. This yields a contradiction.

Remark 3.1. In the above proof we could not apply Proposition 2.2 directly to the function $y(\xi)$, as it may not be the case that $y(\xi)$ approaches its limits $y(\pm \infty)$ exponentially fast.

The next theorem enables us to take limits of connecting solutions, which will be crucial in establishing global existence of solutions.

Theorem 3.10. Let $\rho_n \in V$ and $\gamma_n \in \mathbb{R}_{>0}$ be two sequences satisfying $\gamma_n \to \gamma_0$ and $\rho_n \to \rho_0$ as $n \to \infty$, possibly with $\gamma_0 = 0$. Let $(P_n(\xi), c_n)$ denote any connecting solution to (3.1) with $\rho = \rho_n$ and $\gamma = \gamma_n$. Then, after possibly passing to a subsequence, the limit

$$\lim_{n \to \infty} P_n(\xi) = P_0(\xi) \tag{3.28}$$

exists pointwise and also the limit

$$\lim_{n \to \infty} c_n = c_0 \tag{3.29}$$

exists, with $|c_0| < \infty$. Furthermore, $P_0(\xi)$ satisfies the limiting differential difference equation

$$-\gamma_0 P_0''(\xi) - c_0 P_0'(\xi) = F(P_0(\xi), P_0(\xi + r_1), \dots, P_0(\xi + r_N), \rho_0)$$
(3.30)

almost everywhere. In addition, we have the limits

$$\lim_{\xi \to \pm \infty} P_0(\xi) = \pm 1. \tag{3.31}$$

Proof. Using the fact that the functions $P_n(\xi)$ satisfy $P'_n > 0$, we may argue in a standard fashion that, after passing to a subsequence, the pointwise limit $P_0(\xi) = \lim_{n \to \infty} P_n(\xi)$ exists for all $\xi \in \mathbb{R}$. Due to the limits $\lim_{n \to \infty} P_n(\xi) = \pm 1$, we have $\int_{-\infty}^{\infty} P'_n(s) ds = 2$. Writing $F(\xi) = \liminf_{n \to \infty} P'_n(\xi)$ we obtain, using Fatou's Lemma,

$$\int_{-\infty}^{\infty} F(s)ds \le 2. \tag{3.32}$$

In particular, this implies that the measure of the set for which $F(s) = \infty$ is zero. Letting β_n be any sequence with $\beta_n \to 0$ as $n \to \infty$, we have that, if we choose ξ_0 appropriately,

$$\lim_{n \to \infty} \inf \beta_n (P'_n(\xi) - P'_n(\xi_0)) = 0 \quad \text{almost everywhere} . \tag{3.33}$$

Now suppose that $\liminf_{n\to\infty} |c_n| = \infty$. Without loss assume $c_n > 0$. Write $q_0 = q(\rho_0)$ and fix a point

$$q_* \in (q_0, 1). \tag{3.34}$$

Let $x_n(\xi) = P_n(c_n\xi + \xi_n)$, where $\xi_n \in \mathbb{R}$ is such that $P_n(\xi_n) = q_*$. Then (3.1) in integrated form gives us

$$-\gamma_n c_n^{-2} \left(x_n'(\xi) - x_n'(\xi_0) \right) - \left(x_n(\xi) - x_n(\xi_0) \right) = \int_{\xi_0}^{\xi} F\left(x_n(s), x_n(s + r_1 c_n^{-1}), \dots, x_n(s + r_N c_n^{-1}), \rho_n \right) ds.$$
(3.35)

Again, because the x_n are monotonically increasing functions, we can pass to a subsequence for which the pointwise limit $x(\xi) = \lim_{n\to\infty} x_n(\xi)$ exists and is continuous at all but countably many points. We have seen above that $\liminf_{n\to\infty} \beta_n c_n^{-1} x_n'(\xi) = 0$ almost everywhere, for a sequence $\beta_n \to 0$. After taking the limit $\liminf_{n\to\infty} \infty$ we thus obtain, using $\beta_n = c_n^{-1} \to 0$,

$$-(x(\xi) - x(\xi_0)) = \int_{\xi_0}^{\xi} F(x(s), x(s), \dots, x(s), \rho_0) ds,$$
 (3.36)

which holds almost everywhere. By redefining x on a set of measure zero, which does not affect the right hand side of (3.36), we can assume this identity to hold everywhere. From this identity we also see that $x(\xi)$ is differentiable and satisfies

$$-x'(\xi) = \Phi(x(\xi), \rho_0). \tag{3.37}$$

Since $x(\xi) \leq q_*$ for almost all $\xi \leq 0$, we cannot have $x(\xi) = 1$ for some ξ , as this would imply $x(\xi) = 1$ for all ξ . Now $x_n(\xi) \geq q_*$ for all $\xi \geq 0$, hence also $1 > x(\xi) \geq q_*$ for $\xi \geq 0$ and thus $x'(\xi) = -\Phi(x(\xi), \rho_0) < 0$ whenever $\xi \geq 0$. On the other hand, $x'_n(\xi) > 0$, hence $x'(\xi) \geq 0$, for all ξ . This contradiction implies that $\liminf_{n \to \infty} |c_n| < \infty$. Thus, after passing to a subsequence, the limit $c_0 = \lim_{n \to \infty} c_n$ exists.

Integration of (3.1) yields

$$-\gamma_n \left(P'_n(\xi) - P'_n(\xi_0) \right) - c_n \left(P_n(\xi) - P_n(\xi_0) \right) = \int_{\xi_0}^{\xi} F\left(P_n(s), P_n(s+r_1), \dots, P_n(s+r_N), \rho_n \right) ds.$$
 (3.38)

Consider the case where $\gamma_0 > 0$. Notice that $y_n(\xi) = 1 - P_n(\xi)$ is a monotone decreasing function on the real line, which satisfies the linear equation (2.1) with coefficients given by (3.9), with $x_1 = 1$ and $x_2 = P_n$. Referring to these coefficients as $A_{j,n}(\xi)$, we see that (2.2) satisfies the conditions of Lemma A.1 and we hence obtain from the proof of this lemma

$$y_n'(\xi) \ge -B_n y_n(\xi),\tag{3.39}$$

in which $B_n = \sqrt{\frac{c_n^2}{4\gamma_n^2} - \frac{\alpha_{0,n}}{\gamma_n}} + \frac{c_n}{\gamma_n}$. Now there exists α_0 such that $0 \ge \alpha_{0,n} \ge \alpha_0$, as the functions $y_n(\xi)$ are uniformly bounded and D_1F is a continuous function, which attains its maxima and minima on compact sets. This means that the constants B_n are bounded, $0 \le B_n \le B$ for some B. From (3.39) we now see that y'_n and hence P'_n are uniformly bounded. From the differential equation (3.1) it now also follows that the functions P''_n are uniformly bounded. Thus P'_n is an equicontinuous family, allowing us to pass to a subsequence for which $P'_n(\xi) \to P'_0(\xi)$ and $P_n(\xi) \to P_0(\xi)$ uniformly on compact intervals.

Thus, taking the limit $\liminf_{n\to\infty}$ in (3.38), we now obtain for all $\gamma_0 \geq 0$

$$-\gamma_0 \left(P_0'(\xi) - P_0'(\xi_0) \right) - c_0 \left(P_0(\xi) - P_0(\xi_0) \right) = \int_{\xi_0}^{\xi} F\left(P_0(s), P_0(s+r_1), \dots, P_0(s+r_N), \rho_0 \right) ds, \quad (3.40)$$

which holds for all $\xi \in \mathbb{R}$ if $\gamma_0 \neq 0$ and almost everywhere if $\gamma_0 = 0$. In case $\gamma_0 = 0$ and $c_0 \neq 0$ we can again by redefining P_0 on a set of measure zero ensure that (3.40) holds for all $\xi \in \mathbb{R}$. After differentiation we see that $P_0(\xi)$ satisfies the differential difference equation stated in the theorem.

We now set out to prove the limits (3.31). Because $P_0(\xi)$ is a bounded monotonically increasing function, the limits $\lim_{\xi \to \pm \infty} P_0(\xi)$ exist. We will refer to these limits as $P_0(\pm \infty)$. When $c_0 \neq 0$, the function $P'_0(\xi)$ decays exponentially, and when $\gamma_0 \neq 0$, the function $P''_0(\xi)$ decays exponentially. Taking the limits $\xi \to \pm \infty$ in equation (3.30) we obtain

$$0 = F(P_0(\pm \infty), P_0(\pm \infty), \dots, P_0(\pm \infty), \rho_0) = \Phi(P_0(\pm \infty), \rho_0), \tag{3.41}$$

which implies that

$$P_0(\pm \infty) \in \{-1, q(\rho_0), 1\}.$$
 (3.42)

Since we know that $P_n(\xi) < 0$ if $\xi < 0$ and $P_n(\xi) > 0$ if $\xi > 0$, we have that $P_0(\xi) \le 0$ if $\xi < 0$ and $P_0(\xi) \ge 0$ if $\xi > 0$ almost everywhere. In particular, if $q(\rho_0) = \pm 1$ then the proof is complete as then necessarily $P_0(\pm \infty) = \pm 1$. Thus assume that $q(\rho_0) \in (-1, 1)$. Fix any points q_1 and q_2 satisfying $-1 < q_1 < q(\rho_0) < q_2 < 1$ and let $\xi_n, \zeta_n \in \mathbb{R}$ be such that

$$P_n(\xi) \le q_1 \text{ for } \xi < \zeta_n, \qquad q_1 \le P_n(\xi) \le q_2 \text{ for } \zeta_n < \xi < \xi_n, \qquad P_n(\xi) \ge q_2 \text{ for } \xi > \xi_n.$$
 (3.43)

Without loss (we may always pass to a subsequence) we may assume that the limits $\xi_n \to \xi_0$ and $\zeta_n \to \zeta_0$ both exist, although they may possibly be infinite. It is enough to show that the difference $\xi_n - \zeta_n$ is bounded. Indeed, if this is the case, and if ξ_n and hence also ζ_n are bounded themselves, so that ξ_0 and ζ_0 are both finite, then $P_0(\xi) \leq q_1$ for all $\xi < \zeta_0$ and $P_0(\xi) \geq q_2$ for all $\xi > \xi_0$, which with (3.42) implies the limits (3.31). The case $\xi_0 = \zeta_0 = \pm \infty$ cannot occur, since then either $P_0(\xi) \leq q_1$ or $P_0(\xi) \geq q_2$, hence $P_0(\xi) = \pm 1$ for all $\xi \in \mathbb{R}$, which is a contradiction.

To prove that $\xi_n - \zeta_n$ is bounded, assume $\xi_n - \zeta_n \to \infty$ and define

$$x_{n+}(\xi) = P_n(\xi + \xi_n), \ x_{n-}(\xi) = P_n(\xi + \zeta_n).$$
 (3.44)

Upon passing to a subsequence and taking limits $x_{n\pm} \to x_{\pm}$ as above, we obtain solutions of (3.30) which satisfy the four boundary conditions in (3.25) with $q(\rho_0)$ replacing $q(\rho)$. However, this is impossible by Lemma 3.9.

Lemma 3.11. Suppose that the function $q: \overline{V} \to \mathbb{R}$ associated to (3.1) satisfies $q(\rho^*) = 0$ for some $\rho^* \in \overline{V}$. Then (3.1) with $\rho = \rho^*$ has a connecting solution $(P(\xi), c)$ for some $c \in \mathbb{R}$.

Proof. First we consider the specific equation for some k > 0,

$$-\gamma x''(\xi) - x'(\xi) = \beta^{-1} (x(\xi - k) - x(\xi)) - f(x(\xi)), \tag{3.45}$$

in which f is given by

$$f(x) = \frac{\beta x(x^2 - 1)}{1 - \beta x} + 2\gamma x(x^2 - 1), \quad \beta = \tanh k,$$
 (3.46)

for $x \in [-1, 1]$. Outside this interval f is modified to be a nonzero C^1 function on the real line. It is routine to check that $x = \tanh \xi$ satisfies (3.45).

Now let $g:[0,1]\to [0,1]$ be any C^1 smooth function satisfying $g(\frac{1}{4})=0$ and $g(\frac{3}{4})=1$ and consider the family of equations

$$-\gamma x''(\xi) - cx'(\xi) = (1 - g(\rho)) \Big(\beta^{-1} \big(x(\xi - k) - x(\xi) \big) - f \big(x(\xi) \big) \Big)$$

$$+ g(\rho) F \big(x(\xi + r_0), \dots, x(\xi + r_N), \rho^* \big)$$
(3.47)

for $\rho \in [0, 1]$. It is easy to see that this family satisfies the conditions (b1) through (b5), with $q(\rho) = 0$ for all $\rho \in [0, 1]$. We know that at $\rho = \frac{1}{4}$ the equation (3.47) has a connecting solution, namely c = 1, $x = \tanh \xi$. Due to Proposition 3.2, we see that solutions to (3.47) exist in a neighbourhood of $\rho = \frac{1}{4}$ and Theorem 3.10 allows us to extend this continuation to the interval (0, 1). This proves the claim, as at $\rho = \frac{3}{4}$ the system reduces to the specified equation (3.1) with $\rho = \rho^*$.

In case there is no value ρ^* for which $q(\rho^*) = 0$, the following lemma shows that we can choose an arbitrary value $\rho_0 \in V$ and embed the differential difference equation (3.1) with $\rho = \rho_0$ into a new family which does have $q(\rho_*) = 0$ for some ρ^* . We can then apply the same reasoning as in the proof of Lemma 3.11 to the new family to obtain a connecting solution to our original family at $\rho = \rho_0$.

Lemma 3.12 (see [28, Lemma 8.6]). Consider the system

$$-\gamma x''(\xi) - cx'(\xi) = F_0(x(\xi + r_0), \dots, x(\xi + r_N))$$
(3.48)

satisfying the conditions (b1) through (b5) without the parameter ρ . Assume that $q = q_0 \in (-1,1)$ for the quantity in condition (b5). Then there exists a family (3.1), with V = (-1,1) and $q(\rho) = \rho$, satisfying the conditions (b1) through (b5), which reduces to (3.48) at $\rho = q_0$.

We now have all the ingredients to complete the proof of Theorem 3.1.

Proof of Theorem 3.1. One can use Lemma's 3.11 and 3.12 to establish the existence of a solution at some parameter $\rho_* \in V$, after which a global continuation for all $\rho \in V$ of this solution can be constructed using Theorem 3.10 and Proposition 3.2. Uniqueness follows from Lemma 3.8. Here we have assumed V is connected, if not, use this construction for each connected component of V. \square

4 The Algorithm

In this section we present and analyze a numerical method for solving the nonlinear autonomous differential difference equation

$$-\gamma x''(\xi) - cx'(\xi) = F(x(\xi), \overline{x}(\xi)), \tag{4.1}$$

where we have introduced the notation $\overline{\phi}(\xi) = (\phi(\xi + r_1), \phi(\xi + r_2), \dots, \phi(\xi + r_N)) \in \mathbb{R}^N$. As in the previous section, we demand that $\gamma > 0$, $r_i \neq r_j$ if $i \neq j$ and $r_i \neq 0$ for $i = 1 \dots N$, where $N \geq 1$. Throughout this section we will also assume F satisfies the conditions (b1) through (b5) from Section 3.

Following Definition 3.1, a connecting solution to (4.1) is a pair $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ that satisfies (4.1) and has the limits

$$\lim_{\xi \to +\infty} \phi(\xi) = \pm 1. \tag{4.2}$$

Solutions to (4.1) correspond to zeroes of the operator \mathcal{G} defined in (4.3), which in the present notation is given by

$$\mathcal{G}(\phi, c)(\xi) = -\gamma \phi''(\xi) - c\phi'(\xi) - F(\phi(\xi), \overline{\phi}(\xi)). \tag{4.3}$$

The numerical method we use to solve the differential difference equation (4.1) consists of applying a variant of Newton's method to find a zero of the operator \mathcal{G} which satisfies the boundary conditions (4.2). Normally, applying Newton's method to seek a zero of \mathcal{G} would involve an iteration step of the form

$$(\phi_{n+1}, c_{n+1}) = (\phi_n, c_n) - [D_{1,2}\mathcal{G}(\phi_n, c_n)]^{-1}\mathcal{G}(\phi_n, c_n). \tag{4.4}$$

To execute this step one would have to solve the linear differential difference equation

$$D_{1,2}\mathcal{G}(\phi_n, c_n)(\phi_{n+1}, c_{n+1}) = D_{1,2}\mathcal{G}(\phi_n, c_n)(\phi_n, c_n) - \mathcal{G}(\phi_n, c_n). \tag{4.5}$$

Since this is a computationally expensive procedure due to the presence of the shifted arguments [1], we want to reduce their contribution as much as possible. To this end, we fix a relaxation parameter $\mu \in [0,1]$ and introduce the linear operator $D_{1,2}\mathcal{F}^{\mu}: W^{2,\infty} \times \mathbb{R} \to L^{\infty}$, given by

$$D_{1,2}\mathcal{F}^{\mu}(\phi,c)(\psi,b)(\xi) = -\gamma\psi''(\xi) - c\psi'(\xi) - D_1F(\phi,\overline{\phi})\psi(\xi) - \mu D_2F(\phi,\overline{\phi})\overline{\psi}(\xi) - b\phi'(\xi). \tag{4.6}$$

Here $D_1F(x, \overline{x})$ denotes the derivative of F with respect to the first unshifted argument and $D_2F(x, \overline{x})$ denotes the derivative with respect to the shifted arguments. This operator $D_{1,2}\mathcal{F}^{\mu}(\phi, c)$ will play an important role in the variant of Newton's method we employ to solve (4.1). In particular, the iteration step in our method consists of solving the linear differential difference equation

$$D_{1,2}\mathcal{F}^{\mu}(\phi_n, c_n)(\phi_{n+1}, c_{n+1}) = D_{1,2}\mathcal{F}^{\mu}(\phi_n, c_n)(\phi_n, c_n) - \mathcal{G}(\phi_n, c_n). \tag{4.7}$$

We note here that when $\mu = 1$, the iteration step (4.7) is equivalent to the Newton iteration defined in (4.4). However, when $\mu = 0$, (4.7) is just an ordinary differential equation, which can be solved efficiently using standard techniques.

It will be useful to rewrite (4.7) in the form

$$(\phi_{n+1}, c_{n+1}) = (\phi_n, c_n) - [D_{1,2}\mathcal{F}^{\mu}(\phi_n, c_n)]^{-1}\mathcal{G}(\phi_n, c_n). \tag{4.8}$$

At this point it is not yet clear if this iteration step is well-defined. In particular, we will show that for μ close enough to 1, the operator $D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)$ is invertible for all pairs (ϕ_*, c_*) sufficiently close to the solution (ϕ, c) . The main theorem of this section roughly states that the numerical method introduced above converges to a solution of (4.1). In order to make this precise, we need to define what we mean by a point of attraction of the Newton iteration (4.7).

Definition 4.1. A pair $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ is a point of attraction of the Newton iteration (4.7) if there is an open neighbourhood $S \subseteq W_0^{2,\infty} \times \mathbb{R}$, with $(\phi, c) \in S$, such that for any $(\phi_0, c_0) \in S$, the iterates defined by (4.7) all lie in $W_0^{2,\infty} \times \mathbb{R}$ and converge to (ϕ, c) .

Theorem 4.1. Let $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to the nonlinear autonomous differential difference equation (4.1). Then there exists $\epsilon > 0$ such that (ϕ, c) is a point of attraction for the Newton iteration (4.7) for all μ satisfying $|\mu - 1| < \epsilon$.

Theorem 4.1 will be proved in a number of steps. We first prove that the Newton iteration (4.7) is well-defined for appropriate choices of the parameter μ and the initial condition (ϕ_0, c_0). Then we will consider the linearization of (4.8) around the solution (ϕ , c) and prove that the spectral radius of this linearized operator is smaller than one, which will allow us to complete the proof.

The first two lemma's use the fact that $D_{1,2}\mathcal{G}(\phi,c)$ is an isomorphism to show that this also holds for the operator $D_{1,2}\mathcal{F}^{\mu}(\phi_*,c_*)$, for pairs (ϕ_*,c_*) sufficiently close to (ϕ,c) .

Lemma 4.2. Let $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (4.1). Then there exists $\epsilon > 0$ such that $D_{1,2}\mathcal{F}^{\mu}(\phi, c)$ is an isomorphism for all μ satisfying $|\mu - 1| < \epsilon$.

Proof. We start out by noting that $D_{1,2}\mathcal{F}^1(\phi,c) = D_{1,2}\mathcal{G}(\phi,c)$, which is an isomorphism from $W_0^{2,\infty} \times \mathbb{R}$ onto L^{∞} . It follows from [31, Theorem 5.10] that $[D_{1,2}\mathcal{G}(\phi,c)]^{-1}$ is a bounded linear operator. We can thus write $v = \|[D_{1,2}\mathcal{G}(\phi,c)]^{-1}\|$ and since $D_{1,2}\mathcal{G}(\phi,c)$ is a nontrivial operator, $0 < v < \infty$ must hold. Noticing that

$$||[D_{1,2}\mathcal{F}^{\mu_1}(\phi,c)] - [D_{1,2}\mathcal{F}^{\mu_2}(\phi,c)]|| = |\mu_1 - \mu_2| ||D_2F(\phi,\overline{\phi})||$$
(4.9)

and using the fact that $||D_2F(\phi,\overline{\phi})|| < \infty$ as ϕ is bounded, we see that we can choose $\epsilon > 0$ such that

$$||[D_{1,2}\mathcal{F}^{\mu}(\phi,c)] - [D_{1,2}\mathcal{G}(\phi,c)]|| < \frac{1}{2v}$$
(4.10)

whenever $|\mu - 1| < \epsilon$. Now fix $\mu \in (1 - \epsilon, 1 + \epsilon)$ and let I be the identity operator on $W_0^{2,\infty} \times \mathbb{R}$. Since

$$||I - [D_{1,2}\mathcal{G}(\phi, c)]^{-1}[D_{1,2}\mathcal{F}^{\mu}(\phi, c)]||$$

$$= ||[D_{1,2}\mathcal{G}(\phi, c)]^{-1}([D_{1,2}\mathcal{G}(\phi, c)] - [D_{1,2}\mathcal{F}^{\mu}(\phi, c)])|| \le \frac{1}{2n}v = \frac{1}{2} < 1,$$
(4.11)

Neumann's Lemma implies that $[D_{1,2}\mathcal{G}(\phi,c)]^{-1}[D_{1,2}\mathcal{F}^{\mu}(\phi,c)]$ is invertible and hence $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ has a left inverse. Because $D_{1,2}\mathcal{G}(\phi,c)$ is an isomorphism, it has a left and right inverse and so by an analogous argument involving the identity operator on L^{∞} the existence of a right inverse for $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ can be established. This completes the proof that $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ is an isomorphism. \square

For convenience, we define open balls $B_{\psi,b,\delta}$ in $W_0^{2,\infty} \times \mathbb{R}$ given by

$$B_{\psi,b,\delta} = \{ (\phi_*, c_*) \in W^{2,\infty} \times \mathbb{R} \mid ||(\psi, b) - (\phi_*, c_*)|| < \delta \}.$$
 (4.12)

Lemma 4.3. Let $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (4.1). Then there exists $\epsilon > 0$, such that for all $\mu \in \mathbb{R}$ with $|\mu - 1| < \epsilon$, there is an open ball $B = B_{\phi,c,\delta}$, for some $\delta > 0$, with the property that the linear operator $D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)$ is an isomorphism for all $(\phi_*, c_*) \in B$.

Proof. The proof is analogous to the proof of Lemma 4.2. One uses the fact that $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ is invertible and the observation that $\|D_{1,2}\mathcal{F}^{\mu}(\widetilde{\phi},\widetilde{c})\|$ is continuous with respect to $(\widetilde{\phi},\widetilde{c})$ in the norm on $W_0^{2,\infty}\times\mathbb{R}$. To establish this, one needs the local Lipschitz condition (b2) on the derivatives of F, which implies the global Lipschitz continuity of D_1F on compact subsets of \mathbb{R}^{N+1} . Together with the boundedness of all $\phi_*\in W_0^{2,\infty}$, this establishes that for fixed ϕ_* and for all ϕ_{**} with $\|\phi_{**}-\phi_*\|\leq C$, we have $|D_1F(\phi_*,\overline{\phi}_*)(\xi)-D_1F(\phi_{**},\overline{\phi}_{**})(\xi)|\leq D\|\phi_*-\phi_{**}\|$ for some $D<\infty$. With this estimate and a similar one for D_2F , the continuity is easily established.

We remark that Lemma 4.3 guarantees that for μ close enough to 1, there exists $\delta > 0$ such that the Newton iteration step given by (4.7) is well-defined whenever $(\phi_n, c_n) \in B_{\phi,c,\delta}$. We can now define the operator $H^{\mu}: B_{\phi,c,\delta} \to W_0^{2,\infty} \times \mathbb{R}$ given by

$$H^{\mu}(\phi_*, c_*) = (\phi_*, c_*) - [D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)]^{-1}\mathcal{G}(\phi_*, c_*). \tag{4.13}$$

Lemma 4.4. Let $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (4.1). Then there exists $\epsilon > 0$ such that for all μ satisfying $|\mu - 1| < \epsilon$, the operator H^{μ} defined by (4.13) is Frechet differentiable at (ϕ, c) . For these values of μ , the corresponding derivative with respect to ϕ_* and c_* at this point is given by

$$D_{1,2}H^{\mu}(\phi,c) = I - [D_{1,2}\mathcal{F}^{\mu}(\phi,c)]^{-1}D_{1,2}\mathcal{G}(\phi,c). \tag{4.14}$$

Proof. From Lemma 4.2 we know that there exists $\epsilon > 0$ such that for all μ satisfying $|\mu - 1| < \epsilon$, $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ is an isomorphism. From the proof of Lemma 4.2 we also know that for such μ we have $||I - [D_{1,2}\mathcal{G}(\phi,c)]^{-1}D_{1,2}\mathcal{F}^{\mu}(\phi,c)|| < 1$. Now fix μ satisfying $|\mu - 1| < \epsilon$.

Fix $\beta > 0$. We know that G is Frechet-differentiable at (ϕ, c) , hence there exists δ_1 such that

$$\|\mathcal{G}(\phi_*, c_*) - \mathcal{G}(\phi, c) - D_{1,2}\mathcal{G}(\phi, c)[(\phi_*, c_*) - (\phi, c)]\| \le \beta \|(\phi_*, c_*) - (\phi, c)\|$$
(4.15)

for all $(\phi_*, c_*) \in B_{\phi,c,\delta_1}$. From Lemma 4.3 we know that there exists δ_2 such that $D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)$ is an isomorphism for all $(\phi_*, c_*) \in B_{\phi,c,\delta_2}$. In the proof of Lemma 4.3 we have seen that $||D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)||$

is continuous in ϕ_* and c_* . Using this and the continuity of the inverse, we see that there exists $\delta_3 > 0$ such that

$$\|[[D_{1,2}\mathcal{F}^{\mu}(\phi,c)]^{-1} - [D_{1,2}\mathcal{F}^{\mu}(\phi_*,c_*)]^{-1}][D_{1,2}\mathcal{G}(\phi,c)]\| \le \beta \tag{4.16}$$

whenever $\|(\phi, c) - (\phi_*, c_*)\| < \delta_3$. From (4.16) it also follows that when $\|(\phi, c) - (\phi_*, c_*)\| < \delta_3$ we have

$$||[D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)]^{-1}[D_{1,2}\mathcal{G}(\phi, c)]|| \le \beta + ||[D_{1,2}\mathcal{F}^{\mu}(\phi, c)]^{-1}[D_{1,2}\mathcal{G}(\phi, c)]|| = \beta + C$$
(4.17)

for some finite constant C. Using the identity

$$[D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)]^{-1} = [D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)]^{-1}[D_{1,2}\mathcal{G}(\phi, c)][D_{1,2}\mathcal{G}(\phi, c)]^{-1}, \tag{4.18}$$

we see that $\|[D_{1,2}\mathcal{F}^{\mu}(\phi_*, c_*)]^{-1}\| \leq D(\beta + C)$ for some finite constant D, whenever $\|(\phi, c) - (\phi_*, c_*)\| < \delta_3$.

Now choose $\delta = \min(\delta_1, \delta_2, \delta_3)$. Using the fact that $(\phi, c) = H^{\mu}(\phi, c)$ we obtain for all $(\phi_*, c_*) \in B_{\phi, c, \delta}$

$$\begin{aligned} & \|H^{\mu}(\phi_{*}, c_{*}) - H^{\mu}(\phi, c) - [I - [D_{1,2}\mathcal{F}^{\mu}(\phi, c)]^{-1}D_{1,2}\mathcal{G}(\phi, c)][(\phi_{*}, c_{*}) - (\phi, c)] \| \\ &= \|[D_{1,2}\mathcal{F}^{\mu}(\phi, c)]^{-1}D_{1,2}\mathcal{G}(\phi, c)[(\phi_{*}, c_{*}) - (\phi, c)] - [D_{1,2}\mathcal{F}^{\mu}(\phi_{*}, c_{*})]^{-1}\mathcal{G}(\phi_{*}, c_{*}) \| \\ &\leq \|-[D_{1,2}\mathcal{F}^{\mu}(\phi_{*}, c_{*})]^{-1}[\mathcal{G}(\phi_{*}, c_{*}) - \mathcal{G}(\phi, c) - D_{1,2}\mathcal{G}(\phi, c)[(\phi_{*}, c_{*}) - (\phi, c)]] \| \\ &+ \|[[D_{1,2}\mathcal{F}^{\mu}(\phi, c)]^{-1} - [D_{1,2}\mathcal{F}^{\mu}(\phi_{*}, c_{*})]^{-1}][D_{1,2}\mathcal{G}(\phi, c)[(\phi_{*}, c_{*}) - (\phi, c)]] \| \\ &\leq (D(\beta + C)\beta + \beta) \|(\phi_{*}, c_{*}) - (\phi, c)\|. \end{aligned}$$

$$(4.19)$$

This completes the proof that H^{μ} is Frechet differentiable.

We can now use the fact that $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ is an isomorphism to establish the crucial fact that the spectral radius of the linear operator $D_{1,2}H^{\mu}(\phi,c)$ is less than one.

Lemma 4.5. Let $(\phi, c) \in W_0^{2,\infty} \times \mathbb{R}$ be a connecting solution to (4.1). Let $\hat{\sigma}^{\mu}$ denote the spectral radius of $D_{1,2}H^{\mu}(\phi, c)$. Then there exists $\epsilon > 0$, such that for all μ satisfying $|\mu - 1| < \epsilon$, we have $\hat{\sigma}^{\mu} < 1$.

Proof. Writing out the eigenvalue problem for $D_{1,2}H^{\mu}(\phi,c)$, we obtain the equation

$$(1-\mu)[D_{1,2}\mathcal{F}^{\mu}(\phi,c)]^{-1}[D_2F(\phi,\overline{\phi})\overline{\psi}] - \lambda(\psi,b) = (0,0), \tag{4.20}$$

where λ is the eigenvalue and (ψ, b) are the eigenfunctions. After applying $D_{1,2}\mathcal{F}^{\mu}(\phi, c)$ and using the explicit form of $D_{1,2}\mathcal{F}^{\mu}$ this is equivalent to

$$-D_{1,2}\mathcal{F}^{\tilde{\mu}(\lambda)}(\phi,c)(\psi,b) = 0, \tag{4.21}$$

in which

$$\tilde{\mu}(\lambda) = \mu + \frac{1 - \mu}{\lambda}.\tag{4.22}$$

We know from Lemma 4.2 that there exists $\delta > 0$ such that $D_{1,2}\mathcal{F}^{\mu}(\phi,c)$ is an isomorphism for all μ satisfying $|\mu - 1| < \delta$. If we now choose $\epsilon = \frac{\delta}{2}$, we see that for all μ satisfying $|\mu - 1| < \epsilon$ and for all $|\lambda| \ge 1$,

$$|\tilde{\mu}(\lambda) - 1| \le \frac{\delta}{2} + \frac{\delta}{2} |\lambda|^{-1} \le \delta. \tag{4.23}$$

In particular, this means that for these μ and λ equation (4.21) has only the zero solution, as $D_{1,2}\mathcal{F}^{\tilde{\mu}(\lambda)}(\phi,c)$ is an isomorphism. Thus for these μ there cannot be any eigenvalues λ with $|\lambda| \geq 1$, proving that $\hat{\sigma}^{\mu} < 1$.

We are now ready to complete the proof of Theorem 4.1.

Proof of Theorem 4.1. Fix $\beta > 0$ such that for all μ satisfying $|\mu - 1| < \beta$, we have that the operator H^{μ} is well-defined in a neighbourhood of (ϕ, c) and Frechet differentiable at (ϕ, c) , together with the inequality $\hat{\sigma}^{\mu} < 1$, where $\hat{\sigma}^{\mu}$ is the spectral radius of $D_{1,2}H^{\mu}(\phi, c)$. Now fix μ satisfying $|\mu - 1| < \beta$, write $H = H^{\mu}$ and $\hat{\sigma} = \hat{\sigma}^{\mu}$ and choose $\epsilon > 0$ such that $\hat{\sigma} + \epsilon < 1$. Let H^{p} be the p-fold iterate of H. Since H is Frechet-differentiable at (ϕ, c) , so is H^{p} . From the chain rule it follows that $D_{1,2}H^{p}(\phi, c) = [D_{1,2}H(\phi, c)]^{p}$.

From the Gelfand and Mazur formula [32, Theorem 10.13] for the spectral radius $\hat{\sigma}$, it follows that we may choose p such that

$$||[D_{1,2}H(\phi,c)]^p|| \le (\hat{\sigma} + \epsilon)^p,$$

$$(\hat{\sigma} + \epsilon)^p + \epsilon < 1.$$
(4.24)

Let s be an integer. From the Frechet-differentiability of H^s we know that there exists $\delta > 0$, such that for all $(\phi_*, c_*) \in B_{\phi, c, \delta}$ and for all $1 \le s \le p$,

$$||H^{s}(\phi_{*}, c_{*}) - H^{s}(\phi, c) - [D_{1,2}H(\phi, c)]^{s}[(\phi_{*}, c_{*}) - (\phi, c)]|| \le \epsilon ||(\phi_{*}, c_{*}) - (\phi, c)||.$$

$$(4.25)$$

With this we can compute

$$||H^{s}(\phi_{*}, c_{*}) - (\phi, c)|| \leq ||H^{s}(\phi_{*}, c_{*}) - H^{s}(\phi, c) - [D_{1,2}H(\phi, c)]^{s}[(\phi_{*}, c_{*}) - (\phi, c)]|| + ||[D_{1,2}H(\phi, c)]^{s}|| ||(\phi_{*}, c_{*}) - (\phi, c)|| \leq (||[D_{1,2}H(\phi, c)]^{s}|| + \epsilon) ||(\phi_{*}, c_{*}) - (\phi, c)||.$$

$$(4.26)$$

Writing

$$w = \max\left(\epsilon, \max\left\{\|[D_{1,2}H(\phi, c)]^s\| \mid s = 1\dots p\right\}\right),\tag{4.27}$$

we see that we can ensure $H^s(\phi_0, c_0) \in B_{\phi, c, \delta_*}$ for $s = 1 \dots p$ by choosing $(\phi_0, c_0) \in B_{\phi, c, \delta_*/2w}$. For s = p equation (4.26) reduces to

$$||H^{p}(\phi_{*}, c_{*}) - (\phi, c)|| \le [(\hat{\sigma} + \epsilon)^{p} + \epsilon] ||(\phi_{*}, c_{*}) - (\phi, c)||. \tag{4.28}$$

Combining everything, we see that by choosing $(\phi_0, c_0) \in B_{\phi,c,\delta/2w}$ all the Newton iterates lie in the ball $B_{\phi,c,\delta}$. Now choosing $\delta > 0$ so small that H is well-defined on $B_{\phi,c,\delta}$, we see that the Newton process is well-defined and satisfies

$$\lim_{n \to \infty} \|(\phi_n, c_n) - (\phi, c)\| \le \lim_{n \to \infty} (2w) \left((\hat{\sigma} + \epsilon)^p + \epsilon \right)^{\left\lfloor \frac{n}{p} \right\rfloor} \|(\phi_0, c_0) - (\phi, c)\| = 0. \tag{4.29}$$

This concludes the proof of the theorem.

Remark 4.1. It is not clear if Theorem 4.1 holds for $\mu = 0$. Setting $\mu = 0$ in the Newton iteration step (4.7) is easily seen to be equivalent to making the approximation $\overline{\phi}_{n+1} = \overline{\phi}_n$. Intuitively, this approximation should become increasingly accurate as the iterates ϕ_n converge to the solution of (4.1). In addition, the equations (4.9) and (4.10) from the proof of Lemma 4.2 give us information about the values of ϵ which satisfy the claim in Theorem 4.1. In particular, smaller values of $\|D_2F\|$ give us larger possible values for ϵ . Referring back to (1.6), we see there that $\|D_2F\|$ is proportional to the parameter α . Since we are interested in solutions to (1.6) far from the continuous limit, i.e., for small values of the parameter α , these observations lead us to believe we can take $\mu = 0$ in many cases of interest. See Section 5 for a further discussion and some numerical examples.

5 Examples

In this section we present some numerical results obtained by our algorithm in order to illustrate some of the key phenomena encountered in the qualitative study of lattice differential equations, together with some of the technical difficulties involved with the numerical computation of solutions to such equations. We note here that all the Newton iteration steps (4.7) which were executed in order to obtain the results in this section were performed with $\mu = 0$.

In the literature it has by now become somewhat classic to study travelling wave solutions to the spatially discretized reaction diffusion equation (1.2). The simplest corresponding differential difference equation is given by

$$-c\phi'(\xi) = \alpha(\phi(\xi+1) + \phi(\xi-1) - 2\phi(\xi)) - (\phi(\xi)^2 - 1)(\phi(\xi) - \rho), \tag{5.1}$$

where $\alpha > 0$ and $\rho \in (-1,1)$ is a detuning parameter. It has been widely studied both numerically and theoretically [1, 5, 10, 14, 16, 24, 36, 37]. The relative simplicity of (5.1) and the fact that solutions exhibit many of the interesting features mentioned in the introduction ensure that this equation is an ideal test problem for any differential difference equation solver.

In [20] (5.1) was solved numerically by adding a small diffusion term $-\gamma\phi''(\xi)$ to the left-hand side of (5.1) and our results were compared to previously established solutions in [1, 16]. In particular, we remark that our implementation allows us to choose $\gamma = 3 \times 10^{-10}$, while up to now the smallest possible choice for γ was given by $\gamma = 10^{-6}$ [1]. The phenomenon of propagation failure is clearly visible from the results for $\alpha = 0.1$ and the corresponding wave profiles already reach their limiting forms at $\gamma = 10^{-5}$.

We wish to empasize here that, in contrast to the presentation in [16], the formulation of the algorithm given in the previous section allows us to consider differential difference equations which involve a nonlinear mixing of shifted terms and ordinary terms. In this section we illustrate this feature by numerically studying the differential difference equation

$$-\gamma \phi''(\xi) - c\phi'(\xi) = \alpha \tanh(\phi(\xi + 1) + \phi(\xi - 1) - 2\phi(\xi)) - f(\phi(\xi), \rho).$$
 (5.2)

Here $\gamma, \alpha > 0$ are two positive parameters and f is the cubic nonlinearity given by

$$f(x,\rho) = (x^2 - 1)(x - \rho), \tag{5.3}$$

where $\rho \in (-1,1)$ is a continuation parameter. The solutions of (5.2) were required to satisfy the limits

$$\lim_{\xi \to -\infty} \phi(\xi) = -1, \quad \lim_{\xi \to \infty} \phi(\xi) = 1 \tag{5.4}$$

and were normalized to have $\phi(0) = 0$. Equations similar to (5.2) play an important role when studying Glauber type Ising models [12] in material science.

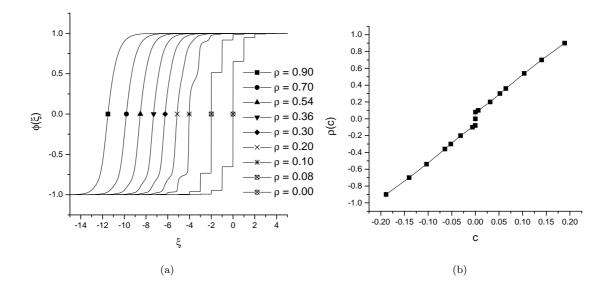


Fig. 2: In (a) the waveprofiles $\phi(\xi)$ have been plotted for solutions to the differential difference equation (5.2) with $\gamma = 10^{-6}$ and $\alpha = 0.1$, at different values of the detuning parameter ρ . For presentation purposes the curves have been shifted by different amounts along the ξ -axis. In (b) the $\rho(c)$ relation has been plotted, i.e., for each value of the detuning parameter ρ the corresponding wavespeed c is given. The solid dots represent the wavespeeds corresponding to the curves in (a), which have been continued to $\rho < 0$, using the observation that $\psi(\xi) = -\phi(-\xi)$ is a connecting solution with wavespeed c. From (b) it is easily seen that there exists a nontrivial interval of ρ in which $c \sim 0$, hence propagation failure occurs.

It is easy to verify that the family (5.2) satisfies all the requirements (b1) through (b5). Also note that if $\phi(\xi)$ is a solution to the problem (5.2) satisfying the limits (5.4) at some parameter $\rho = \rho_0$ with wavespeed $c = c_0$, then $\psi(\xi) = -\phi(-\xi)$ is a solution to the same problem with $\rho = -\rho_0$ and wavespeed $c = -c_0$ and also satisfies the limits (5.4).

The phenomenon of propagation failure has been studied extensively in [28]. In particular, in Corollary 2.5 of [28] it is shown that for our family (5.2) with $\gamma = 0$, there exist quantities $-1 \le \rho_- \le \rho_+ \le 1$, such that (5.2) only has connecting solutions with wavespeed c = 0 for $\rho_- \le \rho \le \rho_+$. It may happen that $\rho_- < \rho_+$, that is, that there is a nontrivial interval of the detuning parameter ρ for which the wavespeed vanishes. In this region one generally expects the solutions to become discontinuous. However, since all the numerical computations were performed with $\gamma > 0$, which

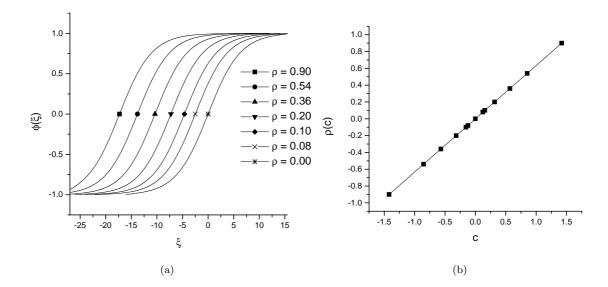


Fig. 3: In (a) the waveprofiles $\phi(\xi)$ have been plotted for solutions to (5.2) with $\gamma = 10^{-4}$ and $\alpha = 5$, at different values of the detuning parameter ρ . The wavespeeds for these solutions are given in (b). The calculations to obtain the solution curves in this figure were performed on the finite interval [-20, 20]. Notice that in (b) there is no nontrivial interval of ρ for which c = 0. Indeed, the solution curves in (a) remain continuous as $\rho \to 0$.

forces the solutions to remain continuous, it is a priori not clear if one can accurately reproduce the solution profiles at $\gamma = 0$ and thus actually uncover the propagation failure. The essential tool here is Theorem 3.10, which establishes that if we have a sequence of solutions $P_n(\xi)$ to (3.1) with $\gamma = \gamma_n$, where $\gamma_n \to 0$, a subsequence of the functions P_n will convergence to a solution at $\gamma = 0$. Ideally, this convergence should occur at a value for the parameter γ which can be handled numerically and the solution curves should remain computationally stable below this value. This was the case for the solutions to (5.1) calculated in [20] and we show here that the same property holds for the problem (5.2) currently under investigation.

In Figure 2 the calculated solutions to (5.2) are presented, together with their wavespeeds. One sees clearly from Figure 2(b) that there is a nontrivial interval of the detuning parameter ρ for which the wavespeed c vanishes. Looking at Figure 2(a), one sees that the solutions for these values of ρ exhibit step-like behaviour. In the calculations we used $\gamma = 10^{-6}$, which thus indicates that for γ small enough, one can be confident that the effects of propagation failure will be observed and

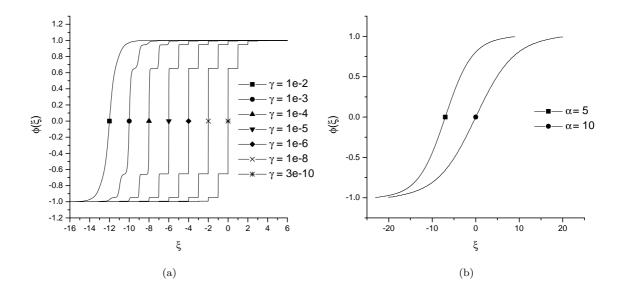


Fig. 4: In (a) waveprofiles $y(\xi)$ for solutions to (5.2) at different values of γ are given, for fixed $\rho = 0$ and $\alpha = 0.1$, demonstrating the robust convergence in the $\gamma \to 0$ limit and showing that already at $\gamma = 10^{-5}$ the waveform has attained its limiting profile. In (b) solutions $y(\xi)$ to (5.2) at $\alpha = 5$ and $\alpha = 10$ in the critical case $\rho = 0$ are given. The parameter γ was fixed at 10^{-4} .

accurate predictions can be made about the parameter values at which it will occur. Propagation failure does not occur at each value of α , as the $\rho(c)$ curve in Figure 3(b) shows. Notice that the solutions in Figure 3(a) indeed remain smooth as $\rho \to 0$. We remark here that the wavespeed necessarily satisfies c = 0 when $\rho = 0$, but it is clear that for this specific system (5.2), the solutions only exhibit discontinuous behaviour when the wavespeed vanishes for a nontrivial interval of the detuning parameter ρ .

In Figure 4(a) the solution curves to (5.2) have been plotted for a number of different values of γ , ranging from $\gamma = 10^{-2}$ to $\gamma = 3 \times 10^{-10}$. The transition from smooth to steplike solutions is clearly visible and already occurs at $\gamma \approx 10^{-3}$. Notice that the solution curves remain stable for $\gamma = 10^{-5}$ to $\gamma = 3 \times 10^{-10}$, while the curve for $\gamma = 10^{-4}$ does not differ too much. One sees here that in this example computations with $\gamma \sim 10^{-5}$ will provide an excellent approximation to the actual solutions with $\gamma = 0$. In particular, the computations indicate that the discontinuous behaviour due to propagation failure, which occurs at $\gamma = 0$ and c = 0, is already visible at $\gamma = 10^{-5}$. Indeed, upon recalculation of the curves in Figure 2 using $\gamma = 10^{-8}$, the results were observed to remain exactly

the same.

When we take $\mu = 0$ in the Newton iteration (4.7), we are neglecting the presence of the shifted terms D_2F . In particular, referring to (4.9) in the proof of Lemma 4.2, one expects that when the norm of the shifted term D_2F becomes large, problems will arise with the invertibility of the operator $D_{1,2}\mathcal{F}^{\mu}$ and hence with the convergence of the algorithm. In our case, the importance of the shifted term is given by the parameter α . For large α , the hyperbolic tangent term in (5.2) becomes increasingly important. Nevertheless, by using a suitable continuation scheme, we are able to obtain solutions to (5.2) for $\alpha = 5$ and $\alpha = 10$ at $\gamma = 10^{-4}$ and $\rho = 0$. These solutions have been plotted in Figure 4(b). At these levels of α the shifted term has become the dominant term. If one wishes to increase α even further, it no longer suffices to take $\mu = 0$ in (4.7). It is however quite satisfactory that this choice for μ can be used for practical purposes up to these levels of α , which are already far from the interesting case $\alpha \approx 0.1$.

6 Extensions

Although all the theory developed in this paper applies only to one dimensional families (1.1) that satisfy the conditions (b1) through (b5), it turns out that the application range of the numerical method is much broader. In addition, interesting models exist which lead to differential difference equations that violate the above assumptions. To gain some insight into these issues, we numerically study two important systems that are not covered by the theory developed in this paper, which both give rise to novel dynamical behaviour.

6.1 Ising models

In this subsection we numerically study the differential difference equation given by

$$-\gamma\phi''(\xi) - c\phi'(\xi) = \alpha\left(-\frac{1}{4}\phi(\xi - 2) + \phi(\xi - 1) + \phi(\xi + 1) - \frac{1}{4}\phi(\xi + 2) - \frac{3}{2}\phi(\xi)\right) - f(\phi(\xi), \rho), (6.1)$$

where f again denotes the bistable cubic nonlinearity $f(x,\rho)=(x^2-1)(x-\rho)$ for some parameter $\rho \in (-1,1)$ and $\alpha > 0$ is a strictly positive parameter. We again impose the limits $\phi(\pm \infty)=\pm 1$ and the normalization condition $\phi(0)=0$ and again take $\mu=0$ when performing the iteration steps

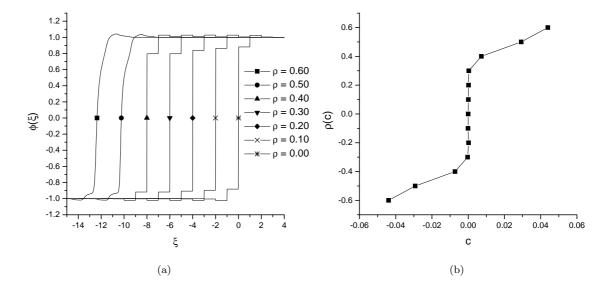


Fig. 5: In (a) the waveprofiles $\phi(\xi)$ have been plotted for solutions to (6.1) with $\gamma = 10^{-6}$ and $\alpha = 0.042$, at different values of the detuning parameter ρ . The corresponding wavespeeds for these solutions are given in (b).

(4.7). The interesting feature in (6.1) is that the coefficients in front of the shifted terms $\phi(\xi \pm 2)$ are now negative, which implies that this equation does not satisfy the assumption (b3) introduced in Section 3. In particular, we no longer have any guarantee that (6.1) in fact has a solution or that the numerical method will be able to find it.

Equation (6.1) with $\gamma = 0$ is an example of a class of differential difference equations which was proposed in [4] to provide a discrete convolution model for Ising-like phase transitions. The equation was derived by considering groups of atoms arranged on a lattice and computing the gradient flow of a Helmholtz free energy functional. This energy functional takes into account interactions within each group of atoms together with interactions between groups, thus incorporating both local and non-local effects into the model. Due to the nature of the physical forces involved, the long-range interaction coefficients can be both positive and negative.

Unnormalized solutions to (6.1) with $\gamma=0,\ c=0$, fixed ρ and sufficiently small $\alpha>0$ were analyzed in [4]. In particular, for each sufficiently small $\alpha>0$ it was shown that there exist three intervals $I_j(\alpha)$ for $1 \leq j \leq 3$, such that for any two disjoint sets $S_1, S_2 \subset \mathbb{Z}$, there exists a unique (unnormalized) solution u to (6.1) that satisfies $u(x) \in I_i$ whenever $\lfloor x \rfloor \in S_i$, for all $1 \leq i \leq 3$. Here

we have defined $S_3 = \mathbb{Z} \setminus (S_1 \cup S_2)$. We remark here that $-1 \in \text{int}(I_1)$ and $1 \in \text{int}(I_2)$. From this it is clear that the set of solutions to (6.1) with $\gamma = c = 0$ has a rich structure.

In Figure 5 the results of an application of the numerical method to (6.1) with $\gamma = 10^{-6}$ and $\alpha = 0.042$ are displayed. The transition from smooth solution curves to discontinuous step functions as ρ approaches the critical value $\rho = 0$ is clearly illustrated. Notice that in contrast to the results from the previous section, the solution curves are no longer monotonic and in addition are no longer restricted to the interval [-1,1]. The values taken by the step functions in Figure 5 are in agreement with the predictions from [4] and these results again illustrate that the algorithm is robust enough to be able to uncover some of the behaviour at $\gamma = 0$.

6.2 Higher Dimensional Systems

Up to now all the theory has been developed for scalar differential difference equations of the form (3.1). The question of course immediately arises if the results can be extended to higher dimensional systems and if the numerical method is able to handle them as well. In this subsection we briefly discuss some of the issues involved, using a bistable reaction-diffusion equation on a one dimensional lattice with spatially varying diffusion coefficients as an example. Specifically, we will study the system

$$\dot{u}_j(t) = \alpha_j \left(u_{j+1}(t) + u_{j-1}(t) - 2u_j(t) \right) - \left(u_j^2(t) - 1 \right) \left(u_j(t) - \rho \right), \quad j \in \mathbb{Z}, \tag{6.2}$$

where $\rho \in (-1,1)$ is a detuning parameter and the coefficients α_j are periodic with period two, i.e., we have $\alpha_{j+2} = \alpha_j$ for all $j \in \mathbb{Z}$.

Lattice differential equations of the form (6.2) arise naturally when modelling diffusion processes in discrete systems which are spatially periodic. As a specific biological example we mention a model that describes the behaviour of nerve fibers by employing an electrical circuit model for the excitable fiber membrane [23, Sec 9.3]. One considers myelinated nerve fibers that have periodic gaps, called nodes, in their coating. Assuming a one dimensional grid of nodes and writing V_j for the voltage at node j, one derives the equations [23]

$$p(C\dot{V}_j + I_{\text{ion}}(V_j)) = \frac{1}{\mu_j LR} (V_{j+1} + V_{j-1} - 2V_j), \quad j \in \mathbb{Z}.$$
(6.3)

Here p is the perimeter length of the fibre, C is the capacitance, L is the length of myelin sheath

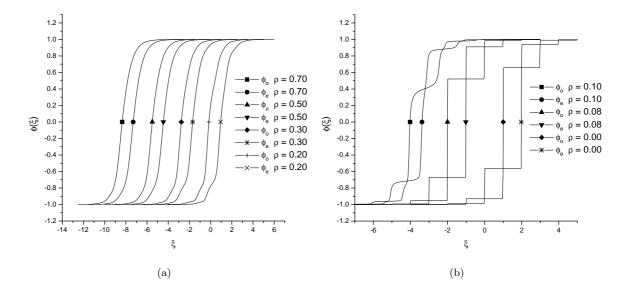


Fig. 6: Waveprofiles $\phi_o(\xi)$ and $\phi_e(\xi)$ have been plotted for solutions to (6.4) with $\alpha_o = 1.5$, $\alpha_e = 1.7$ and $\gamma = 10^{-5}$. In addition to the global shift for different values of ρ , the curves for ϕ_e in (a) have been shifted by 1 along the ξ -axis relative to their accompanying ϕ_o curves. This additional shift has not been applied to the curves in (b).

between nodes, R is the resistance per unit of length and μ_j is the length of node j. Allowing the node length μ_j to vary periodically among nodes and remarking that a cubic nonlinearity is a natural form for the ionic current $I_{\text{ion}}(V)$, one sees that (6.3) transforms into a system of the form (6.2).

As in previous sections, we numerically analyze the system (6.2) by adding a small artificial diffusion term and looking for travelling wave solutions. In particular, the points on the lattice are split into two groups, called even and odd, which admit their own waveforms ϕ_e , ϕ_o and diffusion coefficients α_e , α_o . Substituting the travelling wave anszatz $u_{2k}(t) = \phi_e(2k - ct)$ and $u_{2k+1} = \phi_o(2k+1-ct)$ into (6.2), we arrive at the two dimensional differential difference equation

$$\begin{cases}
-\gamma \phi_o''(\xi) - c\phi_o'(\xi) = \alpha_o \left(\phi_e(\xi+1) + \phi_e(\xi-1) - 2\phi_o(\xi)\right) - 15\left(\phi_o^2(\xi) - 1\right)\left(\phi_o(\xi) - \rho\right), \\
-\gamma \phi_e''(\xi) - c\phi_e'(\xi) = \alpha_e \left(\phi_o(\xi+1) + \phi_o(\xi-1) - 2\phi_e(\xi)\right) - 15\left(\phi_e^2(\xi) - 1\right)\left(\phi_e(\xi) - \rho\right).
\end{cases} (6.4)$$

In addition, we impose the asymptotic limits $\phi_o(\pm \infty) = \pm 1$, $\phi_e(\pm \infty) = \pm 1$ and introduce the phase condition $\phi_o(0) = 0$ in order to control the translational invariance of (6.4).

In contrast to previous sections, it was necessary to take $\mu = 1$ when performing the Newton iterations (4.7) needed to numerically solve (6.4). The results can be found in Figure 6, where

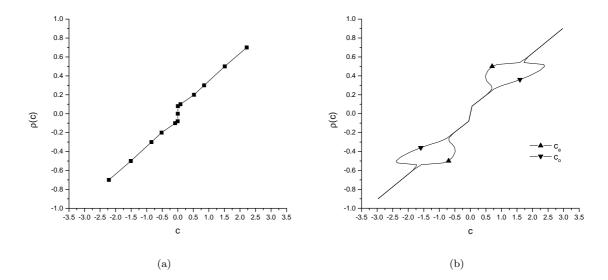


Fig. 7: In (a) the wavespeed plot for the solutions to (6.4) with $\alpha_o = 1.5$, $\alpha_e = 1.7$ and $\gamma = 10^{-5}$ is given. Notice the nontrivial interval of the detuning parameter ρ for which c = 0, indicating that propagation failure occurs for the periodic diffusion problem (6.2). In (b) the wavespeed plot for the constant diffusion system (6.5) with $\alpha = 1.6$ and $\gamma = 10^{-5}$ is given. Notice the existence of two regions for which $c_e \neq c_o$. We call these regions period two bifurcation regions. The presence of these regions demonstrates that, unlike one dimensional systems, higher dimensional systems do not necessarily have unique solutions.

solution curves to (6.4) with $\alpha_o = 1.5$, $\alpha_e = 1.7$ and $\gamma = 10^{-5}$ have been plotted for various values of the detuning parameter ρ . The corresponding wavespeeds can be found in Figure 7(a). It is clear from the latter wavespeed plot and the steplike behaviour exhibited in Figure 6(b) that propagation failure can occur for the discrete periodic diffusion system (6.2). We also mention the interesting fact that as the norm of the detuning parameter ρ increases, the two waveprofiles ϕ_e and ϕ_o become increasingly alike, indicating that the significance of the diffusion term in (6.4) decreases as $|\rho| \to 1$.

At the moment it is unclear if we have existence and uniqueness of solutions to equations of the form (6.4) and if the convergence theory established in this paper for the Newton iteration (4.7) continues to hold. Some of the arguments used to derive the current results are strictly one dimensional in nature and do not generalize trivially to higher dimensions. It will be a topic of future research to address these issues, but for the moment we finish by numerically illustrating that extending the theory to higher dimensions is not simply an exercise in bookkeeping.

Note that when $\alpha_o = \alpha_e$, (6.4) is guaranteed to have at least one solution. This can be seen by choosing $\phi_o = \phi_e$ and applying Theorem 3.1 to the resulting equation. However, in [15, 20] the two dimensional system

$$\begin{cases}
-\gamma \phi_o''(\xi) - c_o \phi_o'(\xi) = \alpha \left(\phi_e(\xi + 1) + \phi_e(\xi - 1) - 2\phi_o(\xi) \right) - 15 \left(\phi_o^2(\xi) - 1 \right) \left(\phi_o(\xi) - \rho \right), \\
-\gamma \phi_e''(\xi) - c_e \phi_e'(\xi) = \alpha \left(\phi_o(\xi + 1) + \phi_o(\xi - 1) - 2\phi_e(\xi) \right) - 15 \left(\phi_e^2(\xi) - 1 \right) \left(\phi_e(\xi) - \rho \right).
\end{cases} (6.5)$$

was analyzed with the boundary conditions $\phi_*(\pm \infty) = \pm 1$ and $\phi_*(0) = 0$ for * = o, e. A corresponding wavespeed plot can be found in Figure 7(b) and the interesting feature is the presence of solutions with $c_o \neq c_e$, indicating that for the two dimensional system (6.5) uniqueness of solutions is lost.

A Proof of Theorem 2.5

The aim of this section is to provide some basic results on the class of scalar differential difference equations encountered when studying (1.1) and to use these results to prove Theorem 2.5. We will mainly be concerned with the subclass of linear equations (2.1) that arises when linearizing (1.1) around solutions. However, we shall also provide a number of comparison principles for solutions to the nonlinear equation (1.1) which can directly be applied to the linear equations mentioned above.

The first result gives conditions under which (2.2) admits no positive solutions which decay superexponentially. This is especially useful in combination with Proposition 2.2, as in the absence of superexponentially decaying solutions this Proposition allows us to obtain asymptotic descriptions of the solutions to (2.2).

Lemma A.1. Consider the homogeneous equation (2.2) and let $x: J^{\#} \to \mathbb{R}$ be a solution to this equation on $J = [\tau, \infty)$ for some $\tau \in \mathbb{R}$. Suppose that Assumption 2.1 holds, possibly with $\alpha_j = 0$ for one or more $1 \le j \le N$. Assume further that $x(\xi) \ge 0$ for all $\xi \in J^{\#}$, but that there does not exist an R > 0 such that $x(\xi) = 0$ for all $\xi \ge R$. Then x does not decay superexponentially. The analogous result for $J = (-\infty, \tau]$ also holds.

Proof. Without loss we shall also assume $J = [\tau, \infty)$, as the case of $J = (-\infty, \tau]$ can be treated by

a change of variables $\xi \to -\xi$, which does not change the sign of γ . For convenience, we introduce the quantity $\widetilde{\alpha}_0 = \min(\alpha_0, \frac{c^2}{4\gamma} - \epsilon)$, where $\epsilon > 0$ is an arbitrary number.

We start out by noting that we can rescale equation (2.6) by defining $y(\xi) = e^{\lambda \xi} x(\xi)$, where λ can be chosen appropriately. It is easy to see that $y(\xi)$ satisfies the following differential difference equation

$$y''(\xi) = (2\lambda - \frac{c}{\gamma})y'(\xi) - \lambda(\lambda - \frac{c}{\gamma})y(\xi) - \frac{1}{\gamma} \sum_{i=0}^{N} A_{j}(\xi)e^{-\lambda r_{j}}y(\xi + r_{j}). \tag{A.1}$$

Since $y(\xi) \geq 0$ for all $\xi \in J^{\#}$, we have the inequality

$$y''(\xi) \le (2\lambda - \frac{c}{\gamma})y'(\xi) + \left(-\lambda(\lambda - \frac{c}{\gamma}) - \frac{\widetilde{\alpha}_0}{\gamma}\right)y(\xi). \tag{A.2}$$

Now choosing $\lambda = \frac{c}{2\gamma}$ we obtain

$$y''(\xi) \le By(\xi), \quad \xi \in J, \tag{A.3}$$

in which $B = \frac{c^2}{4\gamma^2} - \frac{\tilde{\alpha}_0}{\gamma} > 0$. Using a standard argument for ordinary differential equations which can be found in [20, Lemma A.1], one sees that for arbitrary $\xi_0 \in J$,

$$y(\xi) \le C_1 e^{\sqrt{B}(\xi - \xi_0)} + C_2 e^{-\sqrt{B}(\xi - \xi_0)}$$
 (A.4)

holds for all $\xi \geq \xi_0$. The coefficients C_1 and C_2 in this expression are given by

$$C_{1} = \frac{1}{2\sqrt{B}} \left(y'(\xi_{0}) + \sqrt{B}y(\xi_{0}) \right),$$

$$C_{2} = \frac{1}{2\sqrt{B}} \left(-y'(\xi_{0}) + \sqrt{B}y(\xi_{0}) \right).$$
(A.5)

From the nonnegativity of $y(\xi)$ we see that we must have $C_1 \geq 0$, as otherwise (A.4) would imply that $y(\xi) < 0$ for sufficiently large ξ . From this we conclude

$$y'(\xi_0) \ge -\sqrt{B}y(\xi_0), \quad \xi_0 \in J,$$
 (A.6)

which immediately implies that $y(\xi)$ and hence $x(\xi)$ cannot have superexponential decay.

The following lemma will be crucial to establish comparison principles for solutions to the non-linear equation (1.1). It can be easily derived by employing the scaling argument introduced in the proof of Lemma A.1.

Lemma A.2. Let $x:J^{\#}\to\mathbb{R}$ be a solution to (2.1) on $J=[\tau,\infty)$ for some $\tau\in\mathbb{R}$ and suppose that Assumption 2.1 holds, possibly with $\alpha_j=0$ for one or more $1\leq j\leq N$. Assume further that $x(\xi)\geq 0$ for all $\xi\in J^{\#}$. Then if $x(\xi_0)=0$ for some $\xi_0\in J$, we have $x(\xi)=0$ for all $\xi\geq \xi_0$.

We now restrict ourselves to constant coefficient equations

$$-\gamma x''(\xi) - cx'(\xi) - L_0(x_{\xi}) = 0 \tag{A.7}$$

that satisfy Assumption 2.1. Our goal will be to obtain detailed information about the eigenvalues of such systems. This will allow us to give precise asymptotic descriptions of solutions to the nonautomatous linear equation (2.6) and to provide conditions for which (A.7) is hyperbolic. To this end, we introduce the quantity

$$A_{\Sigma} = -\Delta_{c,\gamma,L_0}(0) = \sum_{j=0}^{N} A_{j,0},$$
(A.8)

associated to the constant coefficient operator L_0 . The following lemma relates the existence of complex eigenvalues of (A.7) to the sign of the characteristic function $\Delta_{c,\gamma,L_0}(s)$ for real values of s.

Lemma A.3. Consider the constant coefficient equation (A.7), suppose that Assumption 2.1 holds and in addition assume that $A_{\Sigma} < 0$. Consider an arbitrary $a \in \mathbb{R}$. If $\Delta_{c,\gamma,L_0}(a) \geq 0$, then there do not exist any eigenvalues $\lambda \in \mathbb{C}$ such that $\operatorname{Re} \lambda = a$ except possibly $\lambda = a$ itself.

Proof. Note that $A_{0,0} < 0$, since $A_{\Sigma} < 0$ and $A_{j,0} > 0$ for $1 \le j \le N$. Writing $\lambda = a + i\eta$ with $a, \eta \in \mathbb{R}$, we compute

$$\begin{aligned} \left| c\lambda + \gamma\lambda^2 + A_{0,0} \right|^2 &= \left| ca + \gamma a^2 - \gamma \eta^2 + A_{0,0} + i(2a\gamma\eta + c\eta) \right|^2 \\ &= \left| ca + \gamma a^2 + A_{0,0} \right|^2 + \eta^2 (\eta^2 \gamma^2 + 2a\gamma c + 2a^2 \gamma^2 + c^2 - 2\gamma A_{0,0}) \\ &= \left| ca + \gamma a^2 + A_{0,0} \right|^2 + \eta^2 p(a), \end{aligned}$$

where p is a second degree polynomial. It is elementary to see that

$$p(a) \ge \frac{1}{2}c^2 + \eta^2\gamma^2 - 2\gamma A_0 \ge \eta^2\gamma^2 \ge 0.$$

We thus have

$$|c\lambda + \gamma\lambda^2 + A_{0,0}| \ge |ca + \gamma a^2 + A_{0,0}|,$$
 (A.9)

with equality if and only if $\lambda = a$.

Now suppose that $\lambda = a + i\eta$ satisfies $\Delta_{c,\gamma,L_0}(\lambda) = 0$ for some real η and that $\Delta_{c,\gamma,L_0}(a) \geq 0$. Then using (A.9), we arrive at

$$\left| ca + \gamma a^2 + A_{0,0} \right| \le \left| c\lambda + \gamma \lambda^2 + A_{0,0} \right| = \left| \sum_{j=1}^{N} A_{j,0} e^{\lambda r_j} \right| \le \sum_{j=1}^{N} A_{j,0} e^{ar_j} \le -(ca + \gamma a^2 + A_{0,0}).$$
 (A.10)

By examining the first and last terms in (A.10), we see that the three inequalities have to be equalities. This can only be if $\lambda = a$, from which the claim immediately follows.

Notice that under the assumptions of the previous lemma, we have $\Delta_{c,\gamma,L_0}(0) > 0$ and $\Delta''_{c,\gamma,L_0} < 0$. The behaviour of the characteristic function is thus easy to analyze on the real line and we can use the result above to establish the following two claims about the eigenvalues of (A.7).

Lemma A.4. Consider the equation (A.7) and suppose that $A_{\Sigma} < 0$ and Assumption 2.1 is satisfied. Then equation (A.7) is hyperbolic. Furthermore, there exists precisely one real positive eigenvalue $\lambda^+ \in (0, \infty)$ and precisely one real negative eigenvalue $\lambda^- \in (-\infty, 0)$ and each of these eigenvalues is simple. The eigenvalues λ^- and λ^+ depend C^1 smoothly on c and the coefficients $A_{j,0}$. In addition, we have that

$$\frac{\partial \lambda^{-}}{\partial c} < 0 \quad and \quad \frac{\partial \lambda^{+}}{\partial c} < 0.$$
 (A.11)

All the remaining eigenvalues satisfy

Re
$$\lambda \in (-\infty, \lambda^-) \cup (\lambda^+, \infty)$$
, Im $\lambda \neq 0$. (A.12)

Lemma A.5. Consider the equation (A.7) and suppose that $A_{\Sigma} > 0$ and Assumption 2.1 is satisfied. Then either all real eigenvalues of (A.7) lie in $(0, \infty)$, or else they all lie in $(-\infty, 0)$.

We now shift our focus to nonlinear differential difference equations of the form

$$-\gamma x''(\xi) - cx'(\xi) = G(\xi, x(\xi), x(\xi + r_1), \dots, x(\xi + r_N)). \tag{A.13}$$

In the automatous case we write

$$-\gamma x''(\xi) - cx'(\xi) = F(x(\xi), x(\xi + r_1), \dots, x(\xi + r_N)). \tag{A.14}$$

We will impose the following conditions on (A.13).

Assumption A.1. The parameter γ satisfies $\gamma > 0$ and the shifts satisfy $r_i \neq r_j$ when $i \neq j$ and $r_i \neq 0$. There is at least one shifted argument, i.e. $N \geq 1$. The function $G : \mathbb{R} \times \mathbb{R}^{N+1} \to \mathbb{R}$, written as $G(\xi, u)$, where $u = (u_0, u_1, \dots, u_N)$, is C^1 smooth and the derivative D_2G of G with respect to the second argument $u \in \mathbb{R}^{N+1}$ is locally Lipshitz in u. In addition, for every $\xi \in \mathbb{R}$ we have that

$$\frac{\partial G(\xi, u)}{\partial u_j} > 0, \quad u \in \mathbb{R}^{N+1}, \quad 1 \le j \le N.$$
(A.15)

The following lemma roughly states that solutions to (A.14) are uniquely specified by their initial conditions. The proof is almost completely analogous to that in [28], so we omit it.

Lemma A.6. Let $x_j: J \to \mathbb{R}$ for j=1,2 be two solutions of equation (A.13) with the same parameters c and γ on some interval J. Suppose that Assumption A.1 holds and that

$$x_1(\xi) = x_2(\xi), \quad \tau + r_{\min} \le \xi \le \tau + r_{\max},$$
 (A.16)

for some $\tau \in J$ for which $[\tau + r_{\min}, \tau + r_{\max}] \subseteq J$. Then

$$x_1(\xi) = x_2(\xi), \quad \xi \in J^\#.$$
 (A.17)

We remark here that in combination with Lemma A.2 the above result yields the following useful corollary.

Corollary A.7. Consider the linear differential difference equation (2.1) and suppose that Assumption 2.1 holds. Let $x_j: J \to \mathbb{R}$ for j=1,2 be two solutions to (2.1) with the same parameters c and γ on the interval $J = [\tau, \infty)$ for some $\tau \in \mathbb{R}$. If for all $\xi \in J^{\#}$ we have

$$x_1(\xi) \ge x_2(\xi),\tag{A.18}$$

with equality $x_1(\xi_0) = x_2(\xi_0)$ for some $\xi_0 \in J$, then we have

$$x_1(\xi) = x_2(\xi), \quad \xi \in J^\#.$$
 (A.19)

Suppose that x_1 and x_2 are both bounded solutions of the nonlinear autonomous differential difference equation (A.14) with the same parameters c and γ , where $\gamma > 0$. We have seen in Section 3 that the difference $y(\xi) = x_1(\xi) - x_2(\xi)$ satisfies the linear homogeneous equation (2.2) with coefficients given by

$$A_j(\xi) = \int_0^1 \frac{\partial F(u)}{\partial u_j} \bigg|_{u = t\pi(x_1, \xi) + (1 - t)\pi(x_2, \xi)} dt.$$
 (A.20)

If Assumption A.1 holds for the equation (A.14), it is easy to see that $A_j(\xi) > 0$ for all $\xi \in \mathbb{R}$ and for all $1 \leq j \leq N$. Since the derivatives $\frac{\partial F(u)}{\partial u_j}$ are continuous, we can use the fact that $x_1(\xi)$ and $x_2(\xi)$ are uniformly bounded to establish that the coefficients $A_j(\xi)$ are uniformly bounded for

 $0 \le j \le N$. The continuity of these coefficients follows from the Lipschitz condition on the partial derivatives of F. This means that our linear equation (2.2) with coefficients (A.20) satisfies all the assumptions of Lemma A.2. Applying this result to the difference $x_1(\xi) - x_2(\xi)$ and invoking Lemma A.6, we obtain the following useful comparison principle.

Lemma A.8. Let $x_j: J^\# \to \mathbb{R}$ for j=1,2 be two bounded solutions of the nonlinear differential difference equation (A.14) with the same parameters c and γ on the interval $J=[\tau,\infty)$ for some $\tau \in \mathbb{R}$. Suppose also that Assumption A.1 holds and that

$$x_1(\xi) \ge x_2(\xi), \quad \xi \in J^\#.$$
 (A.21)

Then if $x_1(\xi_0) = x_2(\xi_0)$ for some ξ_0 , we have $x_1(\xi) = x_2(\xi)$ for all $\xi \in J^{\#}$.

In order to establish uniqueness of solutions to (1.1), we shall need a comparison principle for solutions to (A.14) which have different wavespeeds.

Lemma A.9. Let $x_j: J^\# \to \mathbb{R}$ for j=1,2 be two bounded solutions of the nonlinear autonomous differential difference equation (A.14) with parameters $\gamma = \gamma_j$ and $c = c_j$ on some interval $J = [\tau, \infty)$ for some $\tau \in \mathbb{R}$. Suppose that Assumption A.1 holds and that $\gamma_1 = \gamma_2 > 0$, but that $c_1 > c_2$. Also assume that

$$x_1(\xi) \ge x_2(\xi), \quad \xi \in J^\#$$
 (A.22)

and that $x_2(\xi)$ is monotonically increasing. Then if $x_1(\xi_0) = x_2(\xi_0)$ for some ξ_0 , we have that $x_1(\xi) = x_2(\xi)$ is constant for all $\xi \geq \xi_0$.

Proof. We start out by noticing that the difference $y(\xi) = x_1(\xi) - x_2(\xi)$ satisfies the linear equation

$$y''(\xi) = -\frac{c_1}{\gamma} x_1'(\xi) + \frac{c_2}{\gamma} x_2'(\xi) - \frac{1}{\gamma} \sum_{j=0}^{N} A_j(\xi) y(\xi + r_j), \tag{A.23}$$

where the coefficients A_j are again given by (A.20).

We have already seen that the coefficients $A_j(\xi)$ are uniformly bounded for $0 \le j \le N$ and that $A_j(\xi) > 0$ for all $\xi \in \mathbb{R}$ and for $1 \le j \le N$. We can thus write $A_0(\xi) \ge \alpha_0$, for some $\alpha_0 < 0$. Now using the fact that $x_2'(\xi) \ge 0$, we have

$$\frac{c_2}{\gamma}x_2'(\xi) \le \frac{c_1}{\gamma}x_2'(\xi),\tag{A.24}$$

which allows us to conclude

$$y''(\xi) \le -\frac{c_1}{\gamma}y'(\xi) - \frac{\alpha_0}{\gamma}y(\xi). \tag{A.25}$$

Upon defining $z(\xi) = e^{\frac{c_1}{2\gamma}\xi}y(\xi)$, we obtain

$$z''(\xi) \le \left(\frac{c_1^2}{4\gamma^2} - \frac{\alpha_0}{\gamma}\right) z(\xi) = Bz(\xi),\tag{A.26}$$

where B > 0. We now proceed as in the proof of Lemma A.1 to conclude that $z(\xi) = 0$ for all $\xi \ge \xi_0$, which implies $x_1(\xi) = x_2(\xi)$ for all $\xi \ge \xi_0$. Referring back to (A.14), we see that for $\xi \ge \xi_0 + r_{\min}$ we must have $c_1x_1'(\xi) = c_2x_2'(\xi)$. However, as also $x_1'(\xi) = x_2'(\xi)$, we must have $x_1'(\xi) = x_2'(\xi) = 0$. This establishes the claim.

We are now ready to provide the proof of Theorem 2.5 and we note here that the preparations in this section allow us to follow closely the proof of [28, Theorem 4.1].

Proof of Theorem 2.5. Denote the limiting constant coefficient operators at $\pm \infty$ by L_{\pm} . Then it follows from Lemma A.4 that the equations (A.7) with L_{\pm} are both hyperbolic. In fact, the same result holds for the family of constant coefficient operators $\frac{1}{2}((1-\rho)L_{-}+(1+\rho)L^{+})$ for $-1 \leq \rho \leq 1$, which connects L_{-} to L_{+} . Theorem 2.1 thus guarantees that $\Lambda_{c,\gamma,L}$ is a Fredholm operator with $\operatorname{ind}(\Lambda_{c,\gamma,L}) = 0$. Corollary A.7 immediately implies that the nontrivial solution p satisfies p > 0. Using Proposition 2.2 and Lemma A.4, we obtain the asymptotic expressions

$$p(\xi) = \begin{cases} C_{-}^{p} e^{\lambda_{-}^{u} \xi} + O(e^{(\lambda_{-}^{u} + \epsilon)\xi}), & \xi \to -\infty, \\ C_{+}^{p} e^{\lambda_{+}^{s} \xi} + O(e^{(\lambda_{+}^{s} - \epsilon)\xi}), & \xi \to \infty, \end{cases}$$

$$(A.27)$$

for some $\epsilon > 0$, with finite exponents

$$-\infty < \lambda_{+}^{s} < 0 < \lambda_{-}^{u} < \infty. \tag{A.28}$$

Since p does not decay superexponentially and is strictly positive, Proposition 2.2 and Lemma 2.3 imply that both $C_{\pm}^p > 0$. Suppose that there exists some $x \in \mathcal{K}(\Lambda_{c,\gamma,L})$ which is linearly independent of p. By adding some multiple of p and replacing x by -x if necessary, we may assume that x satisfies a similar asymptotic expansion (A.27) with $C_{-}^x \leq 0$ and $C_{+}^x = 0$. Because x is not identically zero, Lemma A.6 implies that there exist arbitrarily large ξ for which $x(\xi) \neq 0$. If $x(\xi) \leq 0$ for all large ξ , then the same reasoning as applied above to conclude that $C_{+}^p > 0$ in the expansion (A.27) leads

to a contradiction with $C_+^x = 0$. This means there even are arbitrarily large ξ for which $x(\xi) > 0$. From this it immediately follows that there exists $\mu_0 > 0$ such that

$$p(\xi) - \mu_0 x(\xi) < 0, (A.29)$$

for some $\xi \in \mathbb{R}$. We now consider the family $p - \mu x \in \mathcal{K}_{c,\gamma,L}$ for $0 \leq \mu \leq \mu_0$. The asymptotic expressions for p and x ensure that there exist τ , K, $\lambda \in \mathbb{R}$ such that

$$p(\xi) - \mu x(\xi) \ge Ke^{-\lambda|\xi|} > 0, \quad |\xi| > \tau, \quad 0 \le \mu \le \mu_0.$$
 (A.30)

Now define

$$\mu_* = \sup \{ \mu \in [0, \mu_0] \mid p(\xi) - \mu x(\xi) \ge 0 \text{ for all } \xi \in \mathbb{R} \}.$$
 (A.31)

By definition it follows from (A.29) that $\mu_* < \mu_0$. Obviously, we have the inequality $\mu_* x(\xi) \leq p(\xi)$ for all $\xi \in \mathbb{R}$, but actually it is easy to see that also $\mu_* x(\xi_0) = p(\xi_0)$ for some $\xi_0 \in [-\tau, \tau]$. From Corollary A.7 it now immediately follows that $\mu_*x(\xi) = p(\xi)$, but this contradicts the linear independence of x and p, establishing dim $\mathcal{K}(\Lambda_{c,\gamma,L}) = 1$. To complete the proof, it is enough to show that there exists a $p^* \in \mathcal{K}(\Lambda_{c,\gamma,L}^*)$ which satisfies $p^* \geq 0$, as the strict positivity then follows immediately from Corollary A.7. Thus assume to the contrary that $p^*(\xi_1) > 0 > p^*(\xi_2)$ for some $\xi_1, \xi_2 \in \mathbb{R}$. Lemma A.6 guarantees that we may assume that $|\xi_1 - \xi_2| \leq r_{\text{max}} - r_{\text{min}}$. This means that there exists a continuous function $h: \mathbb{R} \to \mathbb{R}$ such that $\int_{-\infty}^{\infty} p^*(\xi)h(\xi)d\xi = 0$, with $\mathrm{supp}(h) \subset [\tau_1, \tau_2]$ for some $\tau_1, \tau_2 \in \mathbb{R}$ satisfying $\tau_2 - \tau_1 < r_{\text{max}} - r_{\text{min}}$. Theorem 2.1 now implies that there exists an $x \in W^{2,\infty}$ such that $\Lambda_{c,\gamma,L}x = h$. We now consider the family of such solutions $x + \mu p$ for $\mu \in \mathbb{R}$. Noting that x satisfies the homogeneous equation (2.2) for large $|\xi|$ and using similar arguments as above, one argues that there exists a $\mu^* \in \mathbb{R}$ such that $y = x + \mu^* p$ satisfies $y \geq 0$ and $y(\xi_0) = 0$ for some $\xi_0 \in \mathbb{R}$. Since $(-\infty, \tau_1 + r_{\text{max}}] \cup [\tau_2 + r_{\text{min}}, \infty) = \mathbb{R}$, we may use Lemma A.6 to conclude that $y(\xi)$ does not vanish for all large $|\xi|$. By possibly making the substitution $\xi \to -\xi$, we may assume $y(\xi)$ does not vanish for all large ξ . However, Lemma A.2 now implies $y(\xi) = 0$ for all $\xi \ge \xi_0$, which gives the desired contradiction.

B Implementation Issues

Performing the iteration step defined in (4.7) with $\mu=0$ amounts to solving a boundary value problem on the real line. This observation in principle allows one to perform the Newton iterations requiring the help of a boundary value problem solver for ordinary differential equations only, if one truncates the problem to some appropriate finite interval $[T_-, T_+]$ with $T_- < 0 < T_+$. In our C++ implementation, the boundary value problem solver COLMOD [8] was used at each iteration step. Since the boundary value problem which has to be solved has degree three, three boundary conditions need to be specified at each step. These conditions were chosen to be $\phi(T_\pm) = \pm 1$ and $\phi(0) = 0$, in order to pick out the unique translate. In addition, when evaluating the delay and advanced terms in (4.7), the iterates were taken to satisfy $\phi(\xi) = -1$ whenever $\xi \leq T_-$ and $\phi(\xi) = 1$ for $\xi \geq T_+$. In the literature, other sets of boundary conditions have been proposed, which require that at the boundary points $\xi = T_\pm$ solutions are matched up with the exponential eigenfunctions of the corresponding linearization. However, since solutions have exponential behaviour at $\pm \infty$, the distinction between these two sets of boundary conditions vanishes numerically if the interval is chosen to be large enough.

In order to perform the iteration (4.7) with $\mu \neq 0$, the COLMOD code was adapted, roughly along the lines of [1, 2], to collocate the delay and advance terms directly. This required the usage of extra memory space to accommodate the larger matrices involved and the use of a different linear system solver to allow for non block-diagonal matrices.

It remains to specify how a suitable starting value (ϕ_0, c_0) can be supplied for the Newton iterations. It turns out that this is very hard in general: very often the algorithm requires a very accurate initial guess to converge. One has to use the technique of continuation to arrive at a suitable starting value. In general, this means that one starts by solving an "easy" problem to a certain degree of accuracy and gradually moves toward the "hard" problem, using the solution of one problem as the starting value for the next problem which lies "nearby". As an example, we mention that a continuation scheme for the family (5.2) can involve varying combinations of the detuning parameter ρ , the size of the delay term α and the size of γ . The continuity in parameter space which was established in Proposition 3.2 shows that this is indeed a feasible strategy.

References

- [1] Abell, K. A., Elmer, C. E., Humphries, A. R., and Vleck, E. S. V., Computation of Mixed Type Functional Differential Boundary Value Problems. Submitted to SIAM J. Dyn. Sys.
- [2] Bader, G. (1985), Solving Boundary Value Problems for Functional Differential Equations by Collocation. In: U. M. Ascher and R. D. Russel (eds.): Proceedings in Scientific Computing, Numerical Boundary Value ODEs, Vol. 5. pp. 227–243.
- [3] Bates, P. W., Chen, X., and Chmaj, A. (2003), Traveling Waves of Bistable Dynamics on a Lattice. SIAM J. Math. Anal. 35, 520–546.
- [4] Bates, P. W. and Chmaj, A. (1999), A discrete Convolution Model for Phase Transitions. Arch. Rational Mech. Anal. 150, 281–305.
- [5] Bell, J. (1981), Some Threshold Results for Models of Myelinated Nerves. Math. Biosciences 54, 181–190.
- [6] Cahn, J. W. (1960), Theory of Crystal Growth and Interface Motion in Crystalline Materials. Acta Met. 8, 554–562.
- [7] Cahn, J. W., Mallet-Paret, J., and Van Vleck, E. S. (1999), Traveling Wave Solutions for Systems of ODE's on a Two-Dimensional Spatial Lattice. SIAM J. Appl. Math 59, 455–493.
- [8] Cash, J. R., Moore, G., and Wright, R. W. (1995), An Automatic Continuation Strategy for the Solution of Singularly Perturbed Linear Two-Point Boundary Value Problems. J. Comp. Phys. 122, 266–279.
- [9] Chi, H., Bell, J., and Hassard, B. (1986), Numerical Solution of a Nonlinear Advance-Delay-Differential Equation from Nerve Conduction Theory. J. Math. Bio. 24, 583–601.
- [10] Chow, S. N., Mallet-Paret, J., and Shen, W. (1998), Traveling Waves in Lattice Dynamical Systems. J. Diff. Eq. 149, 248–291.
- [11] Chua, L. O. and Roska, T. (1993), The CNN paradigm. IEEE Trans. Circuits Syst. 40, 147–156.

- [12] Elliott, C. M., Gardiner, A. R., Kostin, I., and Lu, B. (1994), Mathematical and Numerical Analaysis of a Mean-Field Equation for the Ising Model with Glauber Dynamics. In: *Chaotic Numerics*, AMS, Vol. 172. pp. 217–242.
- [13] Elmer, C. E. and Van Vleck, E. S. (1996), Computation of Traveling Waves for Spatially Discrete Bistable Reaction-Diffusion Equations. Appl. Numer. Math. 20, 157–169.
- [14] Elmer, C. E. and Van Vleck, E. S. (1999), Analysis and Computation of Traveling Wave Solutions of Bistable Differential-Difference equations. *Nonlinearity* 12, 771–798.
- [15] Elmer, C. E. and Van Vleck, E. S. (2001), Traveling Wave Solutions for Bistable Differential Difference Equations with Periodic Diffusion. SIAM J. Applied Mathematics 61, 1648–1679.
- [16] Elmer, C. E. and Van Vleck, E. S. (2002), A Variant of Newton's Method for the Computation of Traveling Waves of Bistable Differential-Difference Equations. J. Dyn. Diff. Eqn. 14, 493–517.
- [17] Erneux, T. and Nicolis, G. (1993), Propagating Waves in Discrete Bistable Reaction-Diffusion Systems. Physica D 67, 237–244.
- [18] Fife, P. and McLeod, J. (1977), The Approach of Solutions of Nonlinear Diffusion Equations to Traveling Front Solutions. Arch. Rat. Mech. Anal. 65, 333–361.
- [19] Hankerson, D. and Zinner, B. (1993), Wavefronts for a Cooperative Tridiagonal System of Differential Equations. J. Dyn. Diff. Eq. 5, 359–373.
- [20] Hupkes, H. J. and Verduyn-Lunel, S. M. (2003), Analysis of Newton's Method to Compute Travelling Wave Solutions to Lattice Differential Equations. Technical Report 2003–09, Mathematical Institute Leiden.
- [21] Iooss, G. (2000), Traveling Waves in the Fermi-Pasta-Ulam Lattice. Nonlinearity 13, 849–866.
- [22] Iooss, G. and Kirchgässner, K. (2000), Traveling Waves in a Chain of Coupled Nonlinear Oscillators. Comm. Math. Phys. 211, 439–464.
- [23] Keener, J. and Sneed, J. (1998), Mathematical Physiology. Springer-Verlag, New York.

- [24] Keener, J. P. (1987), Propagation and its Failure in Coupled Systems of Discrete Excitable Cells. SIAM J. Appl. Math. 47, 556–572.
- [25] Laplante, J. P. and Erneux, T. (1992), Propagation Failure in Arrays of Coupled Bistable Chemical Reactors. J. Phys. Chem. 96, 4931–4934.
- [26] Mallet-Paret, J. (1996), Spatial Patterns, Spatial Chaos and Traveling Waves in Lattice Differential Equations. In: Stochastic and Spatial Structures of Dynamical Systems, Royal Netherlands Academy of Sciences. Proceedings, Physics Section. Series 1, Vol. 45. Amsterdam, pp. 105–129.
- [27] Mallet-Paret, J. (1999), The Fredholm Alternative for Functional Differential Equations of Mixed Type. J. Dyn. Diff. Eqn. 11, 1–48.
- [28] Mallet-Paret, J. (1999), The Global Structure of Traveling Waves in Spatially Discrete Dynamical Systems. J. Dyn. Diff. Eqn. 11, 49–128.
- [29] Mallet-Paret, J. (2001), Crystallographic Pinning: Direction Dependent Pinning in Lattice Differential Equations. preprint.
- [30] Mallet-Paret, J. and Verduyn-Lunel, S. M., Exponential Dichotomies and Wiener-Hopf Factorizations for Mixed-Type Functional Differential Equations. to appear in J. Diff. Eq.
- [31] Rudin, W. (1974), Real and Complex Analysis. McGraw-Hill, New York.
- [32] Rudin, W. (1991), Functional Analysis. McGraw-Hill, New York.
- [33] Strunz, T. and Elmer, F. J. (1998), Driven Frenkel-Kontorova model I. Uniform Sliding States and Dynamical Domains of Different Particle Densities. *Phys. Rev. E* 58, 1601–1611.
- [34] Strunz, T. and Elmer, F. J. (1998), Driven Frenkel-Kontorova model II. Chaotic Sliding and Nonequilibrium Melting and Freezing. Phys. Rev. E 58, 1612–1620.
- [35] Wu, J. and Zou, X. (1997), Asymptotic and Periodic Boundary Value Problems of mixed FDE's and Wave Solutions of Lattice Differential Equations. *J. Diff. Eq.* **135**, 315–357.
- [36] Zinner, B. (1992), Existence of Traveling Wavefront Solutions for the Discrete Nagumo Equation. J. Diff. Eq. 96, 1–27.

- [37] Zinner, B. (1992), Stability of Traveling Wavefronts for the Discrete Nagumo Equation. J. Diff. Eq. $\bf 96$, 1–27.
- [38] Zinner, B., Harris, G., and Hudson, W. (1993), Traveling Wavefronts for the Discrete Fisher's Equations. J. Diff. Eq. 105, 46–62.