COMPUTATION OF TRAVELING WAVES FOR SPATIALLY DISCRETE BISTABLE REACTION-DIFFUSION EQUATIONS

by

Christopher Erhart Elmer

A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science (Mathematical and Computer Sciences).

Golden, Colorado
Date Mar 26, 96

Signed: ______________________
Christopher Erhart Elmer

Approved: Erik S. Van Vleck
Dr. Erik S. Van Vleck
Thesis Advisor

Golden, Colorado
Date 3/26/96

Graeme Fairweather
Dr. Graeme Fairweather
Professor and Head,
Department of Mathematical and
Computer Sciences

Abstract

Traveling wave solutions for reaction-diffusion equations on an infinite discrete lattice are considered. Traveling wave equations are derived for the spatial domain, $\mathbb{Z}^n$ for $n = 1, 2$, and 3. All points in the spatial domain contribute explicitly to the solution at any point. Using an idealized nonlinear term, traveling wave solutions are found, the anisotropy and propagation failure introduced by the lattice are analyzed, and fundamental properties of the solutions are studied. Numerical techniques for solving the traveling wave equations are introduced. Finally, some numerical experiments are presented.

Table of Contents

List of Figures

Acknowledgements

Many thanks go to my committee members, Dr. Steven Pruess and Dr. Bernard Bialecki, for their comments and interesting suggestions. I would also like to thank Dr. Graeme Fairweather for the opportunity to publish the numerical portion of this thesis, and Dorothy Nelson for sticking up for me from time to time.

The National Institute for Science and Technology (NIST) deserves my appreciation for its generous financial support on this project.

Finally, I thank Dr. Erik Van Vleck for his time, his patience, and his tolerance which I only hope to be able to repay some day.

Chapter 1

INTRODUCTION

In this thesis, we consider traveling wave solutions of spatially discrete reaction-diffusion equations. In particular, we analyze the phenomena of propagation failure and lattice induced anisotropy. These phenomena occur in the discrete version but not the continuous version of the reaction-diffusion equations. Both of these phenomena have been observed in complex physical systems (see [6, 14, 21, 27, 28, 29]). Discretizing the $n-$dimensional Laplacian often introduces directional dependence, anisotropy, into the equations. In our discretization, we allow for representation of any anisotropy one would wish to model, since anisotropy has been observed in a variety of wave propagation problems. The phenomenon of propagation failure, freezing of wave motion, is the failure of waves to propagate until there is sufficient difference in the energy of the primary states of the waveform.

These spatially discrete reaction-diffusion equations, which are differential-difference equations, appear in many areas of science. The two areas of particular interest to us are materials science and biology. Examples from materials science include crystal growth for diffuse and non-singular surfaces, and phase transition problems such as motion of internal interfaces (faces and edges) in solids [1, 6, 14, 16]. Examples from biology include wave propagation in systems of excitable cells in neurophysiology and cardiophysiology [3, 4, 8, 21, 27, 28, 29].

In the thesis, we are analyzing an idealized system of bistable reaction-diffusion equations with spatial domain $\mathbb{Z}^n$ for $n = 1, 2$, and 3. In particular, we derive equations for traveling wave solutions. These equations have the form of differential-difference two-point boundary problems defined on the real line. We extend the analysis of Cahn et al [7] to $n = 3$, and, for an idealized nonlinearity that corresponds to the reaction term in the system, we illustrate the dependence of the wave speed, c, on the value of a parameter in the system, a, that is often referred to as the detuning parameter. We provide an explicit formula that relates c to a, and characterize the dependence of this formula on the orientation of the wavefront.

Our contribution is in considering arbitrary discretizations of the Laplacian. We are allowing all points in the infinite integer lattice to contribute explicitly to the solution at any point. The main reason for allowing explicit representation of all lattice points is that we wish to model any type of lattice anisotropy and any type of propagation failure.

This thesis consists primarily of two parts (or chapters). The first of these, Chapter 2, addresses the problem of analytically finding traveling wave solutions to the spatially discrete reaction-diffusion equations. The second part, Chapter 3, addresses the problem of finding traveling wave solutions to our differential-difference equations using classical numerical techniques.

In Chapter 2, we not only obtain traveling wave solutions, but also obtain a fundamental relationship between the wave speed c and a detuning parameter of the nonlinear term of our equation, and obtain fundamental properties of the solutions. This chapter consists of three sections. The first section is an introduction to the problem, equations, and notation. In the next section, we present results, including solutions, for the case when the wave speed of our traveling waves is nonzero. The last section covers the case when the wave speed of the traveling waves is zero.

In the numerical solutions chapter, Chapter 3, not only are numerical traveling wave solutions presented (in graphical form), we also present the techniques, methods, and convergence results obtained while computing these solutions. Chapter 3 consists of four sections. In the first section, the implementation and theory of the particular numerical methods used are discussed. In the second section, we discuss convergence results for the methods presented in the first section. In the next section, we present the results of our numerical experiments. Finally, in the last section, we compare and discuss the numerical and analytical results obtained in this thesis.

We conclude this thesis with a section containing conclusions and ideas for future work. In the conclusions section, we discuss the importance of the work presented in this thesis, and its possible uses. In the future work section, we indicate the areas of future research.

Chapter 2

DERIVATION OF TRAVELING WAVE EQUATIONS

The goal of this chapter is two-fold. First, we derive traveling wave equations for the infinite system of ordinary differential-difference reaction-diffusion equations,

$$\dot{u}(\eta,t) = \Delta u(\eta,t) - f(u(\eta,t)) \tag{2.1}$$

where Δ is a discrete Laplacian-like operator and where $\eta \in \mathbb{Z}^n, t \in \mathbb{R}, u : \mathbb{Z}^n \times \mathbb{R} \longrightarrow \mathbb{R}, f : \mathbb{R} \longrightarrow \mathbb{R}$. Note that "$\dot{}$" = "$d/dt$". The function $f(u(\eta,t))$ is the nonlinear reaction term of equation (2.1).

Secondly, we wish to show several fundamental properties of the traveling wave solution, φ, such as monotonicity and continuity, for the derived traveling wave equations of the above system.

We achieve these goals in three sections. In the first, we introduce the problem, notation, and assumptions we use in order to achieve our goals. In the second section, we analyze the case of nonzero wave speed, c, and to conclude this chapter, in the third section, we analyze the case of zero wave speed, c. Analyzing these two cases involves finding the traveling wave solutions and presenting several properties of these solutions.

2.1 The problem

In this section, we introduce the spatially discrete bistable reaction-diffusion equations that will be considered throughout the thesis.

Let $n = 1, 2$, or 3 be the dimension of the problem. Let $f : \mathbb{R} \to \mathbb{R}$ be a bistable function. This means that the "potential" of $f(u)$, $F(u)$, that satisfies $F'(u) = f(u)$, has a double well (Figures 2.1b, 2.2b). A typical example of a bistable function is the cubic

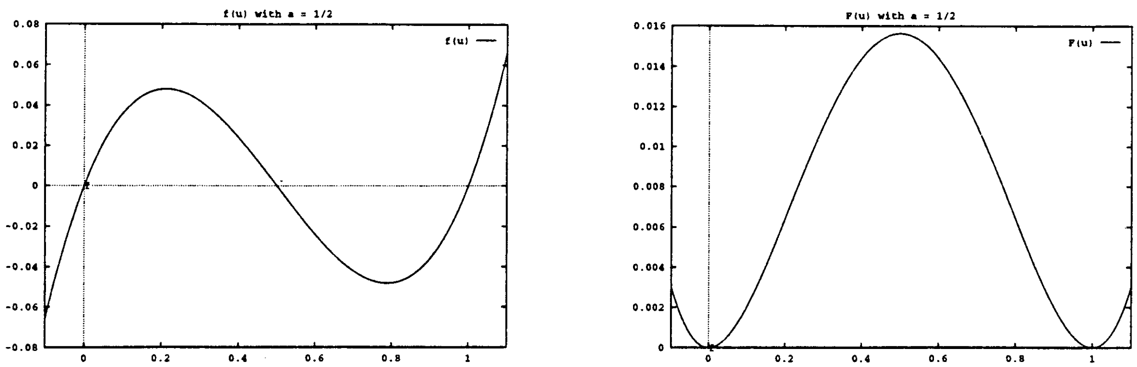
$$f(u) = u(u-a)(u-1), \qquad a \in (0,1), \tag{2.2}$$

where a is is called the "detuning parameter" (Figures 2.1a, 2.2a). The potential for this f is

$$F(u) = \frac{u^4}{4} - \frac{(a+1)}{3}u^3 + \frac{a}{2}u^2, \qquad a \in (0,1), \tag{2.3}$$

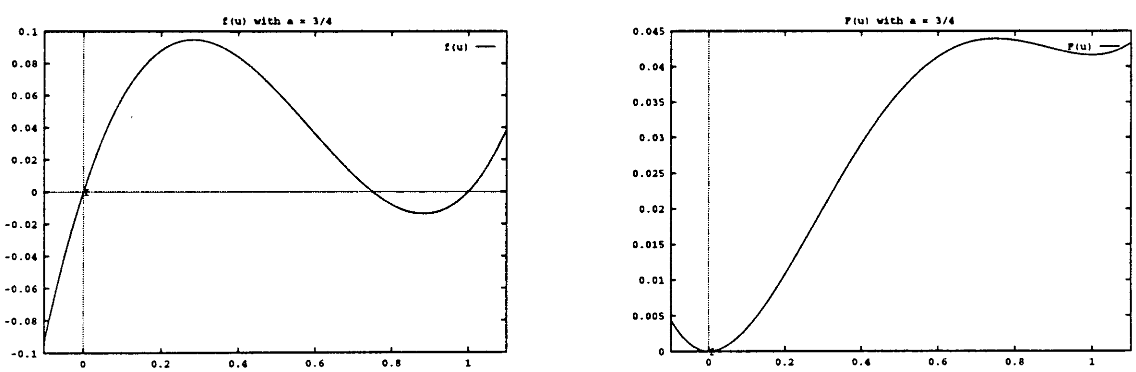
(Figures 2.1b, 2.2b).

Note that when we shift a away from $1/2$, one well of our potential rises above the other (Figures 2.1, 2.2). Let $\eta = (\eta_1, \ldots, \eta_n) \in \mathbb{Z}^n$, and $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$



$f(u)$ with $a = 1/2$ (a) $F(u)$ with $a = 1/2$ (b)

Figure 2.1: The nonlinearity $f(u)$ and its potential $F(u)$ for $a = 1/2$.



$f(u)$ with $a = 3/4$ (a) $F(u)$ with $a = 3/4$ (b)

Figure 2.2: The nonlinearity $f(u)$ and its potential $F(u)$ for $a = 3/4$.

be position vectors. Let $\sigma = (\sigma_1, \ldots, \sigma_n) \in \mathbb{R}^n$ be a vector such that $\sum_{i=1}^{n} \sigma_i^2 = 1$. For $n = 1, 2$, or 3, the elements of the σ vector are:

$$n = 1: \quad \sigma_1 = 1,$$

$$n = 2: \quad \sigma_1 = \cos(\theta), \qquad \sigma_2 = \sin(\theta),$$

$$n = 3: \quad \sigma_1 = \sin(\phi)\cos(\theta), \quad \sigma_2 = \sin(\phi)\sin(\theta), \quad \sigma_3 = \cos(\phi).$$

Define the set

$$D = \{\sigma \cdot l | l \in \mathbb{Z}^n\}, \tag{2.4}$$

where "$\cdot$" represents the dot product of two vectors. Note that if, for any $j \neq k$, σ_k and σ_j are rationally independent, then D is a dense subset of $\mathbb{R}$, while if the $\{\sigma_k\}_{k=1}^{n}$ are rationally dependent (all the σ_k are rational multiples of some nonzero quantity), then there exists a quantity $\nu > 0$ such that $D = \{m\nu | m \in \mathbb{Z}\}$ and so D is a discrete subset of $\mathbb{R}$.

While our desire is to work with spatially discrete equations, let us examine their spatially continuous counterpart, the reaction-diffusion partial differential equation

$$u_t(x,t) = \epsilon \Delta_L u(x,t) - f(u(x,t)), \qquad x \in \mathbb{R}^n, \quad t \in \mathbb{R}, \tag{2.5}$$

where $\epsilon > 0$ is real and Δ_L is the n-dimensional Laplacian operator denoted by

$\Delta_L = \sum_{i=1}^n D_{x_i}^2$. The term $\epsilon\Delta_L u(x,t)$ is the diffusion term in the equation and the function $f(u(x,t))$ is the reaction term. We are looking at the partial differential equation (2.5) in the hope that solution methods for it will be helpful in providing solution techniques for our spatially discrete system.

A solution $u(x,t) = \varphi(x \cdot \sigma - ct)$ of (2.5), where $\varphi : I\!R \to I\!R$ and c is the wave speed, is called a traveling wave solution. We are interested in traveling wave solutions because they are one of the simpliest ways to study movable phase boundaries. Note that here σ represents a vector normal to the wavefront of our traveling wave solution. If we substitute our traveling wave ansatz into the partial differential equation (2.5), we obtain the second order ordinary differential equation

$$-c\varphi'(\xi) = \epsilon(\sum_{i=1}^{n} \sigma_i^2 \varphi''(\xi)) - f(\varphi(\xi))$$

or

$$-c\varphi'(\xi) = \epsilon\varphi''(\xi) - f(\varphi(\xi)), \tag{2.6}$$

where $\xi \equiv (x \cdot \sigma - ct)$. Recalling Figures 2.1 and 2.2, and Equation (2.3), we choose boundary conditions so that the wave flows between the two stable equilibria, $u = 0, 1$. In other words, we choose boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$. We wish to point out that, for this second order ordinary differential equation, the sign of c, the direction of the flow of the wave, can be observed in the potential $F(u)$ of $f(u)$.

When $a = 1/2$, $c = 0$, the wells of $F(u)$ are of equal height, and the wave does not move. When $a < 1/2$, $c < 0$, the well at $u = 0$, of $F(u)$, is higher than the well at $u = 1$, and the wave flows to the left, i.e., the solution flows from 0 to 1; when $a > 1/2$, $c > 0$, the well at $u = 1$, of $F(u)$, is higher than the well at $u = 0$, and the wave flows to the right, i.e., the solution flows from 1 to 0.

In this thesis, we are studying the infinite system of ordinary differential-difference reaction-diffusion equations

$$\dot{u}(\eta, t) = \Delta u(\eta, t) - f(u(\eta, t)) \tag{2.7}$$

on a $n-$dimensional integer lattice. Here

$$\Delta u(\eta, t) = \sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j} [u(\eta + \beta_{k_j}, t) + u(\eta - \beta_{k_j}, t) - 2u(\eta, t)], \tag{2.8}$$

$\eta \in \mathbb{Z}^n, t \in \mathbb{R}, u : \mathbb{Z}^n \times \mathbb{R} \to \mathbb{R}$, and $f : \mathbb{R} \to \mathbb{R}$. Note that $\beta_{k_j} \in \mathbb{Z}^n$ is such that $||\beta_{k_j}||_2^2 = k$, and m_k is the number of such distinct nonzero vectors β_{k_j} for a particular k (note that β_{k_j} and $-\beta_{k_j}$ are not considered distinct). Let α_k denote the vector $\alpha_k = (\alpha_{k_1}, \ldots, \alpha_{k_{m_k}})$ and assume $0 \leq \alpha_{k_j} \in \mathbb{R}$. We assume throughout this thesis that $\sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j} < \infty$.

For a given value of the dimension n and a given value of k, we would like to determine whether or not $m_k = 0$. For $n = 1$, $m_k \neq 0$ provided there exists an integer

z such that $z^2 = k$; for $n = 2$, $m_k \neq 0$ provided there exists integers y and z such that $y^2 + z^2 = k$; and similarly for $n = 3$. To formalize this, we define p_k to be the minimum number of integers such that the sum of the squares of these integers is k. Here are some examples of p_k.

If	$k = 1$	then	$p_1 = 1$	since	$1^2 = 1$,
if	$k = 2$	then	$p_2 = 2$	since	$1^2 + 1^2 = 2$,
if	$k = 3$	then	$p_3 = 3$	since	$1^2 + 1^2 + 1^2 = 3$,
if	$k = 4$	then	$p_4 = 1$	since	$2^2 = 4$,
if	$k = 5$	then	$p_5 = 2$	since	$1^2 + 2^2 = 5$,
and so on.					

Thus $p_k > n$ implies $m_k = 0$. Therefore, if $n = 1$, then $m_k \neq 0$ if and only if $k = 1, 4, 9, 16, 25, 36, 49, \ldots$. If $n = 2$, then $m_k \neq 0$ if and only if $k = 1, 2, 4, 5, 8, 9, 10, \ldots$. And if $n = 3$, then $m_k \neq 0$ if and only if $k = 1, 2, 3, 4, 5, 6, 8 \ldots$.

We choose to use a discretization that allows us to represent every point in the lattice explicitly because we are allowing for any directional variance, along with, in the limit, no lattice anisotropy.

Example 2.1 *Let $m_k = 0$, for $k = 2, \ldots, \infty$, with $\alpha_{1_i} = \alpha \in \mathbb{R}^+$. Then (2.7) with $n = 1$ can be thought of as a discretization of the PDE (2.5) with $\alpha = \frac{\varepsilon}{h^2}$.*

∎

We now present some examples of familiar representations that appear in our ordinary differential-difference equation (2.7).

Example 2.2 *Let* $\alpha \in I\!R^+$. *Let* $m_k = 0$, *for* $k = 2, \ldots, \infty$, *and* $\alpha_{1_i} = \alpha$, *for* $i = 1, \ldots, n$. *Note that* $m_1 = n$. *Then (2.7), (2.8) becomes*

$$\begin{aligned}\dot{u}(\eta, t) &= \sum_{j=1}^{n} \alpha_{1_j}[u(\eta + \beta_{1_j}, t) + u(\eta - \beta_{1_j}, t) - 2u(\eta, t)] - f(u(\eta, t)) \\ &= \alpha \sum_{j=1}^{n}[u(\eta + \beta_{1_j}, t) + u(\eta - \beta_{1_j}, t) - 2u(\eta, t)] - f(u(\eta, t)),\end{aligned}$$

which is the reaction-diffusion equation discretized using the familiar $2n + 1$ *point star.*

■

Example 2.3 *If we take the* $1D$ *case of the above example, we obtain the centered difference approximation.*

■

Example 2.4 *Let's look at the 2D case of Example 2.2, i.e.,* $n = 2$. *Then with* $\beta_{1_1} = (1, 0), \beta_{1_2} = (0, 1), \beta_{2_1} = (1, 1), \beta_{2_2} = (1, -1)$, *we obtain*

$$\dot{u}(\eta, t) =$$

$$\alpha[u(\eta + \beta_{1_1}, t) + u(\eta - \beta_{1_1}, t) + u(\eta + \beta_{1_2}, t) + u(\eta - \beta_{1_2}, t) - 4u(\eta, t)] - f(u(\eta, t)),$$

which is the reaction-diffusion equation discretized using the familiar five-point star.

■

Example 2.5 *Let* $m_k = 0,\ k = 3, 4, \ldots,$ *and* $\alpha \in I\!R^+$, *with* $\alpha_{1_i} = 4\alpha$, *and* $\alpha_{2_i} = \alpha$ *for* $i = 1, \ldots, n$. *Then we have*

$$\dot{u}(\eta, t) = \sum_{k=1}^{2}(\sum_{j=1}^{m_k} \alpha_{k_j}[u(\eta + \beta_{k_j}, t) + u(\eta - \beta_{k_j}, t) - 2u(\eta, t)]) - f(u(\eta, t)).$$

This gives us a "hypercube" representation of the Laplacian. Note that we need n *to be at least 2 in this case.*

■

Example 2.6 *Note that when* $n = 2$ *in the above example we obtain the classical nine-point box discretization with* $\beta_{1_1} = (1, 0), \beta_{1_2} = (0, 1), \beta_{2_1} = (1, 1), \beta_{2_2} = (1, -1)$,

$$\begin{aligned}
\dot{u}(\eta, t) \quad &= \quad \alpha\{4[u(\eta + \beta_{1_1}, t) + u(\eta - \beta_{1_1}, t) + u(\eta + \beta_{1_2}, t) + u(\eta - \beta_{1_2}, t)] \\
&\quad + u(\eta + \beta_{2_1}, t) + u(\eta - \beta_{2_1}, t) + u(\eta + \beta_{2_2}, t) + u(\eta - \beta_{2_2}, t) \\
&\quad - 20u(\eta, t)\} - f(u(\eta, t)).
\end{aligned}$$

■

Example 2.7 *Let $m_k = 0$, for $k = 1, \ldots, i-1, i+1, \ldots$, with $\alpha_i \neq \bar{0}$. Then we obtain a discretization with only the point and its i^{th} nearest neighbors represented:*

$$\dot{u}(\eta, t) = \sum_{j=1}^{m_i} \alpha_{i_j}[u(\eta + \beta_{i_j}, t) + u(\eta - \beta_{i_j}, t) + u(\eta, t)] - f(u(\eta, t)).$$

■

The relationship of (2.7) with the partial differential equation (2.5) prompts us to look at traveling wave solutions for the discrete system of ordinary differential equations (2.7). Here a solution $u(\eta, t) = \varphi(\eta \cdot \sigma - ct)$ of (2.7) is called a traveling wave solution. If we substitute our traveling wave ansatz into (2.7) and let $\eta \cdot \sigma - ct \equiv \xi$, we obtain

$$-c\varphi'(\xi) = L\varphi(\xi) - f(\varphi(\xi)), \tag{2.9}$$

where $L\varphi(\xi) = \sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j}[\varphi(\xi + \beta_{k_j} \cdot \sigma) + \varphi(\xi - \beta_{k_j} \cdot \sigma) - 2\varphi(\xi)]$, with $\beta_{k_j} \in \mathbb{Z}^n$, $\|\beta_{k_j}\|_2^2 = k$, $\alpha_k \in \mathbb{R}^{m_k}$, and $\sigma \in \mathbb{R}^n$ such that $\|\sigma\|_2^2 = 1$. Again we choose the boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$.

At this point, we note that the partial differential equation (2.6) is independent of dimension and direction. This is <u>not</u> true for the discrete version (2.9), which depends directly on the direction of the wavefront and on the dimension of the problem.

2.1.1 Linearizing f

Since we wish to solve our differential-difference equation analytically, we need to simplify the nonlinear term f so that we can use classical solution methods. The particular technique that we make use of is the Fourier transform. However we still wish to have a bistable form for f. Our choice is a piecewise linear function that approximates the smooth cubic nonlinearities discussed earlier (2.2). The specific class of piecewise linear f that we consider is

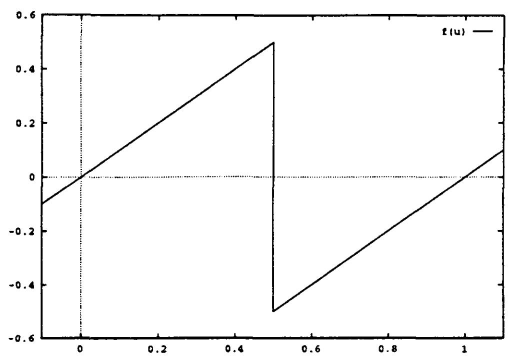
$$f(u) = f(u,a) = u - h(u-a), \qquad \text{with} \quad a \in (0,1) \tag{2.10}$$

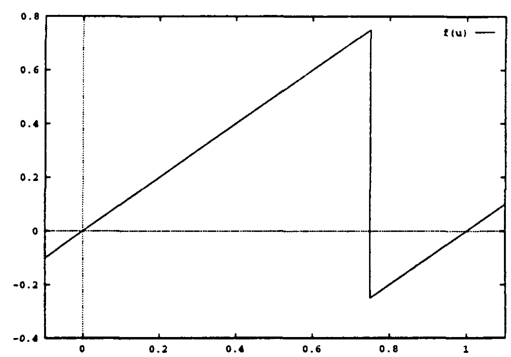
where h denotes the Heaviside function

$$h(v) = \begin{cases} 0 & v < 0, \\ 1 & v > 0. \end{cases} \tag{2.11}$$

Notice that this f, (2.10), models the smooth nonlinearity (2.2) and its potential is double-welled (Figure 2.3).

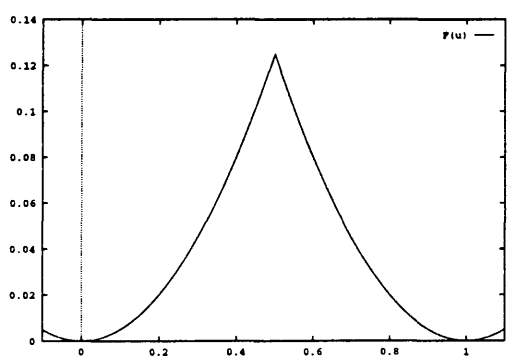
Our new f, defined above, is discontinuous. Now that we are using a discontinuous f, the first thing that needs to be addressed is exactly what is meant by a solution to (2.7). To solve our system of differential equations, it is sufficient to regard both f and h as set valued functions, with $f(u)$ and $h(v)$ singleton sets for $u \neq a$ and

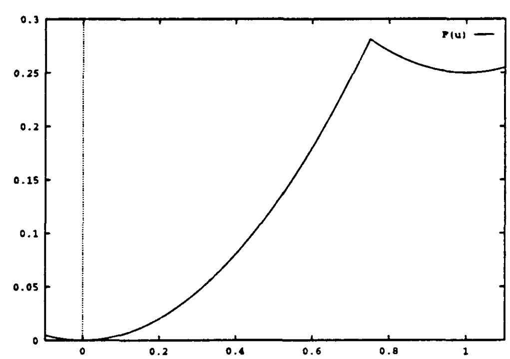




$a = 1/2$ $a = 3/4$

Piecewise linear $f(u)$





$a = 1/2$ $a = 3/4$

$F(u)$

Figure 2.3: Piecewise linear $f(u)$ and its potential $F(u)$.

$v \neq 0$, and $f(a) = [a-1, a]$ and $h(0) = [0,1]$. This amounts to filling in the jump discontinuities in the graphs of f and h. By a solution to (2.7) we mean $u(\eta, t)$, where for any η, say η_0, $u(\eta_0, t)$ is smooth in t and satisfies the differential inclusion

$$\dot{u}(\eta_0, t) \in \Delta u(\eta_0, t) - f(u(\eta_0, t))$$

for almost every t.

2.2 Nonzero Wave Speed

In this section, we derive the solution of (2.9) for $c \neq 0$, for the piecewise linear function f, (2.10), described in the last section. This derivation is a review and extension of the derivation presented in [7], the review because the same concepts are used, the extension since our discrete operator is much more involved than the discrete operator presented in [7]. In particular, our operator consists of an infinite number of points while the operator in [7] consists of finitely many, and we consider dimensions $n \leq 3$ while the analysis in [7] is for $n = 2$. From our derived solution, we obtain a relationship between the detuning parameter, a, and the wave speed, c. Also, from this solution, we present some qualitative results concerning the solution.

In order to construct our solution, we use the Fourier transform. Recall that this was the reason for going to a "linearized" nonlinearity f.

This section begins with the construction of a solution, $\varphi(\xi)$, for (2.9), with boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$, and linear f as in (2.10). The construction consists of defining a function $\varphi_\varepsilon(\xi) = e^{-\varepsilon\xi}\varphi(\xi)$ and transforming (2.9). To the $\varphi_\varepsilon(\xi)$ version of the discrete equation, we apply the Fourier transform, and after some manipulation, we derive a formula for $\varphi(\xi)$. We then show that this solution, $\varphi(\xi)$, is continuous in both ξ and c, and is analytic in c for $c \neq 0$. We also show that $D_c\varphi(\xi)$ is bounded. From the formula for $\varphi(\xi)$, we next derive a relation between a and c, called Γ. The function Γ is odd in c, analytic in c, and discontinuous at $c = 0$. The discontinuity in Γ is a jump discontinuity and is called the range of propagation failure. We let 2γ equal the range of propagation failure, and study how γ depends on the rational dependence/independence of the elements of the normal vector σ. We then show that $\varphi(\xi)$ is strictly increasing on the real line. The last key result of this section is that c depends analytically on a for a outside the interval of propagation failure. This is not true for a in the interval of propagation failure.

At this point, we assume that our solution, φ, satisfies $\varphi(\xi) = a$ for only one value of ξ, call it ξ_0. Without loss of generality, we may assume $\xi_0 = 0$ by translating $\xi \to \xi - \xi_0$, [11]. We will justify these assumptions after we derive a solution.

We let $\varphi(0) = a$, the translate that has been classically chosen in the literature [6, 11]. Basically all this means is that we are assuming that

$$\varphi(\xi) < a, \qquad \xi < 0, \qquad\qquad \varphi(\xi) > a, \qquad \xi > 0. \tag{2.12}$$

This implies that $\varphi(\xi) - a < 0$ if $\xi < 0$, and $\varphi(\xi) - a > 0$ if $\xi > 0$. Thus, for the Heaviside function defined in (2.11), $h(\varphi(\xi) - a) = h(\xi)$ for $\xi \neq 0$. Therefore,

$$f(\varphi(\xi)) = \varphi(\xi) - h(\varphi(\xi) - a) = \varphi(\xi) - h(\xi) \qquad \text{for} \quad \xi \neq 0.$$

Our system now becomes

$$-c\varphi'(\xi) = L\varphi(\xi) - \varphi(\xi) + h(\xi), \tag{2.13}$$

$$\varphi(-\infty) = 0, \qquad \varphi(+\infty) = 1,$$

which is a linear homogeneous equation that can be tackled using Fourier transform methods. We begin our derivation of a solution with a preliminary lemma.

Lemma 2.1 *Let φ be a solution of (2.13) with boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$, for $c \neq 0$. Then there exists an $\varepsilon_0 > 0$ such that, for some $K > 0$,*

$$|\varphi(\xi)| \leq K e^{\varepsilon_0 \xi} \quad \text{for} \quad \xi \leq 0. \tag{2.14}$$

Proof. Let $\psi(\xi) = \varphi(-\xi)$. Then (2.13) becomes

$$c\psi'(\xi) = L\psi(\xi) - \psi(\xi)$$

for all $\xi > 0$. Note that by our boundary conditions, $\psi(\xi) \to 0$ as $\xi \to \infty$. Let $\hat{\psi}$ be the Laplace transform of ψ:

$$\hat{\psi}(s) = \int_0^\infty e^{-s\xi} \psi(\xi) d\xi.$$

Note that $\hat{\psi}(s)$ is analytic for $\Re(s) > 0$. Integrating by parts gives us that

$$\begin{aligned}\hat{\psi}(s) &= \frac{\psi(0)}{s} + \int_0^\infty \frac{e^{-s\xi}}{s}\psi'(\xi)d\xi \\ &= \frac{\psi(0)}{s} + \int_0^\infty \frac{e^{-s\xi}}{cs}(L\psi(\xi) - \psi(\xi))d\xi.\end{aligned}$$

Integrating this relation, we obtain

$$P(s)\hat{\psi}(s) = q(s), \tag{2.15}$$

where

$$P(s) = cs + 1 - H,$$

and

$$q(s) = c\psi(0) - J(s),$$

with $H = \sum_{k=1}^{\infty}\sum_{j=1}^{m_k}\alpha_{k_j}(e^{\beta_{k_j}} + e^{-\beta_{k_j}} - 2)$,

and $J(s) = \sum_{k=1}^{\infty}\sum_{j=1}^{m_k}\alpha_{k_j}(e^{\beta_{k_j}\cdot\sigma}\int_0^{\beta_{k_j}\cdot\sigma} e^{-s\xi}\psi(\xi)d\xi - e^{-\beta_{k_j}\cdot\sigma}\int_{-\beta_{k_j}\cdot\sigma}^{0} e^{-s\xi}\psi(\xi)d\xi)$. Note that by integrating by parts,

$$\int_0^b e^{-s\xi}\psi(\xi)d\xi = -\frac{e^{-s\xi}\psi(\xi)}{s}\Big|_{\xi=0}^{b} + \frac{1}{s}\int_0^b e^{-s\xi}\psi'(\xi)d\xi.$$

Thus the integrals in (2.15) are of order $O(|s|^{-1})$. This implies that $q(s) = c\psi(0) +$

$O(|s|^{-1})$. Note that as $|\Im(s)| \to \infty$, cs dominates $1 - H$ (where $\Im(s)$ is the imaginary part of s). This follows from the fact that $\sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j} < \infty$. Thus,

$$\hat{\psi}(s) = \frac{\psi(0)}{s} + O(|s|^{-2}) \quad \text{as} \quad |\Im(s)| \to \infty.$$

Consequently, we can shift the integration contour around singularities on the imaginary axis. Therefore

$$\begin{aligned}
\psi(\xi) &= \frac{1}{2\pi i} \int_{\varepsilon_0 - i\infty}^{\varepsilon_0 + i\infty} e^{s\xi} \hat{\psi}(s) ds \\
&= \frac{1}{2\pi i} \int_{-\varepsilon_0 - i\infty}^{-\varepsilon_0 + i\infty} e^{s\xi} \hat{\psi}(s) ds + \frac{1}{2\pi i} \sum_{\Im(s)=0} e^{s\xi} \mathrm{Res}(\hat{\psi}, s) \qquad (2.16) \\
&= \frac{1}{2\pi i} \int_{-\varepsilon_0 - i\infty}^{-\varepsilon_0 + i\infty} e^{s\xi} \left(\hat{\psi}(s) - \frac{\psi(0)}{s} \right) ds + \frac{1}{2\pi i} \sum_{\Im(s)=0} e^{s\xi} \mathrm{Res}(\hat{\psi}, s),
\end{aligned}$$

where $\varepsilon > 0$ is sufficiently small, $\mathrm{Res}(g, z)$ denotes the residue of a meromorphic function g at a point z, and the sum in (2.16) is taken over all poles of $\hat{\psi}$ on the imaginary axis, if any exist. The limits of integration denote contour integrals along the vertical lines $t \to \pm\varepsilon_0 + it$, for $t \in I\!R$.

Some explanation may be in order to help justify (2.16). The first equality in (2.16) is due to the Laplace inversion formula. We can use this since $\hat{\psi}$ has no poles in the right half of the complex plane. The second equality in (2.16) comes from shifting the contour of integration, the vertical axis, around any poles of $\hat{\psi}$ on the imaginary axis, and $\varphi_0 > 0$ is small enough that $\hat{\psi}$ has no poles in the strip $-\varepsilon_0 \leq \Re(s) < 0$. The third equality in (2.16) follows from the identity

$$\frac{1}{2\pi i}\int_{\varepsilon-i\infty}^{\varepsilon+i\infty}\frac{e^{s\xi}}{s}ds = \begin{cases} 1, & \varepsilon > 0, \\ 0, & \varepsilon < 0, \end{cases}$$

for $\xi > 0$, which is just the inversion formula for the function $g(\xi) = 1$ and its transform $\hat{g}(s) = 1/s$.

The third integral in (2.16) satisfies

$$\left|\frac{1}{2\pi i}\int_{\varepsilon-i\infty}^{\varepsilon+i\infty} e^{s\xi}\left(\hat{\psi}(s) - \frac{\psi(0)}{s}\right)ds\right| \leq Ke^{-\varepsilon_0\xi} \quad \text{for} \quad \xi \geq 0,$$

for some $K > 0$; in particular, this term approaches zero as $\xi \to \infty$. Recall that $\psi(\xi) \to 0$ as $\xi \to \infty$ by assumption. Each of the residues in the summation vanishes, i.e.

$$\text{Res}(\hat{\psi}, s) = 0 \quad \text{for} \quad \Im(s) = 0.$$

Therefore, $|\psi(\xi)| \leq Ke^{-\varepsilon_0\xi}$ for $\xi \geq 0$, which is equivalent to (2.14).

■

Now we are ready to construct our solution to the traveling wave equation (2.9) with boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$, and reaction term f as in equation (2.10). First, let $\varphi_\varepsilon(\xi) = e^{-\varepsilon\xi}\varphi(\xi)$, with $\varepsilon > 0$, ε small. By Lemma 2.1, if φ is a solution to (2.13), then, as $\xi \to -\infty$,

$$\begin{aligned}\varphi_\varepsilon(\xi) &= e^{-\varepsilon\xi}\varphi(\xi) \le |e^{-\varepsilon\xi}||\varphi(\xi)| \\ &\le |Ke^{(\varepsilon_0-\varepsilon)\xi}| \to 0 \quad \text{for} \quad 0<\varepsilon<\varepsilon_0.\end{aligned}$$

Also as $\xi \to \infty$,

$$\varphi_\varepsilon(\xi) = e^{-\varepsilon\xi}\varphi(\xi) \to 0$$

since $\varphi(+\infty) = 1$. This implies that $\varphi_\varepsilon(-\infty) = 0$ and $\varphi_\varepsilon(+\infty) = 0$. Substituting $\varphi(\xi) = e^{\varepsilon\xi}\varphi_\varepsilon(\xi)$ into (2.13), we obtain

$$-ce^{\varepsilon\xi}(\varepsilon\varphi_\varepsilon(\xi) + \varphi_\varepsilon'(\xi)) = e^{\varepsilon\xi}L_\varepsilon\varphi_\varepsilon(\xi) - e^{\varepsilon\xi}\varphi_\varepsilon(\xi)) + h(\xi),$$

which simplifies to

$$-c\varphi_\varepsilon'(\xi) = L_\varepsilon\varphi_\varepsilon(\xi) - (1-c\varepsilon)\varphi_\varepsilon(\xi) + e^{-\varepsilon\xi}h(\xi), \tag{2.17}$$

where $L_\varepsilon\varphi_\varepsilon(\xi) = \sum_{k=1}^{\infty}\sum_{j=1}^{m_k}(e^{\varepsilon\beta_{k_j}\cdot\sigma}\varphi_\varepsilon(\xi+\beta_{k_j}\cdot\sigma) + e^{-\varepsilon\beta_{k_j}\cdot\sigma}\varphi_\varepsilon(\xi-\beta_{k_j}\cdot\sigma) - 2\varphi_\varepsilon(\xi))$.

Example 2.8 *If we let $m_k = 0, \forall\ k \neq 1$, and $\alpha_{1_j} \neq 0$, then*

$$-c\varphi_\varepsilon'(\xi) \;=\; L_\varepsilon\varphi_\varepsilon(\xi) - (1-c\varepsilon)\varphi_\varepsilon(\xi) + e^{-\varepsilon\xi}h(\xi)$$

$$
\begin{aligned}
&= \sum_{i=1}^{m_1} \alpha_{1_i}[e^{\varepsilon\sigma_i}\varphi_\varepsilon(\xi+\sigma_i)+e^{-\varepsilon\sigma_i}\varphi_\varepsilon(\xi-\sigma_i)-2\varphi_\varepsilon(\xi)] \\
&\quad -(1-c\varepsilon)\varphi_\varepsilon(\xi)+e^{-\varepsilon\xi}h(\xi).
\end{aligned}
$$

■

Example 2.9 *Five point star revisited. If we let* $n = 2$ *and* $\alpha_{1_i} = \alpha \in I\!R, \forall i \in \{1,\ldots,m_1\}$*, in the above example, then*

$$
\begin{aligned}
-c\varphi_\varepsilon'(\xi) &= \alpha\sum_{i=1}^{m_1}[e^{\varepsilon\sigma_i}\varphi_\varepsilon(\xi+\sigma_i)+e^{-\varepsilon\sigma_i}\varphi_\varepsilon(\xi-\sigma_i)-2\varphi_\varepsilon(\xi)] \\
&\quad -(1-c\varepsilon)\varphi_\varepsilon(\xi)+e^{-\varepsilon\xi}h(\xi).
\end{aligned}
$$

■

Example 2.10 *Nine point box revisited. Let* $m_k = 0$*, for* $k = 3, 4, \ldots,$ *and* $\alpha \in I\!R^+$*, with* $\alpha_{1_i} = 4\alpha$*, and* $\alpha_{2_j} = \alpha$ *for* $i = 1,\ldots,m_1$*,* $j = 1,\ldots,m_2$*. Then*

$$
\begin{aligned}
-c\varphi_\varepsilon'(\xi) &= \sum_{k=1}^{2}\sum_{j=1}^{m_k}[e^{\varepsilon\beta_{k_j}\cdot\sigma}\varphi_\varepsilon(\xi+\beta_{k_j}\cdot\sigma)+e^{-\varepsilon\beta_{k_j}\cdot\sigma}\varphi_\varepsilon(\xi-\beta_{k_j}\cdot\sigma)-2\varphi_\varepsilon(\xi)] \\
&\quad -(1-c\varepsilon)\varphi_\varepsilon(\xi)+e^{-\varepsilon\xi}h(\xi).
\end{aligned}
$$

■

Now let's apply the Fourier transform

$$\hat{\varphi}_\varepsilon(s) = \int_{-\infty}^{\infty} e^{-is\xi}\varphi_\varepsilon(\xi)d\xi,$$

where $\varepsilon > 0$ is sufficiently small, to both sides of (2.17). Then

$$\begin{aligned}\hat{\varphi}_\varepsilon(s) &= \int_{-\infty}^{\infty} e^{-is\xi}\varphi_\varepsilon(\xi))d\xi = -\int_{-\infty}^{\infty} \frac{i}{s}e^{-is\xi}\varphi_\varepsilon'(\xi)d\xi \\ &= \frac{i}{sc}[\int_{-\infty}^{\infty} e^{-is\xi}L_{\varepsilon_{k_j}}\varphi_\varepsilon(\xi) - e^{-is\xi}(1-c\varepsilon)\varphi_\varepsilon(\xi) + e^{-is\xi}e^{-\varepsilon\xi}h(\xi)]d\xi\end{aligned}$$

or

$$(-isc + 1 - c\varepsilon - E(s))\hat{\varphi}_\varepsilon(s) = \frac{1}{(is+\varepsilon)},$$

where $E(s) = \sum_{k=1}^{\infty}\sum_{j=1}^{m_k}\alpha_{k_j}(e^{\varepsilon\beta_{k_j}\cdot\sigma}e^{is\beta_{k_j}\cdot\sigma} + e^{-\varepsilon\beta_{k_j}\cdot\sigma}e^{-is\beta_{k_j}\cdot\sigma} - 2)$. This implies that

$$\hat{\varphi}_\varepsilon(s) = \frac{1}{(is+\varepsilon)R(s-i\varepsilon)},$$

where

$$R(q) = -icq + 1 - G(q), \tag{2.18}$$

with $G(q) = \sum_{k=1}^{\infty}\sum_{j=1}^{m_k}\alpha_{k_j}(e^{iq\beta_{k_j}\cdot\sigma} + e^{-iq\beta_{k_j}\cdot\sigma} - 2) = 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k}\alpha_{k_j}[\cos(q\beta_{k_j}\cdot\sigma) - 1]$.

The Fourier inversion theorem gives us

$$\varphi(\xi) = e^{\varepsilon\xi}\varphi_\varepsilon(\xi) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{(is+\varepsilon)\xi}\hat{\varphi}_\varepsilon(s)ds,$$

which is absolutely convergent. This implies

$$\varphi(\xi) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{e^{(is+\varepsilon)\xi}}{(is+\varepsilon)R(s-i\varepsilon)}ds = \frac{1}{2\pi i}\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{is\xi}}{sR(s)}ds.$$

Because of the simple pole at $s = 0$, we break up the integral into

$$\varphi(\xi) = \frac{1}{2\pi i}\left(\int_{C_\varepsilon} + \int_{S_\varepsilon}\right)\frac{e^{is\xi}}{sR(s)}ds, \tag{2.19}$$

where C_ε is $(-\infty, -\varepsilon]$ and $[+\varepsilon, +\infty)$ on the real axis, and S_ε is the half-circle at the origin. First consider the C_ε integral. We have

$$\begin{aligned}
\frac{1}{2\pi i}\int_{C_\varepsilon}\frac{e^{is\xi}}{sR(s)}ds &= \frac{1}{2\pi i}\left(\int_{-\infty}^{-\varepsilon} + \int_{+\varepsilon}^{+\infty}\right)\frac{e^{is\xi}}{sR(s)}ds \\
&= \frac{1}{2\pi i}\int_{+\varepsilon}^{+\infty}\left[\frac{e^{is\xi}}{sR(s)} - \frac{e^{-is\xi}}{sR(-s)}\right]ds \qquad (2.20) \\
&= \frac{1}{\pi}\int_{+\varepsilon}^{+\infty}\frac{A(s)\sin(s\xi)}{s(A^2(s)+c^2s^2)}ds + \frac{c}{\pi}\int_{+\varepsilon}^{+\infty}\frac{\cos(s\xi)}{A^2(s)+c^2s^2}ds,
\end{aligned}$$

where

$$A(s) = 1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k}\alpha_{k_j}[1-\cos(s\beta_{k_j}\cdot\sigma)]. \tag{2.21}$$

Note that for $s \in I\!\!R$, $A(s) = \Re[R(s)]$.

For the S_ε integral, we have

$$\frac{1}{2\pi i}\int_{S_\varepsilon}\frac{e^{is\xi}}{sR(s)}ds = \frac{1}{2\pi i}2\pi i\frac{1}{2}\mathrm{Res}\left(\frac{e^{is\xi}}{sR(s)},0\right) = \frac{1}{2} \tag{2.22}$$

Combining the integral results (2.20) and (2.22) in (2.19), and letting $\varepsilon \to 0$, we obtain an explicit formula for $\varphi(\xi)$. From (2.19), we have the following formula for the solution of (2.9):

$$\begin{aligned}\varphi(\xi) = \frac{1}{2} \quad &+ \quad \frac{1}{\pi}\int_0^\infty \frac{A(s)\sin s\xi}{s(A^2(s)+c^2s^2)}ds \\ &+ \quad \frac{c}{\pi}\int_0^\infty \frac{\cos s\xi}{A^2(s)+c^2s^2}\,ds.\end{aligned} \tag{2.23}$$

Recall that we made the assumption that φ was a solution of (2.9). Since we have constructed such a solution, the assumption has been validated.

Noting that

$$\begin{aligned}1-\varphi(-\xi,-c) &= \frac{1}{2}-\frac{1}{\pi}\int_0^\infty \frac{-A(s)\sin(s\xi)}{s(A^2(s)+c^2s^2)}ds - \frac{-c}{\pi}\int_0^\infty \frac{\cos(s\xi)}{A^2(s)+c^2s^2} \\ &= \varphi(\xi,c),\end{aligned}$$

we see that, for $\varphi(\xi) = \varphi(\xi,c)$, we have the symmetry property $\varphi(\xi,c) = 1 - \varphi(-\xi,-c)$.

Recalling that

$$\varphi(\xi) = \frac{1}{2\pi i} \int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{is\xi}}{sR(s)} ds.$$

we can see that as $\xi \to -\infty$, $\varphi(\xi) \to 0$. Our symmetric property then gives us that $\varphi(+\infty) = 1$.

Proposition 2.1 *Let $\varphi(\xi, c)$ denote the solution function (2.23). Then $\varphi(\xi, c)$ is continuous in both ξ and c, and is analytic in c, for $c \neq 0$. In addition, for $c \neq 0$, the derivative of $\varphi(\xi, c)$ with respect to c,*

$$\psi(\xi) = \psi(\xi, c) = D_c\varphi(\xi, c),$$

is bounded as $\xi \to \pm\infty$. For $\xi \neq 0, \psi(\xi)$ satisfies the equation

$$-\varphi'(\xi) - c\psi'(\xi) = L\psi(\xi) - \psi(\xi),$$

which is the derivative of the equation with respect to c.

Proof. For any compact subset of $\{c \in I\!R | c \neq 0\}$, there exists a uniform lower bound

$$|A^2(s) + c^2 s^2| \geq K_1(1 + s^2) \quad \text{for} \quad s \geq 0, \tag{2.24}$$

and thus, there exists a uniform lower bound for the denominators of the solution $\varphi(\xi)$, (2.23). Note that if $c = 0$, then $A^2(s) + c^2 s^2 = A^2(s) = 0$ for some $s > 0$. This in turn yields an upper bound of the form $K_2(1+s^2)^{-1}$, for bounded ξ, for the two integrands in (2.23). This, and the analyticity of the integrands in c and continuity in (ξ, c) for each s, imply the analyticity and continuity of φ.

The boundedness of ψ is easily proved by differentiating the formula for φ, (2.23), with respect to c, i.e.,

$$\begin{aligned}\psi(\xi,c) &= D_c\varphi(\xi,c)\\ &= -\frac{2c}{\pi}\int_0^\infty \frac{sA(s)\sin(s\xi)}{(A^2(s)+c^2s^2)^2}ds + \frac{1}{\pi}\int_0^\infty \frac{\cos(s\xi)}{A^2(s)+c^2s^2}ds\\ &\quad -\frac{2c^2}{\pi}\int_0^\infty \frac{s^2\cos(s\xi)}{(A^2(s)+c^2s^2)^2}ds.\end{aligned}$$

Therefore, by (2.24), ψ is bounded.

Differentiating (2.13), we obtain

$$-\varphi'(\xi) - cD_c\varphi'(\xi) = D_cL\varphi(\xi) - D_c\varphi(\xi).$$

Along with $\psi(\xi,c) = D_c\varphi(\xi,c)$, this implies that

$$-\varphi'(\xi) - c\psi'(\xi) = L\psi(\xi) - \psi(\xi),$$

as desired.

■

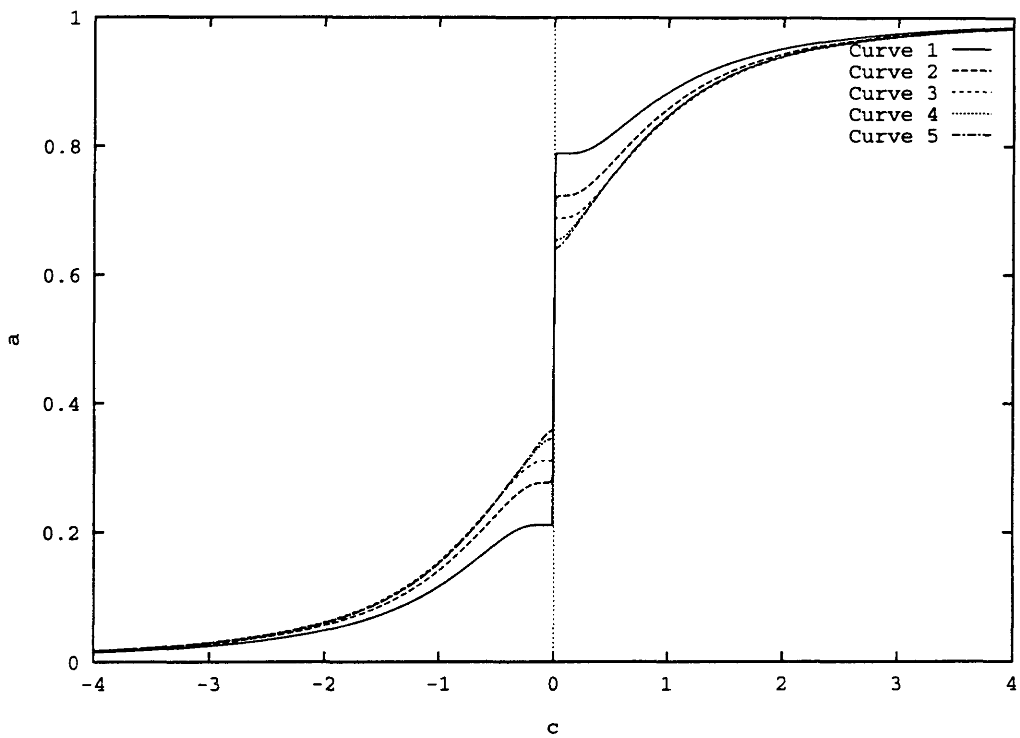


Figure 2.4: Plots of c versus a for various values of σ.

Since for $\varphi(\xi)$ in (2.23), there is an infinite family of wave forms that satisfies this formula, we want to specify an "initial condition" so that we can study an individual translate. As we discussed before, we choose $\varphi(0) = a$. This then gives us the following relation between a and c:

$$\varphi(0, c) = a = \frac{1}{2} + \frac{c}{\pi} \int_0^\infty \frac{ds}{A^2(s) + c^2 s^2}, \tag{2.25}$$

(see Figure 2.4). Note that in Figure 2.4, for Curve 1, $\sigma = (1, 0, 0)$; for Curve 2, $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$; for Curve 3, $\sigma = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$; for Curve 4, $\sigma = (\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}})$; and for Curve 5, $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{6}})$. Set

$$\Gamma(c) := \varphi(0, c) - \frac{1}{2} = \frac{c}{\pi} \int_0^\infty \frac{ds}{A^2(s) + c^2 s^2}, \qquad c \neq 0. \tag{2.26}$$

We now show that Γ is odd in c, analytic in c, and discontinuous at $c = 0$.

Theorem 2.1 *Let $\Gamma(c)$ be defined by (2.26). Then Γ is odd and analytic, moreover*

$$|\Gamma(c)| < \frac{1}{2}$$

for $c \neq 0$. In addition,

$$\lim_{c \to \infty} \Gamma(c) = \frac{1}{2}, \qquad \lim_{c \to 0+} \Gamma(c) = \gamma,$$

where $\gamma > 0$ *is the quantity*

$$\gamma = \lim_{T\to\infty} \frac{1}{2T} \int_0^T \frac{ds}{A(s)}, \tag{2.27}$$

where the limit always exists.

Proof. The proof follows from Theorem 4.3 in [7] with the upper bound of $|A(s) - A_\varepsilon(s)|$ being $2 + 8\omega + \varepsilon$ (where $\omega = \sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j} < \infty$ by assumption) instead of $2 + 16\alpha + \varepsilon$.

■

Note that as $\alpha \to 0$, $1/A(s) \to 1$, thus $\gamma = \lim_{T\to\infty} 1/2 = 1/2$. So as $\alpha \to 0$, the interval of propagation failure, $[1/2 - \gamma, 1/2 + \gamma]$, expands to the interval $(0, 1)$.

Now we wish to study how the range of propagation failure depends on the rational dependence/independence of the $\{\sigma_k\}_{k=1}^n$. First consider $A(s)$, (2.21). Then

$$\begin{aligned}
\frac{1}{A(s)} &= \left(1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}[1 - \cos((\beta_{k_j} \cdot \sigma)s)]\right)^{-1} \\
&= \left(1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j} - \sum_{k=1}^{\infty}\sum_{i=1}^{m_k} \alpha_{k_j}(e^{i(\beta_{k_j}\cdot\sigma)s} + e^{-i(\beta_{k_j}\cdot\sigma)s})\right)^{-1} \\
&= \left(1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}\right)^{-1} \\
&\qquad \sum_{l=0}^{\infty} \left(1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}\right)^{-l} \left(\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}(e^{i(\beta_{k_j}\cdot\sigma)s} + e^{-i(\beta_{k_j}\cdot\sigma)s})\right)^{l}
\end{aligned}$$

$$= \sum_{\mathbf{p}\in\mathbb{Z}^n} \omega_{\mathbf{p}} e^{i(\mathbf{p}\cdot\sigma)s}.$$

The last equality follows since there are at most n frequencies. Note also that $A(s) > 0$ implies $\omega_{\mathbf{p}} > 0$ for all $\mathbf{p} \in \mathbb{Z}^n$.

Example 2.11 *An example of $\omega_{\mathbf{p}}$. Let $m_k = 0$ for $k = 2, 3, \ldots$, and let $n = 2$. Also let $\alpha_{1_1} = \alpha_{1_2} = \alpha \in \mathbb{R}$. Then*

$$\left(1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}\right)^{-1} \sum_{l=0}^{\infty} \left(1 + 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}\right)^{-l} \left(\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}(e^{i(\beta_{k_j}\cdot\sigma)s} + e^{-i(\beta_{k_j}\cdot\sigma)s})\right)^l$$

simplifies to

$$(1+4\alpha)^{-1}\sum_{l=0}^{\infty}(1+4\alpha)^{-l}\alpha^l(e^{i(\beta_{1_1}\cdot\sigma)s} + e^{-i(\beta_{1_1}\cdot\sigma)s} + e^{i(\beta_{1_2}\cdot\sigma)s} + e^{-i(\beta_{1_2}\cdot\sigma)s})^l.$$

Expanding and rearranging the terms in this series, we obtain

$$\sum_{\mathbf{p}\in\mathbb{Z}^n} \omega_{p_1,p_2} e^{i(p_1\sigma_1 + p_2\sigma_2)},$$

where

$$\omega_{p_1,p_2} = \sum_{k=0}^{\infty} \frac{(|p_1|+|p_2|+2k)!(|p_1|+|p_2|+2k)!}{(|p_1|+|p_2|+k)!k!(|p_1|+k)!(|p_2|+k)!} \cdot \frac{\alpha^{(|p_1|+|p_2|+2k)}}{(1+4\alpha)^{(|p_1|+|p_2|+2k+1)}}.$$

■

We can now write γ as

$$
\begin{aligned}
\gamma &= \lim_{T\to\infty} \frac{1}{2T} \int_0^T \frac{1}{A(s)} ds \\
&= \lim_{T\to\infty} \frac{1}{2T} \int_0^T \sum_{\mathbf{p}\in\mathbb{Z}^n} \omega_{\mathbf{p}} e^{i(\mathbf{p}\cdot\sigma)s} ds \\
&= \frac{1}{2} \sum_{\mathbf{p}\cdot\sigma=0} \omega_{\mathbf{p}}. \qquad (2.28)
\end{aligned}
$$

Since $\gamma := \lim_{c\to 0+} \Gamma(c)$, γ determines the range of a for which the wave speed is zero, i.e. the range of propagation failure. Thus the range of propagation failure depends on the rational dependence or independence of the elements of σ, [18].

Example 2.12 *Let the σ_k be rationally independent. Then the summation in (2.28) has only one term, namely $\omega_{\mathbf{0}}$, and*

$$\gamma = \frac{\omega_{\mathbf{0}}}{2},$$

where $\mathbf{0}$ represents the vector of all zeros.

■

Lemma 2.2 *The function $R(s)$ of (2.18) has a simple root $s = -iz_0$ with $z_0 > 0$, and $iR'(-iz_0) > 0$. Moreover, there exists $\epsilon_0 > 0$ such that if, $s \in \mathbb{C}$ is any other root of R satisfying $\Im(s) \leq 0$, then $\Im(s) < -z_0 - \epsilon_0$. (Note $\Im(s)$ is the imaginary part of s).*

Proof. Consider

$$R(-iz) = -cz + 1 - \sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j} 2[\cosh(z\beta_{k_j} \cdot \sigma) - 1]. \tag{2.29}$$

The expression (2.29), considered as a function of $z \geq 0$, is positive at $z = 0$, negative for large z, and has a negative second derivative with respect to z, for all $z \geq 0$. This implies the existence of a unique $z_0 \geq 0$ at which $R(-iz_0) = 0$, and moreover, implies that $s = -iz_0$ is a simple root of R, and that the quantity $iR'(-iz_0)$ is positive. Note that $R(-iz) > 0$ whenever $0 \leq z < z_0$.

Consider now any other $s = u - iz$, where $z \geq 0$ and $R(s) = 0$. From the definition of R, we have that

$$\begin{aligned} 0 &= R(u - iz) \qquad (2.30) \\ &= -icu - cz + 1 - 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}[-1 + \cos(u\beta_{k_j} \cdot \sigma)\cosh(z\beta_{k_j} \cdot \sigma) \\ &\qquad + i\sin(u\beta_{k_j} \cdot \sigma)\sinh(z\beta_{k_j} \cdot \sigma)], \end{aligned}$$

and taking the real part of (2.30) gives

$$\begin{aligned} 0 &= -cz + 1 - \sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j} 2[-1 + \cos(u\beta_{k_j} \cdot \sigma)\cosh(z\beta_{k_j} \cdot \sigma)] \\ &\geq R(-iz), \qquad (2.31) \end{aligned}$$

where we note (2.29). Necessarily $z \geq z_0$, as $R(-iz) > 0$ if $0 \leq z < z_0$ holds.

All that remains now is to show that $z > z_0 + \varepsilon_0$ for some ε_0 independent of the root s, unless $s = -iz_0$. Taking the imaginary part of (2.30)

$$0 = -cu - 2\sum_{k=1}^{\infty}\sum_{j=1}^{m_k} \alpha_{k_j}[\sin(u\beta_{k_j} \cdot \sigma)\sinh(z\beta_{k_j} \cdot \sigma)] \tag{2.32}$$

first shows that there is a bound $|u| \leq K$ on the real parts of all roots s in the strip $z_0 \leq z \leq z_0 + 1$, and so this strip contains only finitely many roots of R. It is therefore enough to prove that the only root of R on the horizontal line $\Im(s) = -z_0$ is the root $s = -z_0$ obtained above. Suppose, therefore, that $z = z_0$. Then the inequality in (2.31) is an equality, and so $\cos(u(\beta_{k_j} \cdot \sigma)) = 1$, for all k, by (2.29). Thus $\sin(u(\beta_{k_j} \cdot \sigma)) = 0$, and so $u = 0$ by (2.32). Thus we have $s = -iz_0$, as desired.

■

Corollary 2.1 *The solution φ of (2.13), given by (2.23), satisfies*

$$\varphi(\xi) = Ce^{z_0\xi} + O(e^{(z_0+\epsilon_0)\xi}) \quad \text{as} \quad \xi \to -\infty, \tag{2.33}$$

where z_0 and ϵ_0 are as in Lemma 2.2, and where $C > 0$. The derivative φ' satisfies the formula

$$\varphi'(\xi) = Cz_0e^{z_0\xi} + O(e^{(z_0+\epsilon_0)\xi}) \quad \text{as} \quad \xi \to -\infty,$$

obtained by formally differentiating (2.33). The analogous results for $\xi \to \infty$, obtained *from the symmetry property, hold. In particular, there exists $T > 0$ such that*

$$\varphi'(\xi) > 0 \quad \text{for} \quad |\xi| \geq T. \tag{2.34}$$

Proof. See Corollary 4.5 in [7].

■

Theorem 2.2 *The solution φ of (2.13), given by (2.23), is strictly increasing on the real line. In particular, φ also satisfies equation (2.9), with boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$, where the nonlinearity f is given by (2.10).*

Proof. We begin by proving that

$$0 < \varphi(\xi) < 1 \tag{2.35}$$

for all $\xi \in I\!R$. Suppose that (2.35) is false, and $\varphi(\xi) \geq 1$ for some ξ. Let T be the same as in Corollary 2.1. Then, by Corollary 2.1, $\varphi'(\xi) > 0$ for $|\xi| \geq T$. This, along with the boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$, implies that $0 < \varphi(\xi) < 1$ for $|\xi| \geq T$. Now let $\eta = \sup\{\varphi(\xi) | \xi \in I\!R\}$, thus $\eta \geq 1$, since $\varphi(\xi) \geq 1$ for some ξ. Thus there must exist an $\xi_0 \in I\!R$ such that $\varphi(\xi_0) = \eta$. Let η_0 be the leftmost such η. Then $\varphi(\xi) < \eta_0$ for all $\xi < \xi_0$. Recall that each centered difference term of the operator

L is $\varphi(\xi + v) + \varphi(\xi - v) - 2\varphi(\xi)$ for some vector v. Because of this, and because $\alpha_{k_i} \geq 0$ $\forall k_i$, and $\alpha_{k_i} > 0$, for some k_i, $L\varphi(\xi_0) < 0$. Then by a continuity argument, $\varphi'(\xi_0 - \epsilon)$ and $\varphi'(\xi_0 + \epsilon)$ are both nonzero and of the same sign for ϵ sufficiently small. But, since $\varphi(\xi)$ is piecewise C^1, this contradicts the fact that η_1 is a point where $\varphi(\xi)$ achieves a maximum. Hence, $0 < \varphi(\xi) < 1$ for all $\xi \in I\!R$.

Using the facts that $0 < \varphi(\xi) < 1$, $\varphi(-\infty) = 0$, and $\varphi(+\infty) = 1$, we may assume that

$$\varphi(\xi) < \varphi(T_0) \quad \text{for} \quad \xi < T_0, \qquad \varphi(\xi) > \varphi(-T_0) \quad \text{for} \quad \xi > -T_0,$$

for some $T_0 \geq T$. Let $\tau > 0$ and define the function

$$\psi_\tau(\xi) = \varphi(\xi + \tau) - \varphi(\xi).$$

From the Corollary 2.1, we have that

$$\psi_\tau(\xi) > 0 \quad \text{if} \quad \text{either} \quad \xi \geq T_0 \quad \text{or} \quad \xi \leq -T_0 - \tau.$$

Suppose that $\tau > 2T_0$. Then, for any $\xi \in I\!R$, either $\xi < T_0$ or $\xi + \tau > T_0$. This implies that $\psi_\tau(\xi) = \varphi(\xi + \tau) - \varphi(\xi) > 0$ for all $\xi \in I\!R$.

Now define the quantity

$$\tau_0 = \inf\{\tau > 0 | \psi_\tau > 0 \quad \text{for} \quad \text{all} \quad \xi \in \mathbb{R}\}.$$

This implies that $\tau_0 \geq 0$ and $\tau_0 \leq 2T_0$, i.e., $\tau_0 \in [0, 2T_0]$. Note that, if $\tau_0 = 0$, then $\varphi'(\xi) > 0$ for all $\xi \in \mathbb{R}$. Now suppose $\tau_0 > 0$. By definition, $\psi_{\tau_0} \geq 0$ for all $\xi \in \mathbb{R}$. Since $\tau_0 = 0$, there exists a point ξ_0 such that $\psi_{\tau_0} = 0$. Since $\psi_\tau(\xi) > 0$ if either $\xi \geq T_0$ or $\xi \leq -T_0 - \tau$, it follows that $\xi_0 \in [-T_0 - \tau_0, T_0]$. Now let ξ_1 be the leftmost such ξ_0; then $\psi_\tau(\xi) > 0$ for $\xi < \xi_0$. This implies that $\psi(\xi_0 + v) + \psi(\xi_0 - v) - 2\psi(\xi_0) > 0$, and as a consequence, $L\psi(\xi_0) > 0$. Now recall (2.13). Subtracting the $\varphi(\xi + \tau_0)$ and the $\varphi(\xi)$ versions of equation (2.13), we obtain

$$-c\psi'_{\tau_0}(\xi) = L\psi_{\tau_0}(\xi) - \psi_{\tau_0}(\xi) + h(\xi + \tau_0) - h(\xi). \tag{2.36}$$

Now notice that at ξ_0 the right hand side of (2.36) is positive. But since ψ_{τ_0} is a minimum at ξ_0, the left hand side is 0. This contradiction implies that $\tau_0 \not> 0$.

■

Theorem 2.3 *The function* Γ *given by (2.26) satisfies*

$$\Gamma'(c) > 0 \quad \text{for} \quad \text{all} \quad c \neq 0. \tag{2.37}$$

In particular, for each $a \in (0,1)$, *equation (2.25) has exactly one solution* $c \neq 0$ *if and only if* $|a - 1/2| > \gamma$, *and has no solution* $c \neq 0$ *if and only if* $|a - 1/2| \leq \gamma$. *The solution* $c = c(a)$ *depends analytically on* a, *for* $|a - 1/2| > \gamma$.

Proof. The proof of this theorem follows from the proof of Theorem 4.7 in [7], with the appropriate change of the operator L.

■

2.3 Zero Wave Speed

In this section, we consider solutions to (2.9), our traveling wave equation, with wave speed $c = 0$. In this case, as opposed to the $c \neq 0$ case, we are only concerned with values $\varphi(\xi)$ for $\xi \in D$, where $D \subseteq \mathbb{R}$ is the countable set (2.4). This is because with $c = 0$, (2.9) becomes just a difference equation. Recall that if the $\{\sigma_k\}_{k=1}^n$ are rationally independent, then D is a dense subset of $\mathbb{R}$, while if $\{\sigma_k\}_{k=1}^n$ are rationally dependent, then $D = \{m\nu | m \in \mathbb{Z}\}$ holds for some quantity $\nu > 0$, and D is a discrete subset of $\mathbb{R}$. Note that both forms of D have measure zero.

This section begins with the construction of a solution $\varphi(\xi)$ from $\mathbb{R}$ to $\mathbb{R}$ of (2.9) by taking the limit as $c \to 0$ of the solution found in the last section. First we take a sequence $c_n \to 0$ which gives us a function φ_* such that $\varphi(\xi, c_n) \to \varphi_*(\xi)$. Since φ_* can (and does) have jump discontinuities, we use the right- and left-hand limits of φ_*, φ_+ and φ_-, respectively. Note that φ_* is defined almost everywhere on $\mathbb{R}$, but we need a function that is defined for all $\xi \in \mathbb{R}$. Thus we construct a function φ_τ as a linear combination of φ_+ and φ_-, which is defined for all $\mathbb{R}$. Next we show that for σ such that the σ_k are rationally independent, φ_τ is strictly increasing on $\mathbb{R}$. For σ such that the σ_k are rationally dependent, we show that φ_τ is constant on the intervals $(n\nu, (n+1)\nu)$, where ν is such that $D = \{m\nu | m \in \mathbb{Z}\}$. Lastly, we see that $\varphi = \varphi_\tau$ on D satisfies $0 = L\varphi(\xi) - f(\varphi(\xi))$.

We construct solutions of (2.9) which satisfy

$$\varphi(\xi) < a \quad \text{for} \quad \xi \in (-\infty, \xi_0) \cap D, \qquad \varphi(\xi) > a \quad \text{for} \quad \xi \in (\xi_0, \infty) \cap D, \tag{2.38}$$

which is a condition analogous to (2.12). Notice that since we need to consider the set D, we do not take $\xi_0 = 0$ as the point where $\varphi(\xi) = a$. We let ξ_0 be arbitrary. This basically gives us two cases for ξ_0, either $\xi_0 \in D$ or $\xi_0 \notin D$.

Although we only need to consider solutions $\varphi : D \to \mathbb{R}$, we shall start out by constructing solutions $\varphi : \mathbb{R} \to \mathbb{R}$. Then we examine the restriction of φ to D and discuss why this is correct.

In the previous section, we derived traveling wave solutions of (2.9) when $c \neq 0$. Now we only need to look at these solutions as $c \to 0$, but first some notation. Let $\tau \in \mathbb{R}$ and define the function $h_\tau : \mathbb{R} \to \mathbb{R}$ by

$$h_\tau(u) = \begin{cases} h(u), & u \neq 0, \\ \tau, & u = 0. \end{cases} \tag{2.39}$$

That is, h_τ is just the Heaviside step function (2.11) with the value τ assigned to $h_\tau(0)$. Notice that while h is set valued, h_τ is single-valued everywhere. Now let

$$h_- = h_0, \qquad h_+ = h_1, \tag{2.40}$$

the function h_τ with $\tau = 0, 1$, respectively. Note that the limit of h as u approaches zero from the right and from the left, $h(0\pm)$, is equal to $h_\pm$.

Let $\varphi(\xi, c)$ denote the solution to (2.13), and consider a sequence $c_n \to 0$ with each $c_n \neq 0$. Because the solution $\varphi(\xi, c)$ is increasing and uniformly bounded in ξ, by Theorem 2.2, we have the limit

$$\varphi(\xi, c_n) \to \varphi_*(\xi)$$

pointwise, for all but countably many $\xi \in I\!R$, for some nondecreasing limit function $\varphi_* : I\!R \to [0, 1]$ (by [25]). One of the first things we encounter is that φ_* has discontinuities. As φ_* is monotone, all of its discontinuities are jumps, and so we may define two other functions $\varphi_\pm : I\!R \to [0, 1]$ by

$$\varphi_-(\xi) = \varphi_*(\xi-), \qquad \varphi_+(\xi) = \varphi_*(\xi+),$$

the left- and right-hand limits of φ_* at each point $\xi \in I\!R$. The functions φ_- and φ_+ are left- and right-continuous on $I\!R$. These limits also equal φ_* almost everywhere.

Since we want to take the limit in (2.13) as $c_n \to 0$, we must rewrite (2.13) in integrated form so that we do not have to deal with the $\varphi'(\xi)$ term. This means that we fix $\xi \in I\!R$ and integrate (2.13) to obtain

$$-c[\varphi(\xi)-\varphi(0)] = \int_0^{\xi}[L\varphi(\zeta)-\varphi(\zeta)+h(\zeta)]d\zeta. \tag{2.41}$$

Now let $c = c_n$ and let $c_n \to 0$. Then the Lebesgue dominated convergence theorem implies that (2.41) converges to

$$0 = \int_0^{\xi}[L\varphi_*(\zeta)-\varphi_*(\zeta)+h(\zeta)]d\zeta,$$

for all ξ. Now we differentiate to obtain

$$0 = L\varphi_*(\xi)-\varphi_*(\xi)+h(\xi),$$

which holds for almost every $\xi \in I\!R$.

But we need a solution function that holds for all $\xi \in I\!R$, because φ_* may fail at points ξ such that $\xi \in D$. Notice that for the functions $\varphi_\pm$, we have

$$0 = L\varphi_\pm(\eta)-\varphi_\pm(\eta)+h_\pm(\eta), \tag{2.42}$$

which holds almost everywhere, with $h_\pm$ as in (2.40). This is because $L\varphi_\pm, \varphi_\pm$, and $h_\pm$ agree almost everywhere with $L\varphi_*, \varphi_*$, and h_*, respectively. Note that φ_+ and h_+ are both right-continuous, and φ_- and h_- are both left-continuous, on $I\!R$. This implies that (2.42) can be obtained at every $\xi \in I\!R$. This implies that, for either choice of $+$ or $-$ of $\pm$, (2.42) holds for all $\xi \in I\!R$.

Define the linear combination

$$\varphi_\tau = \tau\varphi_+(\xi) + (1-\tau)\varphi_-(\xi).$$

Then with (2.42), the definition of h_τ and $h_\pm$, and since $\tau(h_0 - h_1) + h_\tau - h_0 = 0$, the equation

$$0 = L\varphi_\tau(\xi) - \varphi_\tau(\xi) + h_\tau(\xi), \tag{2.43}$$

holds <u>for all</u> $\xi \in I\!R$. Now notice that φ_τ monotone. Taking the limits of $\varphi_\tau(\xi)$ as ξ goes to $\pm\infty$, we obtain

$$\varphi_\tau(-\infty) = 0, \qquad \varphi_\tau(+\infty) = 1, \tag{2.44}$$

which implies that φ_τ satisfies the boundary conditions of (2.13).

Theorem 2.4 *Let $m_k = 0$ for $k = 2, 3, \cdots$, and $\alpha_{1_i} = \alpha, \alpha \in I\!R$. Let $\tau \in [0,1]$. If the $\{\sigma_k\}_{k=1}^n$ are rationally independent, then the function φ_τ is strictly increasing on $I\!R$. If the $\{\sigma_k\}_{k=1}^n$ are rationally dependent, then $\varphi_\tau(\xi) \le \varphi_\tau(\xi+\nu)$ for all $\xi \in I\!R$, where ν is such that $D = \{m\nu | m \in Z\!\!Z\}$. In any case, if we define*

$$\varphi_\tau(\xi, \xi_0) = \varphi_\tau(\xi - \xi_0), \tag{2.45}$$

then for any $\tau \in [0,1]$ *and* $\xi_0 \in \mathbb{R}$, *the function* $\varphi_\tau(\cdot,\xi_0)$ *restricted to the set* D *is strictly increasing.*

Proof. Let $\tau \in [0,1]$ be fixed. We observe that for such a τ, the function φ_τ is nondecreasing everywhere on $\mathbb{R}$, as it is a convex combination of the nondecreasing functions $\varphi_\pm$. Now suppose that $I \subseteq \mathbb{R}$ is an interval on which φ_τ is constant, that is, $\varphi_\tau(\xi_1) = \varphi_\tau(\xi_2)$ for all $\xi_1, \xi_2 \in I$. Recall that $m_1 = n$. From (2.43) and the formula for L in (2.13), we have

$$\begin{aligned} \varphi_\tau(\xi+\sigma_1) = -\varphi_\tau(\xi-\sigma_1) \quad &- \quad \sum_{k=2}^{n}[\varphi_\tau(\xi+\sigma_k)+\varphi_\tau(\xi-\sigma_k)] \\ &+ \quad \frac{1}{\alpha}[(1+2\alpha n)\varphi_\tau(\xi) - h_\tau(\xi)]. \end{aligned} \tag{2.46}$$

Notice that the right-hand side of (2.46) is nonincreasing for $\xi \in I$ (in particular, since h_τ is nondecreasing, by the choice of τ). On the other hand, the left-hand side of (2.46) is nondecreasing for all $\xi \in \mathbb{R}$, and hence is constant for $\xi \in I$. Thus φ_τ is also constant on the interval $I + \sigma_1$, that is, $\varphi_\tau(\xi_1) = \varphi_\tau(\xi_2)$ for all $\xi_1, \xi_2 \in I + \sigma_1$, where $I + \rho = \{\xi + \rho | \xi \in I\}$ for any real ρ.

In the same way, we conclude that φ_τ is constant for all the $I + \sigma_k$ intervals. Thus, using (2.4), φ_τ is constant on the interval $I + \rho$ for each $\rho \in D$.

Now suppose that the interval I on which φ_τ is constant contains two distinct points $\xi_1, \xi_2 \in I$, with $\xi_2 - \xi_1 \in D$. Then the translates $I + \rho$ cover the real line and

φ_τ is constant on all $I\!R$. But this contradicts the facts $\varphi_\tau(-\infty) = 0$ and $\varphi_\tau(+\infty) = 1$. Hence no such ξ_1, ξ_2 exist.

Therefore, if $\xi_1 < \xi_2$ are real numbers such that $\xi_2 - \xi_1 \in D$, then $\varphi_\tau(\xi_1) < \varphi_\tau(\xi_2)$. Now if the σ_k are rationally independent, D is dense in $I\!R$ and φ_τ is strictly increasing. If the σ_k are rationally dependent, $D = \{n\nu | n \in \mathbb{Z}\}$, and for any $\xi \in I\!R$, $(\xi + \nu) - \xi = \nu \in D$; hence, $\varphi_\tau(\xi) < \varphi_\tau(\xi + \nu)$. The theorem now follows.

∎

Note that the function $\varphi(\xi) = \varphi_\tau(\xi - \xi_0)$ satisfies

$$0 = L\varphi(\xi) - \varphi(\xi) + h_\tau(\xi - \xi_0). \tag{2.47}$$

Proposition 2.2 *Let $\tau, \xi_0 \in I\!R$. Then a bounded function $\varphi : D \to I\!R$ satisfies equation (2.47) for all $\xi \in D$ if and only if $\varphi(\xi) = \varphi_\tau(\xi, \xi_0)$ for all $\xi \in D$.*

Proof. See Proposition 5.2 in [7].

∎

Corollary 2.2 *Assume that the $\{\sigma_k\}_{k=1}^n$ are rationally dependent, with ν as in $D = \{n\nu | n \in \mathbb{Z}\}$. Then for each integer n, the function φ_τ is constant on the interval $(n\nu, (n+1)\nu)$.*

Proof. See Corollary 5.3 in [7].

∎

Now that we have the functions

$$\varphi(\xi) = \varphi_\tau(\xi, \xi_0) = \varphi_\tau(\xi - \xi_0) \tag{2.48}$$

which satisfy

$$0 = L\varphi(\xi) - \varphi(\xi) + h_\tau(\xi - \xi_0), \tag{2.49}$$

we now state when these functions satisfy the nonlinear equation

$$0 = L\varphi(\xi) - f(\varphi(\xi)). \tag{2.50}$$

In particular, we determine the relationship between $\tau \in [0,1], \xi_0 \in \mathbb{R}$, and the detuning parameter a.

Recall that h is a set valued function. Since $f(u) = u - h(u-a)$, we want

$$h_\tau(\xi - \xi_0) \in h(\varphi(\xi) - a), \tag{2.51}$$

for all $\xi \in D$. Suppose

$$\varphi(\xi) < a \quad \text{for} \quad \xi \in (-\infty, \xi_0) \cap D, \qquad \varphi(\xi) > a \quad \text{for} \quad \xi \in (\xi_0, \infty) \cap D. \tag{2.52}$$

Now suppose ξ is such that $\xi \in D \backslash \{\xi_0\}$. Then (2.51) holds. Thus, if $\xi_0 \notin D$, then

(2.51) holds for all $\xi \in D$, and hence φ satisfies (2.50) for all $\xi \in D$. On the other hand, if $\xi_0 \in D$, then φ satisfies (2.50) if and only if (2.51) holds at $\xi = \xi_0$. So φ satisfies (2.50) if and only if

$$\tau \in h(\varphi(\xi_0) - a) = h(\varphi_\tau(0) - a).$$

First let's discuss the case when the $\{\sigma_k\}_{k=1}^n$ are rationally dependent. Recall that we are assuming that $\xi_0 \in D$. Also recall that, by Corollary 2.2, φ_τ is constant on each interval $(n\nu, (n+1)\nu)$, between the points of D. One way for (2.50) to hold is if $\varphi_\tau(0) = a$. In this case, the function (2.48) satisfies both inequalities in (2.52), by Theorem 2.4, and consequently is a solution of (2.50). Another way for (2.50) to hold is if $\varphi_\tau(0) < a$. Then we must have $\tau = 0$. Thus $\varphi(\xi) = \varphi_0(\xi, \xi_0) = \varphi_-(\xi - \xi_0)$. This implies that the first inequality in (2.52) holds. We also need the second to hold. The second inequality in (2.52) holds if and only if it holds at $\xi = \xi_0 + \nu$; that is, if and only if

$$a < \varphi(\xi_0 + \nu) = \varphi_-(\nu) = \varphi_+(0), \tag{2.53}$$

where $\varphi_-(\nu) = \varphi_+(0)$ because $\varphi_-(\xi) = \varphi_+(\xi)$ is constant on each interval $(n\nu, (n+1)\nu)$. Thus we have the solution $\varphi(\xi) = \varphi_-(\xi - \xi_0)$ as long as

$$\varphi_-(0) < a < \varphi_+(0). \tag{2.54}$$

Note that, with (2.54), $\varphi(\xi) = \varphi_+(\xi - \xi_0)$ is also a solution to (2.50). Since φ is constant on each $(n\nu, (n+1)\nu)$ interval, $\varphi_+(\xi - \xi_0)$ and $\varphi_-(\xi - \xi_0)$ are equivalent, i.e., $\varphi_+(\xi - \xi_0 - \nu) = \varphi_-(\xi - \xi_0)$. Thus we have two families of solutions, $\varphi(\xi) = \varphi_\tau(\xi - \xi_0)$ when $\varphi_\tau(0) = a$, and $\varphi(\xi) = \varphi_\pm(\xi - \xi_0)$.

Now let's discuss the case when at least two σ_k are rationally independent. Again we assume $\xi_0 \in D$. Using the same argument as in the case which the $\{\sigma_k\}_{k=1}^n$ are rationally dependent, we have that $\varphi(\xi) = \varphi_\tau(\xi - \xi_0)$ when $\varphi_\tau(0) = a$, $\varphi(\xi) = \varphi_-(\xi - \xi_0)$, and $\varphi(\xi) = \varphi_+(\xi - \xi_0)$. Note that here, however, the families containing $\varphi(\xi) = \varphi_-(\xi - \xi_0)$ and $\varphi(\xi) = \varphi_+(\xi - \xi_0)$ are distinct. This is the result of the strict monotonicity of φ. Thus $\varphi(\xi) = \varphi_+(\xi - \xi_0)$ cannot be obtained from $\varphi(\xi) = \varphi_-(\xi - \xi_0)$ by a simple translation (and vise versa). Also, the solution $\varphi_\tau(\xi, \xi_0)$, with $\varphi_\tau(0) = a$, is not equivalent to either $\varphi_\pm(\xi - \xi_0)$. Therefore when $\xi_0 \in D$, three distinct families of solutions satisfy (2.50) when a satisfies (2.54).

Chapter 3

NUMERICS

The goal of this chapter is to present the numerical methods used to solve the discrete traveling wave equation (2.9). The results of this chapter were presented in [10].

This chapter consists of four sections. In the first section we state clearly the problem that we solve numerically. This includes specifying asymptotic boundary conditions, a phase condition, and the methods used in solving our problem. In the first section, we also discuss the problem in terms of the cases $c = 0$ and $c \neq 0$. The first section concludes with a clarification of monotonicity constraints and the equidistributed mesh which they create. The next section discusses convergence of the numerical methods that we use. In the third section, we present actual results obtained. The waveforms, φ, are presented in graphical form. In the last section of this chapter, we compare our numerical results with our analytic results from Chapter 2.

3.1 Numerical Methods

This section begins by discussing how we represent the traveling wave equation (2.9). The first step is to truncate the infinite interval and employ asymptotic boundary conditions (see [2, 5, 12, 22]). Next we discuss the discretization of the traveling wave equations on the truncated interval. In particular, we consider a spline collocation scheme using piecewise cubic C^1 Hermite polynomials. We present an explicit representation of the system to be solved. Since the waveform is known to be monotone (see [7, 26]), we impose monotonicity constraints, which provide a natural mechanism for equidistribution of the mesh. After applying the asymptotic boundary conditions, a phase condition, and the collocation discretization, we solve the nonlinear system using Newton's method. Several different techniques for solving the resulting linear systems are considered, including Jacobi, Gauss-Seidel (GS), and Successive Over Relaxation (SOR). When the wave speed is not zero, we need to find the correct detuning parameter a. We use and present an adaptive quadrature method to approximate the integral term in equation (2.25). For the rest of this chapter, we assume $m_k = 0$ for $k > 1$, $\alpha_{1_i} = \alpha$, where $0 < \alpha \in \mathbb{R}$, and $L_n\varphi(\xi) := L\varphi(\xi) = \alpha \sum_{k=1}^{n}[\varphi(\xi+\sigma_k) + \varphi(\xi - \sigma_k) - 2\varphi(\xi)]$ (recall that $m_1 = n$).

3.1.1 The problem

Let T_- be the lower value and T_+ be the upper value at which we truncate the infinite interval. Let $J = [T_-, T_+]$. Also let $-c\varphi'(\xi) = L_n\varphi(\xi) - f(\varphi(\xi))$ hold for $T_- \leq \xi \leq T_+$. Now we choose asymptotic boundary equations such that $\varphi(\xi)$ is continuously differentiable for $\xi \leq T_-, \xi \geq T_+$; i.e., $\varphi^{(i)}(T_-^-) = \varphi^{(i)}(T_-^+)$ and $\varphi^{(i)}(T_+^-) = \varphi^{(i)}(T_+^+)$ for $i = 0, 1$. We implement the asymptotic boundary conditions using the method described in [2]. In particular, the asymptotic boundary equations are defined as

$$\varphi(\xi) = \kappa_+ e^{-\lambda_+ \xi} + 1, \quad \xi > T_+ \quad \text{and} \quad \varphi(\xi) = \kappa_- e^{\lambda_- \xi}, \quad \xi < T_-, \tag{3.1}$$

where $\kappa_\pm \in I\!R$ and $\lambda_\pm \geq 0$ are chosen so that $\varphi(\xi)$ is continuously differentiable for $\xi = T_\pm$.

Given a mesh

$$T_- = \xi_{-J_-} < \xi_{-J_-+1} < \cdots < \xi_0 = 0 < \cdots < \xi_{J_+-1} < \xi_{J_+} = T_+, \tag{3.2}$$

with meshsize $h_k = \xi_{k+1} - \xi_k$, we write $\varphi_k \approx \varphi(\xi_k)$. In our computations, we approximate φ_k' to second order by

$$\varphi_k' \approx \frac{h_{k-1}(\varphi_{k+1} - \varphi_k)}{h_k(h_k + h_{k-1})} + \frac{h_k(\varphi_k - \varphi_{k-1})}{h_{k-1}(h_k + h_{k-1})}. \tag{3.3}$$

Since the difference operator L_n may consist of any shifts σ_k such that $\sum_{k=1}^{n} \sigma_k^2 = 1$, we employ interpolants to evaluate the difference operator. In particular, we consider the collocation scheme for solving (2.9) based upon piecewise cubic C^1 Hermite polynomials

$$S_k(\xi) = a_k + b_k(\xi - \xi_k) + c_k(\xi - \xi_k)^2 + d_k(\xi - \xi_k)^3, \quad \xi \in [\xi_k, \xi_{k+1}]$$

where

$$\begin{aligned} a_k &= \varphi_k, \quad c_k = \frac{3(\varphi_{k+1} - \varphi_k)/h_k - 2\varphi_k' - \varphi_{k+1}'}{h_k}, \\ b_k &= \varphi_k', \quad d_k = \frac{\varphi_k' + \varphi_{k+1}' - 2(\varphi_{k+1} - \varphi_k)/h_k}{h_k^2}. \end{aligned} \tag{3.4}$$

Note that given (3.3) and (3.4), the b_k, c_k, and d_k are all represented in terms of the a_k.

Now let

$$S(\xi) = \begin{cases} S_k(\xi), & \xi \in [\xi_k, \xi_{k+1}], \quad k = -J_-, \ldots, J_+ - 1, \\ \kappa_- e^{\lambda_- \xi}, & \xi < T_-, \\ \kappa_+ e^{-\lambda_+ \xi} + 1, & \xi > T_+. \end{cases}$$

We want to solve for a particular translate, since all translated versions of the solution are equivalent. We do this by setting a phase condition. In fact, we pick the classical phase condition, $\varphi(0) = a$, as in Chapter 2. Then our problem (2.9), with boundary conditions $\varphi(-\infty) = 0$ and $\varphi(\infty) = 1$, is approximated by the collocation scheme

$$\begin{cases} -cS'(\xi_k) = L_n S(\xi_k) - f(S(\xi_k)), & k = -J_-, \ldots, -1, 1, \ldots, J_+ - 1, \\ S(\xi_0) = a. \end{cases} \tag{3.5}$$

This gives us $J_- + J_+ - 1$ equations in the $J_- + J_+ - 1$ unknowns, $a_{-J_-}, \ldots, a_{-1}, a_1, \ldots, a_{J_+-1}$.

If we write the solution to (3.5) as $G(\hat{a}) = 0$, where $\hat{a} = (a_{-J_-}, \ldots, a_{-1}, a_1, \ldots, a_{J_+-1})$, a Newton iteration then has the form

$$\begin{cases} -DG(\hat{a}^j)\delta^j = G(\hat{a}^j), \\ \hat{a}^{j+1} = \hat{a}^j + \delta^j, \end{cases}$$

where $DG(\hat{a}^j)$ is the Jacobian of G evaluated at $\hat{a}^j$.

Since the waveform is monotone, we enforce monotonicity conditions to obtain accurate approximations of $L_n \varphi_k$. Sufficient conditions for preserving monotonicity have been obtained (see [13, 19] and the references therein). The conditions are

$$\left(\frac{\varphi_{k+1} - \varphi_k}{h_k}\right) \cdot \left(\frac{\varphi_k - \varphi_{k-1}}{h_{k-1}}\right) > 0,$$

$$\theta_k := \varphi'_k \frac{h_k}{\varphi_{k+1} - \varphi_k} < 3, \quad \psi_k := \varphi'_{k+1} \frac{h_k}{\varphi_{k+1} - \varphi_k} < 3. \tag{3.6}$$

We enforce the monotonicity conditions by approximately equidistributing the values of θ_k and ψ_k in (3.6) starting from a uniform mesh by locally halving or doubling the mesh. We update the mesh using the interpolated values after each Newton iterate.

3.1.2 Zero Wave Speed

As we have shown in Section 2.3, in contrast to the traveling wave equations for the continuous case (2.6), the traveling wave equations for the discrete case (2.9) have standing wave solutions for a continuum of values of the parameter a. In fact, for $c = 0, a \in [1/2 - \gamma, 1/2 + \gamma]$. When $c = 0$, (2.9) reduces to a strictly algebraic problem,

$$0 = L_n\varphi(\xi) - f(\varphi(\xi)),$$

as opposed to (2.6) which reduces to a second order differential equation,

$$0 = \epsilon\varphi''(\xi) - f(\varphi(\xi)).$$

If we impose the classical phase condition and neglect the equation centered at $\xi = 0$, then the structure of the Jacobian is identical to the structure of the Jacobian without a phase condition. Neglecting the equation centered at $\varphi(0)$ is legitimate when the waveform is symmetric (as it is for $a = \frac{1}{2}$) or nearly symmetric about $\xi = 0$, because we need only satisfy an inclusion at $\xi = 0$. In one-dimension, at $\xi = 0$, $\alpha(\varphi(\sigma) + \varphi(-\sigma) - 2a) \in (a - 1, a)$ is the inclusion that we wish to satisfy.

3.1.3 Nonzero Wave Speed

In analogy with the case of zero wave speed, for nonzero wave speed, we enforce the classical phase condition, $\varphi(0) = a$, and neglect the equation centered at $\xi = 0$. Again, the structure of the Jacobian is preserved, and the differential inclusion may or may not be satisfied at $\xi = 0$. In one-dimension, at $\xi = 0$, $\alpha(\varphi(\sigma) + \varphi(-\sigma) - 2a) + \varphi'(0) \in (a-1, a)$ is the inclusion that we wish to satisfy.

When the wave speed is nonzero, we need to compute, *a priori*, the value of the detuning parameter a as a function of the wave speed c. This is done using an adaptive quadrature scheme based upon the composite trapezoidal rule to approximate the integral term

$$a - \frac{1}{2} = \frac{c}{\pi} \int_0^\infty \frac{ds}{A^2(s) + c^2 s^2}.$$

Step halving and step doubling is used to control the local error in the quadrature approximation starting from $s = 0$. The end point of the integration is determined by integrating until the integrand is sufficiently small and the global error in the quadrature is proportional to the error tolerance for G.

3.2 Convergence of Iterative Methods

We employ iterative solvers to solve the linear systems. Since the elements of σ are fixed and the mesh is typically nonuniform, we do not expect uniform bandwidths in the Jacobian, $-DG(\hat{a})$. In particular, we expect the bandwidth to be large near

$\xi = 0$ and smaller near T_+ and T_-. In the discretization of the Laplacian, the S that are evaluated at shifted points require four mesh points each to evaluate them. There are $2n$ shifted points in each equation. The $S'(\xi_k)$ term requires three mesh points to evaluate it. Since the mesh point at which $S(\xi_k)$ is evaluated, ξ_k, is one of the mesh points at which $S'(\xi_k)$ is evaluated, there are at most $8n + 3$ nonzero elements in any row of the Jacobian. In order to analyze the convergence of the Jacobi, Gauss-Seidel, and SOR methods, we present some background material on the convergence of iterative methods. Subsequently, the convergence of these methods for our particular cases of zero and nonzero wave speed is analyzed.

Let $-DG(\hat{a}^j) = M - N$. We solve for δ^j in the Newton iteration using the matrix splitting iteration scheme

$$M\delta^j_{i+1} = N\delta^j_i + G(\hat{a}^j). \tag{3.7}$$

Let $-DG(\hat{a}^j) = D - L - U$, where D is diagonal, L is strictly lower triangular, and U is strictly upper triangular. For the Jacobi method, $M = M_{Jac} = D$ and $N = N_{Jac} = L + U$. For the SOR method, $M = M_\omega = \frac{1}{\omega}D - L$ and $N = N_\omega = (\frac{1}{\omega} - 1)D + U$ for $\omega \neq 0$. Note that the Gauss-Seidel method is SOR with $\omega = 1$; thus $M_{GS} = D - L$ and $N_{GS} = U$.

Definition 3.1 *A matrix $A = (a_{ij}) \in I\!R^{n\times n}$ is diagonally dominant if*

$|a_{ii}| > \sum_{j\neq i} |a_{ij}|$ *for $i = 1, \ldots, n$.*

Definition 3.2 *A matrix* $A \in \mathbb{R}^{n\times n}$ *is an M-matrix if*

- $a_{ii} > 0$ *for* $i = 1, \ldots, n$,
- $a_{ij} \leq 0$ *for all* $i \neq j$,
- *the spectral radius* $\rho(D^{-1}(L+U)) < 1$, *and*
- *the entries of* $D^{-1}(L+U)$ *are nonnegative.*

Proposition 3.1 *If* $-DG(\hat{a}^j)$ *is an M-matrix, then the Jacobi and SOR (for* $\omega \in (0,1]$*) iterative methods converge.*

Proof. See Hackbusch [17], pp. 160–163.

∎

Definition 3.3 *Let* $A \in \mathbb{R}^{n\times n}$ *and let* $B = |D| - |A-D|$ *where* $|C|$ *denotes the matrix whose entries are the absolute values of the corresponding entries of the matrix* C*. The matrix* A *is called an H-matrix if* B *is an M-matrix.*

Proposition 3.2 *If* $-DG(\hat{a}^j)$ *is an H-matrix, then the Jacobi and Gauss-Seidel iterative methods converge.*

Proof. See Hackbusch [17], pp. 163–164.

∎

We now investigate the structure of the Jacobian, $-DG(\hat{a})$. For simplicity, we consider the case of a linear interpolant and the approximation $(\varphi_{j+1} - \varphi_{j-1})/(h_j +$

h_{j-1}) for the derivative φ'_j. The Jacobian using the cubic interpolant may be obtained as a perturbation of the Jacobian analyzed here.

Theorem 3.1 *Given a mesh* $\{\xi_j\}_{j=-J_-}^{J+}$, *let* $\omega_j^i = \xi_j - \sigma_i - \xi_k$, *where* ξ_k *denotes the left mesh point in the interval containing* $\xi_j - \sigma_i$, *and* $\chi_j^i = \xi_j + \sigma_i - \xi_l$, *where* ξ_l *denotes the left mesh point of the interval containing* $\xi_j + \sigma_i$. *Assume that piecewise linear interpolation with a first order approximation of the derivative, the classical phase condition, and asymptotic boundary conditions are employed. Note that*

$$- DG(\hat{a})_{j,j-1} = \frac{c}{h_j + h_{j-1}} - \alpha \sum_{i \in I_j} \frac{h_{j-1} - \omega_j^i}{h_{j-1}}, \tag{3.8}$$

where I_j *denotes those values of* i *for which* $\xi_j - \sigma_i \in [\xi_{j-1}, \xi_j)$. *Then* $-DG(\hat{a})$ *is an M-matrix if, for all* j,

$$- DG(\hat{a})_{j,j-1} < 0. \tag{3.9}$$

Otherwise, $-DG(\hat{a})$ *is an H-matrix if, for all* j,

$$\frac{2|c|}{h_j + h_{j-1}} < 1. \tag{3.10}$$

Proof. To prove that $-DG(\hat{a})$ is an M-matrix given condition (3.9), here it is sufficient to show that $-DG(\hat{a})$ is diagonally dominant. Since we are using linear interpolants, the terms multiplying α cancel and since $-DG(\hat{a})_{j,j-1} < 0$, the term multiplying c in $|-DG(\hat{a})_{j,j-1}|$ cancels with the term multiplying c in $|-DG(\hat{a})_{j,j+1}|$. Since $f'(\xi_j) = 1$ for $\xi_j \neq 0$, $-DG(\hat{a})$ is diagonally dominant.

To prove that $-DG(\hat{a})$ is an H-matrix given (3.10), note that, in this case, the terms multiplying α cancel, but the terms multiplying c do not.

■

Remark 3.1 *When $c = 0$, Theorem 3.1 shows that $-DG(\hat{a})$ is an M-matrix, thus $-DG(\hat{a})$ is an M-matrix for $|c|$ sufficiently small.*

Remark 3.2 *The contraction factor for the Jacobi method when $c = 0$ increases to 1 as $\alpha \rightarrow \infty$.*

Corollary 3.1 *If the Jacobi iteration converges, then Newton's method using the Jacobi method to solve the linear systems converges. Similarly, if for a value of ω the SOR iteration converges, then Newton's method using SOR converges.*

Proof. See Ortega and Rheinboldt [24], pp. 321–332.

■

3.3 Numerical Results

In this section, we present the results of some numerical experiments. All of our calculations were obtained on a Silicon Graphics Indigo^2 workstation using double precision (i.e. machine epsilon $\epsilon_M \approx 2.2 * 10^{-16}$). We set tolerances for Newton's method and the iterative method, and upper and lower tolerances for the values of θ and ψ in (3.6). We employ inverse tangent and hyperbolic tangent functions as initial guesses. All computations were performed using Gauss-Seidel as the iterative method, although similar results were obtained using Jacobi, and SOR.

In Figure 3.1, we plot waveforms obtained for $\alpha = \frac{1}{2}$, $c = 0$, and various values of σ and a. Using the same values of σ employed in Figure 3.1, we choose the parameter a to be slightly smaller than $\frac{1}{2} + \gamma(\sigma, \alpha)$ (see (2.25) and (2.27)). For Waveform 1, we set $\sigma = (1, 0, 0)$ and $a = 0.78$; for Waveform 2, we set $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$ and $a = 0.71$; for Waveform 3, we set $\sigma = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$ and $a = 0.68$; for Waveform 4, we set $\sigma = (\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}})$ and $a = 0.65$; and for Waveform 5, we set $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{6}})$ and $a = 0.64$. The results obtained are consistent with the results in Section 5 of [7] that show that φ is piecewise constant when the elements of σ are rationally dependent. In particular, for $c = 0$ and $\sigma = (1, 0, 0), (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, and $(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$, we expect the waveform to be constant on the intervals $(k\nu, (k+1)\nu)$, $k \in \mathbb{Z}$, with $\nu = 1, \frac{1}{\sqrt{2}}$, and $\frac{1}{\sqrt{3}}$, respectively. As such, we have chosen the initial mesh to include those values of $k\nu$ contained within the interval $[T_-, T_+]$. Note that the waveforms appear to be symmetric even though $a \neq \frac{1}{2}$. When the elements of σ are not rationally dependent, the waveforms should be strictly monotone, although computationally the numerical approximations of the elements of σ are always rationally dependent.

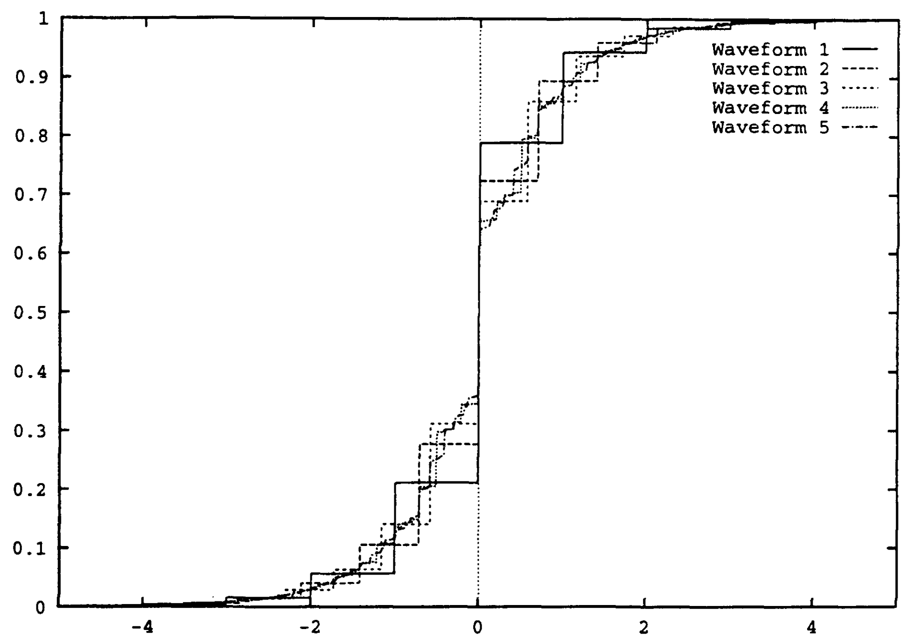


Figure 3.1: Plots of waveforms for $\alpha = \frac{1}{2}$, $c = 0$, and various values of σ and a.

In Figure 3.2, we plot waveforms obtained for $\alpha = \frac{1}{2}$, $c = 0.01$, and various values of σ and a. Note that since the waveforms become independent of σ as $c \to \pm\infty$ we have chosen c relatively small in magnitude to highlight the dependence on σ. Using the same values of σ employed in Figures 3.1 and 3.2, we choose $a \equiv a(\sigma, \alpha, c)$ (again see (2.25) and (2.27)) that corresponds to the particular value of σ. For Waveform 1, we set $\sigma = (1, 0, 0)$ and have $a \approx 0.7884$; for Waveform 2, we set $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$ and have $a \approx 0.7223$; for Waveform 3, we set $\sigma = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$ and have $a \approx 0.6887$; for Waveform 4, we set $\sigma = (\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}})$ and have $a \approx 0.6545$; and for Waveform 5, we set $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{6}})$ and have $a \approx 0.6411$.

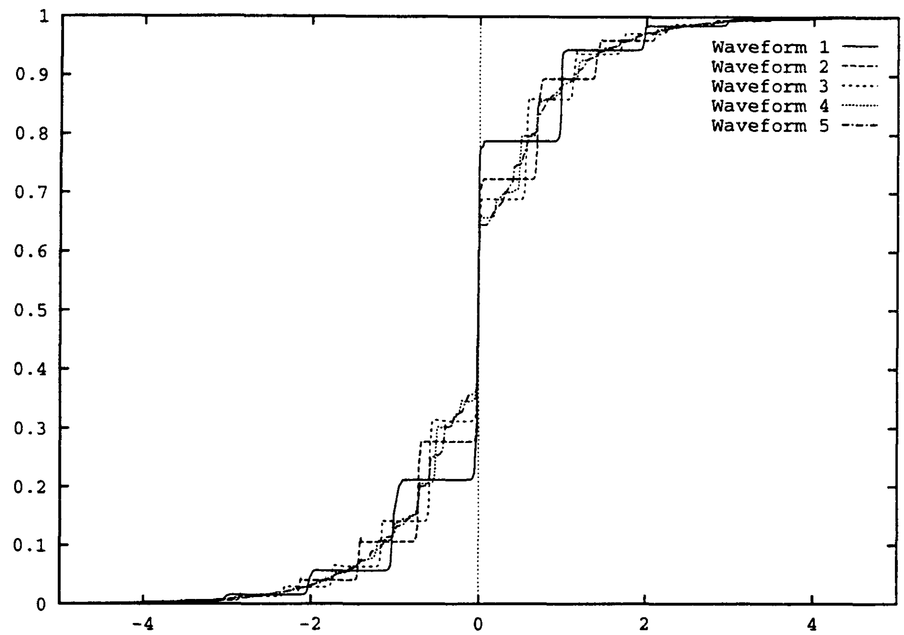


Figure 3.2: Plots of waveforms for $\alpha = \frac{1}{2}$, $c = 0.01$, and various values of σ and a.

3.4 Comparison

We begin by examining at the $c = 0$ solutions. In Figure 3.1, Waveforms 1, 2, and 3, are the numerical solutions to (3.5) when $\sigma = (1, 0, 0)$, $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, and $\sigma = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$, respectively. The elements of these three σ are rationally dependent. Recall that we showed in Section 2.3 that if we assume that the σ_k are rationally dependent, with ν as in (2.4), then for each integer n, the function φ is constant on the interval $(n\nu, (n+1)\nu)$. Thus the analytic solution is constant on intervals of width $\nu = 1$ for $\sigma = (1, 0, 0)$, intervals of width $\nu = \frac{1}{\sqrt{2}}$ for $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, and intervals of width $\nu = \frac{1}{\sqrt{3}}$ for $\sigma = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$. The numerical and analytic solution seem to agree in these three cases.

The last two curves in Figure 3.1, Waveform 4 and Waveform 5, have elements of σ that are rationally independent. For Waveform 4, where $\sigma = (\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}})$, $\frac{1}{2}$ and $\frac{1}{\sqrt{2}}$ are rationally independent. For Waveform 5, where $\sigma = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{6}})$, all three σ_k are rationally independent. Recall that in Section 2.3 we showed that if any two of the σ_k are rationally independent, then φ is strictly increasing. Again we see that we have some agreement between the numerical and analytic solutions. However, for the numerical solutions, we can only use "computer numbers" and consequently the σ_k are not truly rationally independent.

For the $c \neq 0$ solutions, recall that Theorem 2.2 states that φ is strictly increasing. This is true for all σ. The waveforms in Figure 3.2 are strictly monotone for $c \neq 0$, which is consistent with the analysis. However, the waveforms are obviously perturbations of the waveforms obtained in Figure 3.1 for $c = 0$.

Chapter 4

CONCLUSIONS AND FUTURE WORK

4.1 Conclusions

In the first half of this thesis, we defined an infinite lattice discretization for the reaction-diffusion equation. We then developed and extended the analysis that J. Cahn et al [7] carried out for the nearest neighbor discretization of the reaction-diffusion equation. After converting the equation into a traveling wave equation, we then presented the analysis and derivation of a traveling wave solution to our traveling wave equation for two cases, when $c \neq 0$, and when $c = 0$.

In the $c \neq 0$ case, we constructed a solution, φ, and a relationship Γ between the wave speed c and the detuning parameter a of the reaction term f, for a piecewise linear f. We showed that $\varphi(\xi)$ is strictly increasing on $I\!R$, continuous in both ξ and c, and analytic in c. We also showed that $D_c\varphi(\xi)$ is bounded. We showed that Γ is odd in c, analytic in c, and discontinuous at $c = 0$. The discontinuity in Γ turned out to be the interval of propagation failure for the solution of the discretized equation.

We also saw that the range of propagation failure depended on the direction of σ, the normal vector to the wavefront, as well as the rational dependence/independence of the elements of σ.

In the $c = 0$ case, our discrete traveling wave is just a difference equation. We found the solution φ by taking $c \to 0$ for the solution of the $c \neq 0$ case. With some care, we found that such a solution is valid on all of D. The rational dependence/independence of the elements of σ play an even stronger role in this case. In particular, if the σ_k are rationally dependent, then $\varphi(\xi)$ has intervals on which it is no longer strictly increasing; in fact, $\varphi(\xi)$ is constant on the intervals.

The second half of this thesis consisted of numerically solving the discrete reaction-diffusion traveling wave equation for the nearest neighbor discretization. This consisted of using Newton's method, since our problem is nonlinear. In turn, Newton's method required linear solvers to solve each Newton step. We used the Jacobi, the GS, and the SOR methods with success. Our numerical results were in agreement with our analytical results and the analytical results found in [7]. While perhaps the numerical techniques used were not the most sophisticated, they were chosen to assure confidence in the results.

Reaction-diffusion equations appear in nearly every field of science. Discrete versions of reaction-diffusion equations are useful because they mimic the propagation failure and lattice anisotropy inherent in many systems. Our results are general enough to be applied to systems of bistable type with any propagation failure and any anisotropy.

4.2 Future Work

There are four main areas of future work;

- continuation of the present analysis to include smooth nonlinearities f,
- detailed analysis of the relationship between the wavespeed c and σ, the direction of travel,
- stability of solutions,
- application of our results to the nonlinear discrete wave equation, $u_{tt} = \Delta u - f(u)$.

To make our work even more useful and accepted, extending our results to general smooth nonlinearities f is important. The Fourier techniques, used in this thesis to find a traveling wave solution, do not work in general for smooth f. But using the numerical solver we presented, we hope to be able to understand how a solution behaves, which may help us in developing analytical solutions for smooth f.

With our infinite lattice discretization, we can study the relationship between the wave speed c and σ, the direction of travel more carefully. This study should produce a Wulff diagram of the behavior of the solution and the direction we travel through the lattice. From such a study we would also hope to gain further insight into the stability and how it depends on σ.

The results from the $c = 0$ sections of this thesis should apply to nonlinear discrete wave equation, $u_{tt} = \Delta u - f(u)$, for $c^2 < K \sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j}$ for some finite K. This is because for $c^2 < K \sum_{k=1}^{\infty} \sum_{j=1}^{m_k} \alpha_{k_j}$, the nonlinear discrete wave equation is of same form as the discrete reaction-diffusion equation with $c = 0$.

Bibliography

[1] S. Allen and J. W. Cahn, A Microscopic Theory for Antiphase Boundary Motion and its Application to Antiphase Domain Coarsening, *Acta Metallurgica* **27** (1979) 1084–1095.

[2] U. Ascher, R. M. Mattheij, and R. D. Russell, *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations* (Prentice Hall, Englewood Cliffs, N.J., 1988)

[3] J. Bell, Some Threshold Results for Models of Myelinated Nerves, *Math. Biosciences* **54** (1981) 181–190.

[4] J. Bell and C. Cosner, Threshold Behavior and Propagation for Nonlinear Differential-Difference Systems Motivated by Modeling Myelinated Axons, *Quart. Appl. Math.* **42** (1984) 1–114.

[5] W. J. Beyn, The Numerical Computation of Connecting Orbits in Dynamical Systems, *IMA J. Numer. Anal.* **9** (1990) 379–405.

[6] J. W. Cahn, Theory of Crystal Growth and Interface Motion in Crystalline Materials, *Acta Metallurgica* **8** (1960) 554–562.

[7] J. W. Cahn, J. Mallet-Paret, and E. S. Van Vleck, Traveling Wave Solutions for Systems of ODE's on a Two-Dimensional Spatial Lattice, submitted (1995).

[8] H. Chi, J. Bell, and B. Hassard, Numerical Solution of a Nonlinear Advance-Delay- Differential Equation from Nerve Conduction Theory, *J. Math. Biol.* **24** (1986) 583-601.

[9] D. B. Duncan and M. A. M. Lynch, Jacobi Iteration in Implicit Difference Schemes for the Wave Equation, *SIAM J. Numer. Anal.* **28** (1991) 1661–1679.

[10] C. E. Elmer and E. S. Van Vleck, Computation of Traveling Wave Solutions for Spatially Discrete Bistable Reaction-Diffusion Equations, to appear *Appld. Numer. Math.* **20** (1996).

[11] P. Fife and J. McLeod, The Approach of Solutions of Nonlinear Diffusion Equations to Traveling Front Solutions, *Arch. Rat. Mech. Anal.* **65** (1977) 333–361.

[12] M. J. Friedman and E. J. Doedel, Numerical Computation and Continuation of Invariant Manifolds Connecting Fixed Points, *SIAM J. Numer. Anal.* **28** (1991) 789–808.

[13] F. N. Fritsch and R. E. Carlson, Monotone Piecewise Cubic Interpolation, *SIAM J. Numer. Anal.* **17** (1980) 238–246.

[14] W. -Z. Gao, Threshold Behavior and Propagation for a Differential-Difference System, *SIAM J. Math. Anal.* **24** (1993) 89–115.

[15] G. H. Golub and C. Van Loan, *Matrix Computations* (Johns Hopkins University Press, Baltimore, MD, 1989).

[16] C. P. Grant and E. S. Van Vleck, Slowly-Migrating Transition Layers for the Discrete Allen-Cahn and Cahn-Hillard Equations, *Nonlinearity* **8** (1995) 861–876.

[17] W. Hackbusch, *Iterative Solution of Large Sparse Systems of Equations* (Springer-Verlag, New York, 1994).

[18] J. K. Hale, *Ordinary Differential Equations* (Krieger, Malabar, FL, 1980).

[19] H. T. Huynh, Accurate Monotone Cubic Interpolation, *SIAM J. Numer. Anal.* **30** (1993) 57–100.

[20] D. Hankerson and B. Zinner, Wavefronts for a Cooperative Tridiagonal System of Differential Equations, *J. Dyn. Diff. Eq.* **5** (1993) 359–373.

[21] J. P. Keener, Propagation and its Failure in Coupled Systems of Discrete Excitable Cells, *SIAM J. Appl. Math.* **22** (1987) 556–572.

[22] M. Lentini and H. B. Keller, Boundary Value Problems on Problems on Semi-Infinite Intervals and Their Numerical Solution, *SIAM J. Numer. Anal.* **17** (1980) 577–604.

[23] H. McKean, Nagumo's Equation, *Adv. Math.* **4** (1970) 209–223.

[24] J. Ortega and W. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables* (Academic Press, San Diego, CA, 1970)

[25] W. Rudin, *Principles of Mathematical Analysis* (McGraw-Hill Publishing Company, New York, N.Y., 1976).

[26] A. I. Volpert, V. A. Volpert, and V. A. Volpert, *Traveling Wave Solutions of Parabolic Systems* (American Mathematical Society, Providence, RI, 1994)

[27] B. Zinner, Stability of Traveling Wavefronts for the Discrete Nagumo Equation, *SIAM J. Math. Anal.*, **22** (1991) 1016–1020.

[28] B. Zinner, Existence of Traveling Wavefront Solutions for the Discrete Nagumo Equation, *J. Diff. Eq.* **96** (1992) 1–27.

[29] B. Zinner, G. Harris, and W. Hudson, Traveling Wavefronts for the Discrete Fisher's Equation, *J. Diff. Eq.* **105** (1993) 46–62.