Traveling waves in rapid solidification *

Karl Glasner

Abstract

We analyze rigorously the one-dimensional traveling wave problem for a thermodynamically consistent phase field model. Existence is proved for two new cases: one where the undercooling is large but not in the hypercooled regime, and the other for waves which leave behind an unstable state. The qualitative structure of the wave is studied, and under certain restrictions monotonicity of front profiles can be obtained. Further results, such as a bound on propagation velocity and non-existence are discussed. Finally, some numerical examples of monotone and non-monotone waves are provided.

1 Introduction

Continuum descriptions of phase transitions known as phase field models have become popular in describing solidification processes [15, 9, 18, 21, 7, 23]. All phase field models introduce an abstract order parameter ϕ which designates the phase of the system. Without any loss of generality we will take these to be $\phi = 1$ (solid, for example) and $\phi = -1$ (liquid, for example). The construction of these models typically begins with an assumption about the free energy (or alternatively, the negative entropy) of the system as a function of the phase ϕ and the internal energy density e. We will consider the specific functional [18, 21]

$$\mathcal{F}(\phi, e) = \int \tfrac{1}{2}|\nabla \phi|^2 + F(\phi, e)dx$$

which has been written in nondimensional form. The gradient part accounts for surface energy, and the function $F(\phi, e)$ is the bulk free energy density.

We will consider a form for F similar to that proposed by Wang *et al.* [21]:

$$F(\phi, e) = g(\phi) + \lambda u^2 = \frac{\lambda}{2}\left(e + \tfrac{1}{2}p(\phi)\right)^2. \tag{1.1}$$

The constitutive function $g(\phi)$ is typically a positive, symmetric, double well potential with minima at ± 1, but we shall not always require this. The parameter λ designates the coupling between the two fields; for narrow phase interfaces,

it is physically the ratio of interface width to capillary length [14]. We assume $F(\phi; e) \in C^2$ and has the following properties:

- For each fixed value of e, the function $F(\phi, e)$ will have have exactly two minima at ± 1. Specifically we suppose that

$$\frac{\partial^2}{\partial \phi^2} F(\pm 1, e) = \sigma_\pm^s(e) > 0. \tag{1.2}$$

- For each fixed value of e, $F(\phi, e)$ possesses a unique intermediate maximum at some point $\hat{\phi}$ (as an example, see figure 6).

- Outside of the interval $\phi \in (-1, 1)$, $\partial F/\partial \phi$ will be set to zero without any loss of generality.

To complete the model's description, a relationship between internal energy and temperature u is needed. The choice we make has the general form

$$e = u + \tfrac{1}{2} p(\phi)$$

where we will take p to be an increasing function of ϕ. The dependence on ϕ accounts for latent heat released during the phase change. It can always be assumed (by a linear change of the variable u, for example) that

$$p(\pm 1) = \pm 1.$$

The dynamics which arise from the above constitutive model result from a gradient flow of $\mathcal{F}$ which simultaneously conserves total internal energy. In one dimension this yields the system (see [21] for the derivation)

$$\phi_t = \phi_{xx} + f(\phi, u) \tag{1.3}$$
$$e_t = D u_{xx} \tag{1.4}$$

where

$$f(\phi, u) = \left. \frac{\partial F}{\partial \phi} \right|_e (\phi, u)$$

and the parameter D is a nondimensional diffusion coefficient.

The problem we are interested in is where a phase interface is propagating from left to right into the state $\phi = -1$. We also suppose that temperature approaches constants u_-, u_+ far to the left and right, respectively. If we look for constant velocity traveling wave solutions of the form $\phi = \phi(x - Vt)$, $u = u(x - Vt)$, we obtain the traveling wave problem

$$\phi'' + V\phi' + f(\phi, u) = 0 \tag{1.5}$$
$$Du' + Vu - \frac{1}{2} Vp(\phi) - Ve_\infty = 0 \tag{1.6}$$
$$\phi \to -1, \quad u \to u_+ \quad \text{as} \quad x \to +\infty \tag{1.7}$$
$$\phi \to 1, \quad u \to u_- \quad \text{as} \quad x \to -\infty \tag{1.8}$$

where $e_\infty = u_- - \frac{1}{2}p(1)$ is a constant which comes from one integration of the second equation. Since $u_x \to 0$ as $x \to \pm\infty$, u_-, u_+ must satisfy

$$u_- - u_+ = \tfrac{1}{2}[p(1) - p(-1)] = 1. \tag{1.9}$$

We define the nondimensional "undercooling" Δ to be to be

$$\Delta \equiv -u_+ = -e_\infty + \tfrac{1}{2} \tag{1.10}$$

so that $u_- = -\Delta + 1$. We shall talk about the parameters Δ and e_∞ interchangeably.

For certain singular limits of phase field models, u is approximately constant near the phase interface, and an asymptotic analysis can be conducted to determine the wave profile and propagation velocity [5]. When the rate of phase change is rapid, however, this is not the case. In particular, both fields will vary simultaneously, so the problem must be treated as a system rather that a single equation. This gives rise to a number of features not seen in the one component case, including non-existence, non-uniqueness and non-monotone behavior. We therefore adopt an approach different from that of other traveling wave problems.

Several other authors have studied traveling waves in phase field systems. Caginalp and Nishiura [6] prove existence when the coupling between the two variables is weak, allowing for the use of a perturbative argument. In a more recent study, Bates *et al.* [2, 3] establish existence of waves under the hypothesis of hypercooling, when $\Delta > 1$. In contrast, we are principally concerned with the case $\Delta < 1$ and where the coupling between the variables is significant.

The model we discuss here is quite general, and may very well pertain to other phase transition phenomena, such as solidification of binary alloys [22, 7] and superconductivity [8]. In one dimension at least, all of these models have a similar mathematical structure.

The layout of the paper is as follows. In section 2 we establish some basic properties of solutions. Existence results appear in section 3. We then prove a bound on propagation velocity in section 4. With certain restrictions, monotonicity is established in section 5. In section 6, it is shown that in a critical region of parameter space, no solutions may be obtained. Finally, in section 7, some computational examples of both monotone and non-monotone waves are shown.

2 Preliminary Results

We can rewrite the system (1.5 - 1.6) as a third order dynamical system by introducing $\psi = \phi_x$:

$$\phi_x = \psi \tag{2.1}$$

$$\psi_x = -V\psi - f(\phi, u) \tag{2.2}$$

$$u_x = \frac{V}{D}(-u + \tfrac{1}{2}p(\phi) + e_\infty) \tag{2.3}$$

For convenience, we set $\eta = (\phi, \psi, u)$, $\eta_- = (1, 0, u_-)$, $\eta_+ = (-1, 0, u_+)$, and write the system compactly as $\eta_x = G(\eta)$. The task of finding a traveling wave solution is the same as finding a trajectory connecting η_- to η_+.

Because of the gradient construction of the original model, there is a natural Lyapunov function for the system (2.1-2.3):

Lemma 1

$$\frac{d}{dx}\left\{ F(\phi; e_\infty) - \tfrac{1}{2}\phi_x^2 - \lambda\left(\frac{Du_x}{V}\right)^2 \right\} = V\psi^2 + \frac{\lambda D}{V}u_x^2 \qquad (2.4)$$

Proof. This is just a straightforward calculation. □

We can now establish a necessary condition for existence.

Proposition 1 *Any solution to (1.5 -1.8) must satisfy*

$$F(-1, e_\infty) - F(1, e_\infty) = V\int_{-\infty}^{\infty}\psi^2(x)dx + \frac{\lambda D}{V}\int_{-\infty}^{\infty}u_x^2(x)dx. \qquad (2.5)$$

In particular, forward moving solutions have

$$F(-1, e_\infty) > F(1, e_\infty). \qquad (2.6)$$

Proof. This is simply obtained by integrating (2.4). □

The final result of this section pertains to estimates for derivatives of ϕ, u.

Proposition 2 *Suppose ϕ, u solve equations (1.5),(1.6), and (1.8). There exist positive constants C_1, C_2, depending only on e_∞, so that*

$$|\phi_x| < C_1, \quad |u_x| < C_2.$$

Proof. Integrating (2.4) from $-\infty$ to x, we can get

$$\tfrac{1}{2}\phi_x^2(x) < F(\phi(x), e_\infty) - F(1, e_\infty)$$

which establishes the first bound. For the second, we take the derivative of (2.3), multiply by the integration factor $K(x) = V/D\exp(Vx/D)$ and integrate, giving

$$u_x(x) = \tfrac{1}{2}\int_{-\infty}^{x} K(x - x')p(\phi(x'))_x dx. \qquad (2.7)$$

We can bound the term $p(\phi)_x$ by a constant, and the remaining integral evaluates to exactly 1. □

3 Existence of traveling waves

In a separate paper [12], traveling wave solutions are constructed by formal asymptotic expansions. The conclusions which were drawn from this analysis are the following:

- Solutions may not exist for all parameters. When the ratio D/λ is small, a saddle-node bifurcation in the non-hypercooled ($\Delta < 1$) regime gives rise to two monotone solution branches, a stable one where V is large, and an unstable one where V is small.

- When D/λ is large, ϕ is approximately the solution to

$$\phi_{xx} + V\phi_x + f(\phi, u_-) = 0 \tag{3.1}$$
$$\phi(-\infty) = 1, \quad \phi(+\infty) = -1 \tag{3.2}$$

This is a standard traveling wave problem, and much is known about solutions (see [10] for example). For forward-moving ($V > 0$) solutions to exist, it is required that

$$\int_{-1}^{1} f(\phi, u_-)\, d\phi > 0 \tag{3.3}$$

which is (provided $g(\phi)$ is an even double well potential) the same as requiring $\Delta > 1$. This is the hypercooled situation for which existence, and sometimes uniqueness, is guaranteed [2].

- When D is small, the u variable is essentially slaved to the ϕ variable on the fast solution branch. Then ϕ is approximately the solution to

$$\phi_{xx} + V\phi_x + f(\phi, e_\infty + \tfrac{1}{2}p(\phi)) = 0 \tag{3.4}$$
$$\phi(-\infty) = 1, \quad \phi(+\infty) = -1 \tag{3.5}$$

This the same traveling wave problem as (3.1), but with a different source term. The analog of condition (3.3) is actually the same as the earlier condition (2.6) in this case since

$$f(\phi, e_\infty + \tfrac{1}{2}p(\phi)) = \frac{\partial F(\phi; e_\infty)}{\partial \phi}$$

Provided (2.6) holds, there is a forward moving solution to this problem [11]:

Proposition 3 *The traveling wave problem (3.4 - 3.5) posses a solution pair $(\phi, V) = (\Phi_s(x), V_s)$. Φ_s is decreasing and unique up to translation. V_s is positive and uniquely determined.*

We shall now specify two types of traveling waves, each corresponding to different types of source terms $f(\phi, u)$.

Waves of Type I: The first case is where, for fixed u, the function $f(\phi, u)$ is of "bistable" type (see figure 1a). This is the usual situation where both phases $\phi = \pm 1$ are stable. We will further assume that $g(\phi)$ is an even function, with

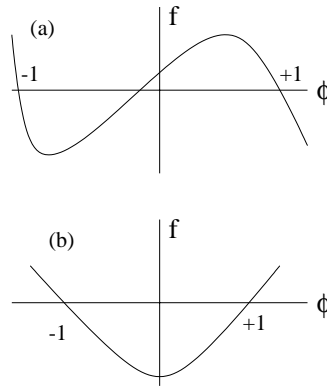$$g'(\phi) \begin{cases} > 0 & \phi < 0 \\ < 0 & \phi > 0. \end{cases}$$

Figure 1: (a) Type I waves. The nonlinear function $f(\phi, u_-)$ is of bistable type for each fixed value of u_-. (b) the function $f(\phi, u_-)$ for waves of type II.

The results of sections 5-7 will pertain specifically to this case.

Waves of Type II: The second case is where $f(\phi, u_-)$ is of monostable type (figure 1b). The phase $\phi = 1$ is actually now unstable, but this type of wave has been exhibited in numerical simulations [1, 24, 13].

Typically, traveling wave problems are viewed as eigenvalue problems in the propagation velocity V. In view of the first conclusion above, however, solutions may not always exist when all other parameters are fixed. The approach we adopt instead is to regard V as fixed. We then have two difference existence results by regarding either D or $\Delta = -e_\infty + \frac{1}{2}$ as the unknown parameter.

In the first of two existence theorems, we take D to be unknown. There are two properties which will be required:

$$F(-1, e_\infty) > F(1, e_\infty) \tag{P1}$$

and

$$\int_{-1}^{1} f(\phi, u_-)\, d\phi < 0. \tag{P2}$$

Property P1 is just the necessary condition established in proposition 1. For waves of type I, properties P1 and P2 will hold when

$$\tfrac{1}{2} < \Delta < 1.$$

For type II waves, property P1 takes the form

$$\lambda > \lambda_s > 0.$$

where λ_s is the value of λ making $F(-1, e_\infty) = F(1, e_\infty)$. In general, λ_s will depend on Δ. Notice that property P2 is automatically satisfied, since $f(\phi, u_-) < 0$. The theorem is

Theorem 1 *Suppose $V \in (0, V_s)$ and properties P1, P2 hold. Then there exists a triple $(\phi(x), u(x), D)$ solving the problem (1.5 - 1.8), with the property that $-1 \le \phi \le 1$.*

In other words, non-hypercooled type I waves always exist in a range of velocities, provided we can adjust D, typically by making it small. The same is true of type II waves, provided λ is large.

The second existence theorem pertains only to waves of type I. We take the undercooling Δ to be unknown, giving the following result:

Theorem 2 *Suppose $V, D > 0$. Then there exists a triple $(\phi(x), u(x), \Delta)$ solving the problem (1.5 - 1.8), with the property that $-1 \le \phi \le 1$.*

This means that any velocity is accessible, provided the undercooling is chosen properly.

The proofs are similar, and are given in a series of steps which we shall outline. The idea is to construct a shooting method with D (or Δ) as the shooting parameter. The system (2.1 - 2.3) possesses a one dimensional unstable manifold near the fixed point η_-. When D is very large (or Δ small), the trajectory which is formed from the unstable manifold never reaches a point where $\phi = -1$. But for small enough D (or large Δ), the trajectory will "overshoot", that is continue below $\phi = -1$. Consequently, there should be some intermediate value which gives $\phi(+\infty) \to -1$.

3.1   Behavior at infinity

We begin by considering the linearization of the third order system (2.1 - 2.3) near the point η_-. Setting $\eta' = \eta - \eta_-$ we obtain the linear system $\eta'_x = \mathcal{L}\eta'$ where

$$\mathcal{L} = \begin{bmatrix} 0 & 1 & 0 \\ \sigma_+ & -V & \rho_+ \\ \frac{V}{2D}p'(1) & 0 & -\frac{V}{D} \end{bmatrix}$$

and we define

$$\sigma_\pm = -\frac{\partial f}{\partial \phi}(\mp 1, u_\pm), \quad \rho_\pm = -\frac{\partial f}{\partial u}(\mp 1, u_\pm),$$

Note that σ, ρ and σ^s are related by

$$\sigma^s_\pm = \sigma_\pm + \tfrac{1}{2}p'(\mp 1)\rho_\pm.$$

Lemma 2 *Assume that condition (1.2) holds. Then $\mathcal{L}$ has one eigenvalue μ with positive real part and two with negative real part and μ depends continuously on D and Δ.*

Proof. A straightforward calculation gives for an eigenvalue μ the characteristic polynomial

$$\mu^3 + (V + V/D)\mu^2 + (V^2/D - \sigma)\mu - V/D(\sigma^s_+) = 0. \tag{3.6}$$

It follows that the product of the roots is positive and their sum is negative by the requirement (1.2). The only possibility is that one of the roots is real and positive, leaving the other two possibly complex with negative real part. Continuous dependence follows from the formula for roots of a cubic equation.
$\square$

We may conclude that for the linear system, there is a one dimensional unstable manifold $\mathcal{M}$ which is the subspace

$$\mathcal{M} = \{\alpha\eta_u | \alpha \in \mathbb{R}\}$$

where η_u is the eigenvector corresponding to μ:

$$\eta_u = \begin{bmatrix} -1 \\ -\mu \\ -\frac{p'(1)}{2(1+\mu D/V)} \end{bmatrix}. \tag{3.7}$$

Notice that η_u depends on D and Δ in a continuous manner.

Let $\mathcal{T}$ be the two dimensional subspace orthogonal to the linear unstable manifold so that $\mathcal{T} \oplus \mathcal{M} = \mathbb{R}^3$. We now state the existence of the unstable manifold for the nonlinear system.

Proposition 4 *In a sufficiently small neighborhood of η_-, say*

$$B_\alpha = \{|\eta'| < \alpha\},$$

there is a unique C^2 map

$$T(\eta'; D, \Delta) : \mathcal{M} \cap B_\alpha \to \mathcal{T},$$

which has the following properties:
(a) $T(0) = 0$
(b) $\nabla T(0) = 0$
(c) T continuously depends on D and Δ
(d) If $\eta'(x)$ is a solution to the linear system lying on $\mathcal{M}$, then $T(\eta'(x))+\eta'(x)+\eta_-$ is a solution to the nonlinear system.
(e) Upper bounds on α^{-1} and $\|T\|_{C^2}$ depend only on $\|G\|_{C^2}$.

The proof of this is a standard result of the theory of dynamical systems.

Since we will be concerned about what happens when $D \to 0$, the bounds on α and $\|T\|_{C_2}$ are not sufficient. These bounds are, however, somewhat artificial.

Corollary 1 *For all $D \in (0, \infty)$ there are constants $C_1, C_2 > 0$ such that α can be chosen so that*

$$\alpha > C_1, \quad \|T\|_{C^2} < C_2$$

Proof. We can multiply the entire system by the factor

$$\beta = \frac{D}{D+1}$$

and introduce the variable $X = x/\beta$, giving a new system $\eta_X = \beta G(\eta)$. The unstable manifold of the new system is also one for the old as well since only the scale of the independent variable was changed. But for the new system, $\beta \| G \|_{C^2}$ has a uniform bound for all $D \in (0, \infty)$ as required. $\square$

A starting point for the shooting method can now be given, by constructing a trajectory which sits on the unstable manifold near the point η_-.

Proposition 5 *There exists a solution $\eta(x) : (-\infty, 0] \to \mathbb{R}^3$ to (2.1-2.3) with the following properties:*
(a) There is a $K > 0$ such that

$$|\eta(x) - \eta_- - Ke^{\mu x}\eta_u| \leq CK^2 e^{2\mu x}$$

for some constant $C > 0$ independent of D.
(b) $\eta(0)$ continuously depends on D, Δ.
(c) There is some fixed $\phi_0 < 1$, so that $\phi(0) = \phi_0$.

Proof. For arbitrary but small K and $x \leq 0$, the function

$$\eta(x; K, D, \Delta) = \eta_- + Ke^{\mu x}\eta_u + T(Ke^{\mu x}\eta_u; D, \Delta)$$

is well defined. Choose $\phi_0 < 1$ so that it is in the range of η_ϕ for all $D > 0$, the subscript denoting the ϕ-component. For small K, the function

$$\phi(0; K, D, \Delta) = 1 - K + T_\phi(K\eta_u; D, \Delta)$$

is decreasing in K, and therefore has a unique continuous inverse $K(\phi(0); D, \Delta)$. We can then set $K = K(\phi_0; D, \Delta)$, so that properties (b) and (c) are satisfied. The estimate (a) follows from Taylor's theorem and properties (a),(b) and (e) in proposition 4. $\square$

3.2   The limit as $D \to 0$ and overshooting

For proof of theorem 1, we will be concerned about what happens in the limit $D \to 0$. The goal of this section is to show that when D is near zero, the trajectory formed from the extension of the solution obtained in proposition 5 will eventually decrease past the value $\phi = -1$, provided $V < V_s$.

Formally setting $D = 0$, we have $u \equiv \frac{1}{2}p(\phi) + e_\infty$ and obtain the reduced system

$$\phi_x = \psi \tag{3.8}$$
$$\psi_x = -V\psi + F_\phi(\phi, e_\infty) \tag{3.9}$$

As long as ϕ is monotone decreasing, it will be useful to work in phase space, viewing ϕ as the independent variable. Then $\psi(\phi)$ solves the non-autonomous equation

$$\frac{d\psi}{d\phi} = -V + \frac{F_\phi(\phi, e_\infty)}{\psi}. \tag{3.10}$$

Given a solution to this equation, the traveling wave profile may be obtained by inverting the one to one function

$$x(\phi) = \int_0^x dx = \int_{\phi_0}^{\phi} \frac{d\phi}{\psi(\phi)}. \tag{3.11}$$

The constant ϕ_0 is the value ϕ takes at $x = 0$; choosing it removes the translation invariance of the original problem.

When $V = V_s$ there is a unique decreasing solution Φ_s given by proposition 3, whose derivative Ψ_s must satisfy (3.10). We will first construct a trajectory which decreases "faster" than Φ_s.

Proposition 6 *When $V < V_s$ there is a solution $\Psi : (-1, 1) \to \mathbb{R}$ of equation (3.10) with the following properties:*
(a) $\Psi(\phi) < \Psi_s(\phi) < 0$.
(b) $\Psi(\phi) \to 0$ as $\phi \to 1$.
(c) For any $\phi_0 \in (-1, 1)$,

$$\int_{\phi_0}^{-1} \frac{d\phi}{\Psi(\phi)} \quad \text{is bounded.}$$

(d) For any $\phi_0 \in (-1, 1)$,
$$\int_{\phi_0}^{1} \frac{d\phi}{\Psi(\phi)} = -\infty.$$

Proof. Let $\Psi_n(\phi)$ be the backwards solution to the initial value problem (3.10) with $\Psi_n(1) = -1/n$, which exists down to a point where $\Psi_n \to 0$. We claim that $\Psi_n(\phi) < \Psi_s(\phi)$. This must be true near $\phi = 1$ since Ψ_s approaches zero there. Suppose then that there is some largest $\phi = \phi^*$ at which $\Psi(\phi^*) = \Psi_s(\phi^*)$. At that point we have

$$\frac{d\Psi_n}{d\phi}(\phi^*) = -V + \frac{F_\phi(\phi^*, e_\infty)}{\Psi_n} > -V_s + \frac{F_\phi(\phi^*, e_\infty)}{\Psi_s} = \frac{d\Psi_s}{d\phi}(\phi^*) \tag{3.12}$$

which is impossible since $\Psi_n < \Psi_s$ when $\phi > \phi^*$. Ψ_n therefore exists on the the whole interval $(-1, 1)$.

We now pass to a limit as $n \to \infty$. A uniform bound on $\|\Psi_n\|_{C^1}$ is obtained by noticing that

$$\left| \frac{d\Psi_n}{d\phi} \right| < |V| + \left| \frac{F_\phi(\phi, e_\infty)}{\Psi_n} \right| < |V| + \left| \frac{F_\phi(\phi, e_\infty)}{\Psi_s} \right| < |V| + |V_s| + \left| \frac{d\Psi_s}{d\phi} \right|$$

There exists some subsequence which converges uniformly in C^1 to a limit we shall simply call Ψ, solving equation (3.10).

Now to verify that Ψ has the stated properties. For (a), clearly we have $\Psi^* \leq \Psi_s$. But if they are equal at some point, an argument similar to that in equation (3.12) would give a contradiction.

For (b), we observe that

$$0 \geq \Psi_n(\phi) \geq -1/n - C(1 - \phi)$$

where C is a positive uniform bound on the derivatives of Ψ_n. Taking $n \to \infty$ gives

$$0 \geq \Psi(\phi) \geq -C(1 - \phi) \tag{3.13}$$

which proves (b).

For (d), the inequality (3.13) gives

$$\int_{\phi_0}^1 \frac{d\phi}{\Psi(\phi)} < C^{-1} \int_{\phi_0}^1 \frac{d\phi}{\phi - 1} = -\infty.$$

For (c), suppose instead

$$\int_{\phi_0}^{-1} \frac{d\phi}{\Psi(\phi)} = +\infty.$$

Formula (3.11) then may be used to obtain a solution $\phi(x)$ to the traveling wave problem (3.4-3.5) with speed $V \neq V_s$, which is impossible. $\square$

We can use formula (3.11) to obtain a solution $x(\phi)$ from Ψ, and by property (d) above, $x \to -\infty$ as $\phi \to 1$. The inverse of this function, $\Phi(x)$, is a solution to the system (3.8 -3.9) with

$$\lim_{x \to -\infty} \phi(x) = 1.$$

Additionally, by virtue of property (c) in the proposition, there is some x at which both $\Phi(x) = -1$ and $\Psi(x) < 0$. Consequentially there is some ϵ, x^* for which

$$\Phi(x^*) = -1 - \epsilon.$$

We next study the limit of the full system as $D \to 0$. It will be shown that the limit of solutions to the full system will be the solution of (3.8-3.9). The first result shows that u can approximately be regarded as a function of ϕ.

Proposition 7 *Let (ϕ, ψ, u) be a solution to the system (2.1-2.3) satisfying (1.8). Then there exists a positive constant k, so that*

$$|u(x) - \tfrac{1}{2}p(\phi(x)) - e_\infty| \leq kD\overline{\psi}(x)$$

where

$$\overline{\psi}(x) = \sup_{(-\infty, x)} |\psi|.$$

Proof. Multiplying (2.3) by the integrating factor

$$K(x) = \frac{V}{D} \exp(Vx/D)$$

and integrating gives

$$u(x) = \int_{-\infty}^{x} K(x - x') \left[\tfrac{1}{2} p(\phi(x')) + e_\infty \right] dx'. \qquad (3.14)$$

An exact Taylor expansion of the $p(\phi(x'))$ term around x gives

$$
\begin{aligned}
u(x) &= \int_{-\infty}^{x} K(x - x') \left[\tfrac{1}{2} p(\phi(x)) + e_\infty \right] dx' \\
&\quad + \int_{-\infty}^{x} K(x - x') p(\phi(x^*(x')))_x (x' - x) dx'
\end{aligned}
$$

where $x^*(x') \in (x', x)$. The first integral explicitly integrates to $\tfrac{1}{2} p(\phi(x)) + e_\infty$. For the second integral, we may bound term involving x^* by a constant times $\overline{\psi}(x)$, and the remaining term integrates to exactly D/V. $\qquad \square$

Now let (ϕ, ψ, u) be the solution obtained in proposition 5. Since ϕ is monotone decreasing at least up to $x = 0$, we may again regard it as the independent variable, and $\psi(\phi), u(\phi)$ solve

$$\frac{d\psi}{d\phi} = -V + \frac{g'(\phi) + \tfrac{1}{2}\lambda u(\phi)p'(\phi)}{\psi} \qquad (3.15)$$

We will also write $\overline{\psi}(\phi)$ for the function defined in the previous proposition. It is important to note that, at least when ϕ is near 1, property (a) in proposition 5 indicates that ψ is also monotone decreasing, and consequentially

$$\overline{\psi} = |\psi| = -\psi.$$

We may now show that a solution of this equation approaches the expected limit as $D \to 0$.

Proposition 8 *Let $\psi(\phi)$ be a solution to equation (3.15) obtained in proposition 5, and let $\Psi(\phi)$ be a solution to equation (3.10) as obtained in proposition 6. There is a positive constant k_1 so that*

$$|\psi(\phi) - \Psi(\phi)| < k_1 D, \quad \phi > \phi_0.$$

Proof. Set $\Theta = \psi - \Psi$. Using proposition 7, Θ solves the equation

$$\frac{d\Theta}{d\phi} + \frac{F_\phi(\phi, e_\infty)}{\Psi\psi} \Theta = \frac{U(\phi)}{\psi}$$

where

$$U(\phi) = \frac{\lambda}{2} p'(\phi)[u(\phi) - \tfrac{1}{2}p(\phi) - e_\infty]$$

For any $\phi_0 < 1$, we can define the integrating factor

$$K_2(\phi) = \exp\left(\int_{\phi_0}^{\phi} \frac{F_\phi(\phi', e_\infty)}{\Psi(\phi')\psi(\phi')} d\phi' \right).$$

Note that since Ψ, ψ and F_ϕ are all negative near $\phi = 1$, $K_2 \leq 1$ for $\phi \geq \phi_0$. Multiplying by K_2 and integrating from ϕ_0 to some $\tilde\phi$ yields

$$K_2(\tilde\phi)\Theta(\tilde\phi) - \Theta(\phi_0) = \int_{\phi_0}^{\tilde\phi} K_2(\phi)\frac{U(\phi)}{\psi}d\phi.$$

Taking the limit $\tilde\phi \to 1$, we obtain

$$|\Theta(\phi_0)| = \left|\int_{\phi_0}^1 \frac{U(\phi)}{\psi}d\phi\right| < k_1 D.$$

$\square$

We conclude this section by showing that the solution to the full problem overshoots when D is small precisely because the "slaved" $(D \to 0)$ limit is being approached.

Proposition 9 *Let (ϕ, ψ, u) be the solution obtained in proposition 5. There exists x^*, so that if D is small enough, $\phi(x^*) = -1$ for some $x \leq x^*$.*

Proof. By an appropriate translation of the limit solution $\Phi(x)$, we can make $\Phi(0) = \phi(0) = \phi_0$. Using proposition 8 we have $\Psi(0) = \psi(0) + \mathcal{O}(D)$. Since ψ has a uniform bound, $u(x) = \frac{1}{2}\phi(x) + e_\infty + \mathcal{O}(D)$, therefore (ϕ, ψ) solve a system of the form

$$\begin{aligned}
\phi_x &= \psi \\
\psi_x &= -V\psi + F_\phi(\phi, e_\infty) + R(x)
\end{aligned}$$

where $R = \mathcal{O}(D)$. Now suppose that $\Phi(x^*) = -1 - \epsilon$. By elementary theory, solutions are continuous both with respect to initial data and perturbations of the equation. Consequentially for D small enough we have $\phi(x^*) < \Phi(x^*) + \epsilon = -1$. $\square$

3.3 Proof of Theorem 1

We now formally define the shooting procedure which is used to obtain a solution. For $M > 0$ set

$$\Sigma_M(D) = \phi(M)$$

where $\eta = (\phi, \psi, u)$ is the solution to (2.1-2.3) obtained in proposition 5. Since ϕ varies continuously both with respect to its initial data and parameters, it follows $\Sigma(D)$ is also continuous. For each M, we will vary D so that $\Sigma = -1$, and so obtain a solution η_M. We will conclude by passing to the limit $M \to \infty$ and showing that the limiting solution has the correct asymptotic behavior.

Proof of Theorem 1.   *Step 1:* Overshooting

For large M, we have already shown that ϕ can obtain the value -1 when D is small. Past this point, it is easy to see that $\phi < -1$ since ψ converges to zero in an exponential fashion because $f \equiv 0$. This ensures $\Sigma < -1$.

Step 2: Undershooting

When $D = \infty$ (i.e. $D^{-1} = 0$) we claim that $\Sigma > -1$. Suppose instead there exists some x^* for which $\phi(x^*) = -1$. $u(x)$ is constant in this case, taking the value u_-. Multiplying (2.2) by ψ and integrating from $-\infty$ to x^* gives

$$\tfrac{1}{2}\psi^2(x^*) = \int_{-1}^{1} f(\phi, u_-)\, d\phi - V \int_{-\infty}^{x^*} \psi^2(x) dx < 0$$

by virtue of property P2, which is impossible.

   Step 3: Uniform bounds and passing to the limit

We now define
$$D_M = \sup\{D | \Sigma_M(D) = -1\}$$

which must exist by steps 1 and 2 and the fact that Σ is continuous. Associated with each D_M is a solution $\eta_M = (\phi_M, \psi_M, u_M)$ of (2.1 - 2.3) with $D = D_M$. Since ϕ_M may not decrease past -1, we have

$$-1 \leq \phi_M \leq 1.$$

We claim that D_M is non-decreasing in M. For ϵ small, let $M_1 = M + \epsilon$. Then

$$\Sigma_{M_1}(D_M) = \phi_M(M + \epsilon) \leq \phi_M(M) = -1$$

so that $D_{M_1} \leq D_M$. This uniformly bounds D_M from below. Using the uniform bounds on ϕ_x and u_x, there is a constant C so that

$$\| \eta_M \|_{C^1([-M,M])} < C.$$

We can find a subsequence $M_j \to \infty$ so that $D_{M_j} \to D$ and $\eta_{M_j} \to \eta = (\phi, \psi, u)$ locally in the C^1 norm, giving a solution to (2.1-2.3) on $(-\infty, \infty)$.

   By construction, the limiting solutions must satisfy the left hand far field conditions (1.7). We need only show that the right hand conditions (1.8) hold.

Step 4: Behavior as $x \to +\infty$

The existence of a limit follows from the gradient character of the system by the following lemma:

Lemma 3 *Suppose $\lim_{x \to \infty} I(x) = I^*$, and that there is some positive constant C so that $|I_{xx}(x)| < C$. Then $\lim_{x \to \infty} I_x(x) = 0$.*

Proof. For $\epsilon > 0$, let x_1 be so large that

$$|I^* - I(x)| \leq \epsilon^2, \quad x \geq x_1.$$

For any $x \geq x_1$,

$$I(x) = I(x_1) + I_x(x_1)(x - x_1) + \int_{x_1}^{x} \int_{x_1}^{x'} I_{xx}(x'') dx'' \, dx'.$$

Then using the bound on the second derivative and setting $x - x_1 = \epsilon$, we have

$$\epsilon |I_x(x_1)| \leq |I(x) - I(x_1)| + \frac{C}{2}\epsilon^2 \leq (1 + \frac{C}{2})\epsilon^2$$

which means $I'(x_1) \leq C\epsilon$. □

To continue the proof, let $I(x)$ be the Lyapunov function in lemma 1. Since I is increasing and bounded from above, the limit $\lim_{x\to\infty} I(x)$ exists. A bound on the second derivative of I follows from the bounds on derivatives of ϕ and u. Therefore $\psi, u_x \to 0$ as $x \to \infty$, and consequentially $\lim_{x\to\infty} F(\phi; e_\infty)$ exists. Since ϕ is continuous, it must also approach a limit $\overline{\phi}$. Using equation (2.3) it follows that

$$\lim_{x\to\infty} u(x) = e_\infty + \tfrac{1}{2}p(\overline{\phi}) \equiv \overline{u}.$$

Then $(\overline{\phi}, 0, \overline{u})$ must be a fixed point of the system (2.1 - 2.3), which is the same as saying that $\overline{\phi}$ is a critical point of the function $F(\phi; e_\infty)$. Three possibilities exist:
(a) $\overline{\phi} = 1$.
(b) $\overline{\phi} = \hat{\phi}$, the intermediate maximum of $F(\phi; e_\infty)$.
(c) $\overline{\phi} = -1$ and $\overline{u} = -\Delta$.
We can show that the first two are impossible.

If (a) holds, then equation (2.5) implies that $\psi, u_x \equiv 0$, which is impossible. Suppose instead that (b) holds. Let ϵ to be small enough that

$$F(\phi, e_\infty) - F(-1, e_\infty) \geq \epsilon \tag{3.16}$$

when ϕ is in some small neighborhood of $\hat{\phi}$; this is always possible since $\hat{\phi}$ is a maximum of $F(\phi, e_\infty)$. Since $\psi, u_x \to 0$ as $x \to \infty$, there must exist some point X for which (3.16) holds for $\phi = \phi_M(X)$ and

$$\tfrac{1}{2}\psi_M^2(X) + \lambda \frac{D_M^2}{V^2}(u_M)_x^2(X) < \epsilon \tag{3.17}$$

for large values of M. By integrating (2.4) from X to M for each η_M, we get

$$\tfrac{1}{2}\psi_M^2(X) + \lambda \frac{D^2}{V^2}(u_M)_x^2(X) > F(\phi_M(X); e_\infty) - F(-1; e_\infty) > \epsilon \tag{3.18}$$

which is a contradiction of (3.17).
This concludes the proof of Theorem 1.

3.4   Proof of Theorem 2

The proof of theorem 2 is very similar to the first existence theorem, so we will only point out the differences. We again construct the "shooting" function

$$\Sigma_M(\Delta) = \phi(M)$$

which is continuous in Δ. The steps in completing the proof are the same as above:

Step 1: Overshooting

We will first establish a comparison solution by an existence result for the one-component equation.

Proposition 10 *Let V be given. There exists $\tilde{V} > V, U < 0, \Phi$ solving*

$$\Phi_{xx} + \tilde{V}\Phi + f(\phi, U) = 0 \tag{3.19}$$

with the boundary conditions $\Phi(\pm\infty) = \mp 1$, where Φ is decreasing.

Proof. Notice that (since we are dealing only with waves of type I) the term $f(\phi, U)$ is of bistable type for each U. Therefore (3.19) has a solution pair $(\Phi, \tilde{V})$ for each fixed U, where Φ is decreasing. We need only show

$$\tilde{V} \to +\infty \quad \text{as} \quad U \to -\infty.$$

Regarding Φ as the independent variable, the derivative of Φ, call it $\Psi(\Phi)$, will solve

$$\frac{d\Psi}{d\Phi} = -\tilde{V} + \frac{g'(\Phi) + \frac{\lambda}{2}Up'(\Phi)}{\Psi}. \tag{3.20}$$

Suppose that as $U \to -\infty$, $\tilde{V}$ remains bounded. Multiplying (3.20) by Ψ yields

$$
\begin{aligned}
\frac{d}{d\Phi}\left(\frac{1}{2}\Psi^2\right) &= g'(\Phi) + \frac{\lambda}{2}Up'(\Phi) - \tilde{V}\Psi \\
&\leq C_1\left(\frac{1}{2}\Psi^2\right) + C_2 U + C_3
\end{aligned}
$$

where C_1, etc. will denote positive constants. Applying the usual Gronwall lemma gives

$$|\Psi(\phi)| \leq C_4|U|^{\frac{1}{2}} + C_5 \quad \text{for } \phi \in (-1, 1).$$

Now multiplying (3.20) by ψ and integrating from $\phi = -1$ to $\phi = +1$, we obtain

$$
\begin{aligned}
\tilde{V} &= \frac{\lambda U}{\int_{-1}^{1}\Psi(\phi)d\phi} \tag{3.21} \\
&\geq C_6|U|^{\frac{1}{2}} - C_7. \tag{3.22}
\end{aligned}
$$

But then $\tilde{V} \to \infty$ as $U \to -\infty$, a contradiction. $\square$

With this comparison solution we can easily show, provided Δ is large enough, that the solution to the full system will overshoot.

Proposition 11 *Let (ϕ, ψ, u) be a solution obtained in proposition 5, with $\Delta \geq -U + 1$. Then there exists x^*, so that $\phi(x^*) = -1$.*

Proof. We will again work in phase space, so as before $\psi(\phi), u(\phi)$ solves

$$\frac{d\psi}{d\phi} = -V + \frac{g'(\phi) + \frac{\lambda}{2}u(\phi)p'(\phi)}{\psi} \tag{3.23}$$

which is valid so long as ϕ is decreasing; in particular, it is true near $\phi = 1$.

First we claim that if $\psi(\phi^*) = \Psi(\phi^*)$ at some point ϕ^*, then $\psi(\phi) > \Psi(\phi)$ when $\phi > \phi^*$. This follows from the inequality

$$
\begin{aligned}
\frac{d\Psi}{d\phi}(\phi^*) &= -\tilde{V} + \frac{g'(\phi^*) + \frac{\lambda}{2}Up'(\phi^*)}{\Psi} \\
&< -V + \frac{g'(\phi^*) + \frac{\lambda}{2}u(\phi)p'(\phi^*)}{\psi} = \frac{d\psi}{d\phi}(\phi^*).
\end{aligned} \tag{3.24}
$$

As a consequence, there is some small neighborhood of $\phi = 1$ where Ψ and ψ do not cross. Suppose that $\Psi < \psi$ there. Then by virtue of $g'(\phi) < 0$, just as in (3.24) we obtain that

$$\frac{d\psi}{d\phi} > \frac{d\Psi}{d\phi}. \tag{3.25}$$

But integrating $d\psi/d\phi$ from ϕ_0 up to $\phi = 1$ gives

$$\lim_{\phi \to 1} \psi(\phi) > \lim_{\phi \to 1} \Psi(\phi) = 0,$$

which is impossible since $\psi \to 0$ as $\phi \to 1$.

It follows that $\psi(\phi)$ exists on the whole interval $(-1, 1)$, and that $\psi(\phi) < \Psi(\phi)$. Finally near $\phi = -1$, by virtue of $g'(\phi) > 0$ we obtain (3.25) again, and consequentially

$$\lim_{\phi \to -1} \psi(\phi) < \lim_{\phi \to -1} \Psi(\phi) = 0.$$

This means, according to formula (3.11) that there is some x^* for which $\phi(x^*) = -1$. $\square$

Step 2: Undershooting

We claim, with $\Delta = \frac{1}{2}$, that ϕ never reaches -1. Suppose that it does, at $x = x^*$. Then integrating (2.4) from $-\infty$ to x^* gives

$$-\frac{1}{2}\psi^2(x^*) - \lambda\frac{D^2}{V^2}u(x^*) = V\int_{-\infty}^{x^*}\psi^2(x)dx + \frac{\lambda D}{V}\int_{-\infty}^{x^*}u_x^2(x)dx$$

which is impossible.

Step 3: Uniform bounds and passing to the limit

By steps 1 and 2, we may find Δ_M, which is some value of Δ satisfying

$$\tfrac{1}{2} < \Delta_M \le -U + 1$$

giving $\Sigma(\Delta_M) = -1$. The C^1 bounds on ϕ, u are as before, and we pass to a limit via a subsequence M_j in the same manner, obtaining a solution on $(-\infty, \infty)$ which we again call $\eta = (\phi, \psi, u)$ and set $\overline{\Delta} = \lim_{M_j \to \infty} \Delta_{M_j}$.

Step 4: Behavior as $x \to +\infty$

The existence of the limit is obtained as before, and the rest of the proof is essentially unaltered, with one exception. In equation (3.16), the quantity e_∞ is replaced by the limiting value $\overline{e_\infty} = -\overline{\Delta} + 1$. Then (3.18) is still true as long as M is large enough so that $(e_\infty)_M = -\Delta_M + 1$ is sufficiently close to $\overline{e_\infty}$. □

4   A Bound on the Propagation Velocity

In theorem 1, it was required that the propagation velocity be less than that of the slaved system, which has a unique velocity V_s. In fact, we can show that V_s is actually an upper bound, at least for monotone waves. The proof of this relies on a comparison technique, commonly called the "sliding method" [4]. The main result is the following:

Theorem 3 *Suppose Φ_s is the decreasing solution given by proposition 3 and suppose ϕ is a decreasing solution to the problem (1.5 - 1.8). If there is some translate of ϕ such that $\phi(x) < \Phi_s(x)$, then $V < V_s$.*

Proof. Suppose that $\phi(x) < \Phi_s(x)$ already holds. By a suitable translation, we can ensure that $\phi(x) \le \Phi_s(x)$ and that there is at least one point x^* where $\phi(x^*) = \Phi_s(x^*)$. At this point, $\Phi_x = \phi_x = -c < 0$ and the following holds:

$$0 \le (\Phi_s - \phi)_{xx} = (V - V_s)(-c) + \tfrac{1}{2}\lambda p'(\phi)\left(\tfrac{1}{2}p(\phi) + e_\infty - u\right). \qquad (4.1)$$

Since $p(\phi(x))$ is decreasing, formula (3.14) implies

$$u(x^*) > \int_{-\infty}^{x^*} K(x' - x^*)\left[\tfrac{1}{2}p(\phi(x^*)) + e_\infty\right] dx' = p(\phi(x^*)) + e_\infty.$$

Using this in (4.1) gives $V - V_s < 0$ as required.   □

The fact that ϕ may be translated so that $\phi < \Phi_s$ depends on the decay rates of each function at $\pm\infty$. In particular, as $x \to \pm\infty$, we have

$$\phi \sim \mp(1 - C\exp(\mu_\pm x))$$

and

$$\Phi_s \sim \mp(1 - C\exp(\mu_\pm^s x))$$

where $\mu_-, \mu_-^s > 0$ and $\mu_+, \mu_+^s < 0$ may be obtained by linearizing about the fixed points $\phi_\pm$. Rather than exhibiting lengthy proofs, we merely describe the outcome of this analysis in a brief, informal fashion.

As $x \to -\infty$, the decay rate μ_- is simply the positive eigenvalue found in section 3.1. We can rewrite the characteristic polynomial (3.6) as

$$(\mu + V/D)(\mu^2 + V\mu - \sigma_s) = -\frac{1}{4}\lambda p'(\phi_-)^2$$

so that

$$\mu_-^2 + V\mu_- - \sigma_-^s \leq 0. \tag{4.2}$$

It is easy to obtain a similar characteristic polynomial for the slaved system, and the positive decay rate μ_-^s solves

$$(\mu_-^s)^2 + V_s\mu_-^s - \sigma_-^s = 0$$

Using (4.2) we have

$$\mu_-(\mu_- + V) \leq \mu_-^s(\mu_-^s + V_s). \tag{4.3}$$

To analyze what happens as $x \to +\infty$ we will assume that $p'(\phi_-) = 0$ for the sake of simplicity. Then $\sigma = \sigma_s$ and μ_+, μ_+^s solve

$$(\mu_+)^2 + V\mu_+ - \sigma_+^s = 0$$

and

$$(\mu_+^s)^2 + V_s\mu_+^s - \sigma_+^s = 0$$

so that

$$\mu_+(\mu_+ + V) = \mu_+^s(\mu_+^s + V_s) = \sigma_+^s. \tag{4.4}$$

Suppose now that $V \geq V_s$. From (4.3) and (4.4) we obtain

$$0 < \mu_- \leq \mu_-^s, \quad \mu_+ \leq \mu_+^s < 0.$$

This means that Φ_s decays faster than ϕ as $x \to -\infty$ and ϕ decays faster that Φ_s as $x \to +\infty$, ensuring that a suitable translation of ϕ to the left will give $\phi < \Phi_s$. We may now employ the theorem, which of course contradicts our hypothesis that $V \geq V_s$.

5 The uniform structure of solutions

For the remainder this paper, we will only discuss type I waves. The discussion will also be limited to $e_\infty \in E$, where E is some bounded interval of admissible values. It follows that traveling wave solutions have $u \in E + (-\frac{1}{2}, \frac{1}{2})$. With the

further assumption of λ being small, we will show that solutions are monotone and there are uniform bounds on the width of the interface profile.

We begin by describing three different ϕ intervals. This first corresponds to the interface layer, and it is defined as

$$L = \{\phi | F(\phi, e) - F(-1, e) \geq \gamma, \quad e \in E\}. \qquad (5.1)$$

where we arbitrarily choose $\gamma = \frac{1}{2}g(0)$. When λ is small, L is nearly centered at zero and has a width bounded away from zero. The other two intervals correspond to the "tails" of the phase profile. We define them to be

$$T_+ = \{\phi | f(\phi, u) \geq \frac{\sigma_+^s}{2}(1 - \phi) \quad \text{for} \quad u \in E + (-\frac{1}{2}, \frac{1}{2})\} \qquad (5.2)$$

and

$$T_- = \{\phi | f(\phi, u) \leq -\frac{\sigma_-^s}{2}(1 + \phi) \quad \text{for} \quad u \in E + (-\frac{1}{2}, \frac{1}{2})\}. \qquad (5.3)$$

We will assume that these intervals overlap, that is

$$(-1, 1) \subset L \cup T_- \cup T_+. \qquad (5.4)$$

It is easy to show this happens when λ is small (how small depending of course on the interval E). Corresponding to each of these intervals are the sets

$$\begin{aligned}
L^x &= \{x | \phi(x) \in L\} \\
T_-^x &= \{x | \phi(x) \in T_-\} \\
T_+^x &= \{x | \phi(x) \in T_+\}
\end{aligned}$$

so that $L^x \cup T_-^x \cup T_+^x = (-\infty, \infty)$.

We can prove the following about the structure of ϕ:

Theorem 4 *Assume that (5.4) holds. Then*
(a) ϕ and u are both monotone decreasing
(b) There are constants w, W, depending only on the functions g and p, for which $w \leq |L^x| \leq W$.

Proof. Suppose first that $\phi(x) \in L^x$. Integrating (2.4) from x to ∞ gives the bound

$$\tfrac{1}{2}\psi^2(x) > F(\phi(x), e_\infty) - F(-1, e_\infty) - \lambda \left(\frac{Du_x}{V}\right)^2.$$

Notice that Du_x/V has a uniform bound by using (2.3), so for small λ we can ensure that there is a constant B_1 with

$$|\psi(x)| > B_1 \qquad (5.5)$$

Therefore ϕ is monotone on each connected component of L^x. Also, multiplying (2.2) by the integrating factor $K_1 = \exp(Vx)$ and integrating from $-\infty$ to x gives

$$\psi(x) = -\int_{-\infty}^x K_1(x' - x) f(\phi(x'), u(x')) \, dx',$$

which is negative provided ϕ is in the tail region T_+. A similar argument shows ϕ is also decreasing in the other tail region T_+, therefore ϕ decreases everywhere. Using the formula (2.7), it follows that u is also decreasing.

For part (b), suppose the interval $L^x = (\phi_a, \phi_b)$. Then

$$\left| \int_{L^x} \phi_x dx \right| = \phi_b - \phi_a = |L|$$

Denote the lower and upper bounds on $|\phi_x|$ in the interval L^x by B_1 and C_1 respectively. Then it follows that $|L^x| < |L|/B_1$ and $|L^x| > |L|/C_1$. □.

6 Criticality and non-existence

When $\Delta > 1$, traveling waves always exist, but this is not necessarily true when $\Delta < 1$ [19, 16, 17]. In fact, there is a critical value of the ratio λ/D, below which no solutions exist. On the other hand, if D is small, solutions must exist by virtue of Theorem 1.

Two technical bounds are needed to prove the main result, which are given in the following lemma. They both depend on the monotone structure of section 5, so we assume that λ is small enough so that theorem 4 holds.

Lemma 4 *There exists positive constants I, J, depending only on g and p, for which*

$$\int_{-\infty}^{\infty} \phi_x^2 \, dx \geq I, \quad \int_{-\infty}^{\infty} 1 - p(\phi)^2 \, dx \leq J. \tag{6.1}$$

Proof. Setting B to be the lower bound on ϕ_x in the interval L^x, we have

$$\int_{-\infty}^{\infty} \phi_x^2 \, dx \geq \int_{L^x} \phi_x^2 \, dx \geq wB^2.$$

For the second bound, note that by the definition of the tail regions (5.2-5.3) there must be some constant C so that when $\phi \in T_\pm$,

$$|1 - p(\phi)^2| \leq C|f(\phi, u)|.$$

We can split the integral into integrals over the sets L^x, T_-^x and T_+^x. Then

$$\int_{L^x} 1 - p(\phi)^2 \, dx < |L_x| < W$$

and

$$\int_{T_-^x} 1 - p(\phi)^2 \, dx < C \int_{T_-^x} f(\phi, u) dx = C \int_{T_-^x} \phi_{xx} + V\phi_x \, dx.$$

The last integral is evidently bounded by some constant which depends only on V_s. A bound on the integral over T_+^x is obtained in the same way. □

Theorem 5 *Suppose that $\Delta < 1$. There exists a constant C, so that if*

$$\frac{\lambda}{D} \leq \frac{2I}{J}$$

then there is no solution to the traveling wave problem (1.5-1.8).

Proof. We will show that when λ/D is small, the equation (2.5) can't hold. Suppose that (ϕ, u) is some solution. The the right hand side of (2.5) has the estimate

$$\text{rhs} = \frac{\lambda}{2}(2\Delta - 1) < \frac{\lambda}{2}. \tag{6.2}$$

For the left hand side, we introduce the negative constant

$$\delta = \Delta - 1.$$

Notice that the function $u + \delta$ is always negative, and has the asymptotic behavior

$$u + \delta \to \begin{cases} 0 & \text{as} \quad x \to -\infty \\ -1 & \text{as} \quad x \to \infty \end{cases} \tag{6.3}$$

We can transform the integral of u_x^2 as follows:

$$\int_{-\infty}^{\infty} u_x^2 \, dx = -\int_{-\infty}^{\infty} u_{xx}(u + \delta) dx \tag{6.4}$$

$$= \frac{V}{D} \int_{-\infty}^{\infty} u_x(u + \delta) - \tfrac{1}{2}p(\phi)_x(u + \delta) \, dx \tag{6.5}$$

$$= \frac{V}{2D} - \frac{V}{2D} \int_{-\infty}^{\infty} p(\phi)_x(u + \delta) dx \tag{6.6}$$

where we have integrated by parts and used equation (1.6). By using formula (3.14) we have

$$(u + \delta)(x) = \tfrac{1}{2} \int_{-\infty}^{x} K(x' - x)[p(\phi(x')) - 1]dx.$$

Using (6.6), we can therefore obtain the estimate

$$\frac{D\lambda}{V} \int_{-\infty}^{\infty} u_x^2 dx = \frac{\lambda}{2} - \frac{\lambda V}{2D} \int_{-\infty}^{\infty} p(\phi(x))_x \int_{-\infty}^{x} e^{\frac{D}{V}(x'-x)}[p(\phi(x')) - 1]dx' \, dx$$

$$\geq \frac{\lambda}{2} - \frac{\lambda V}{2D} \int_{-\infty}^{\infty} p(\phi(x))_x \int_{-\infty}^{x} [p(\phi(x')) - 1]dx' \, dx$$

$$= \frac{\lambda}{2} - \frac{\lambda V}{2D} \int_{-\infty}^{\infty} [1 - p(\phi(x))^2]dx$$
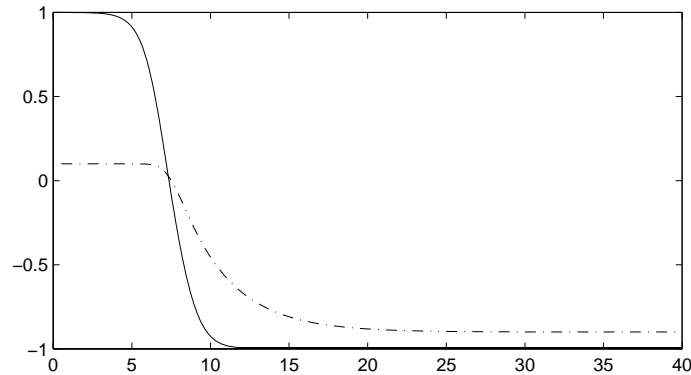
$$\geq \frac{\lambda}{2} - \frac{\lambda V}{2D}J$$

Figure 2: A monotone traveling wave. The phase variable ϕ is solid, temperature u is dashed. In this case, $D = .0628$.

where integration by parts was used for the second equality. Then an estimate for the left hand side of (2.5) is

$$\text{lhs} \geq VI + \frac{\lambda}{2} - \frac{\lambda V}{2D}J. \tag{6.7}$$

Comparing this to the right hand side estimate (6.2), it follows that for (2.5) to hold, one needs

$$\frac{\lambda}{D} > \frac{2I}{J}.$$

$\square$

Remark. Sharp values for I and J can be obtained by letting ϕ solve

$$\phi_{xx} - g'(\phi) = 0$$

and setting $I = \int \phi_x^2 dx$ and $J = \int 1 - p(\phi)^2 dx$.

7 Numerical examples

In this section, we discuss some numerical computations of both monotone and non-monotone wave profiles. The numerical method for obtaining these was, in fact, identical to the proof of theorem 1. All parameters but D were fixed, and a trajectory of the system (2.1-2.3) was computed forward for some fixed amount of time, starting at a point near η_-. Then D was adjusted so that the trajectory tended toward η_+. There was always at least one value of D which gave this behavior, and sometimes several. In any case, the smallest value of D corresponded to a monotone profile, where larger values gave oscillatory wavefronts.
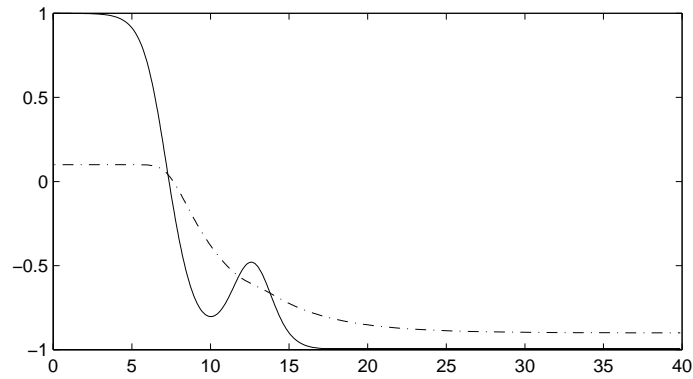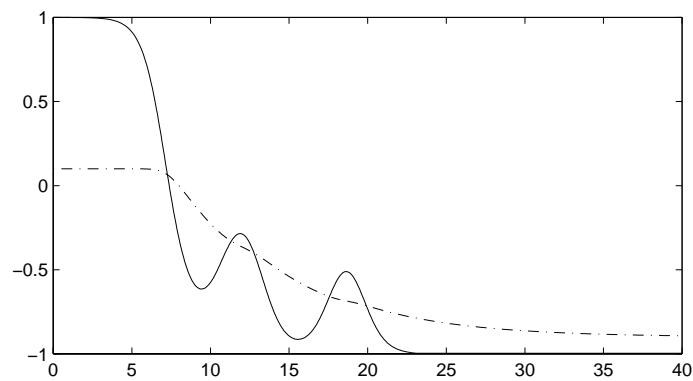
Figure 3: An oscillatory wave, $D = .077$.
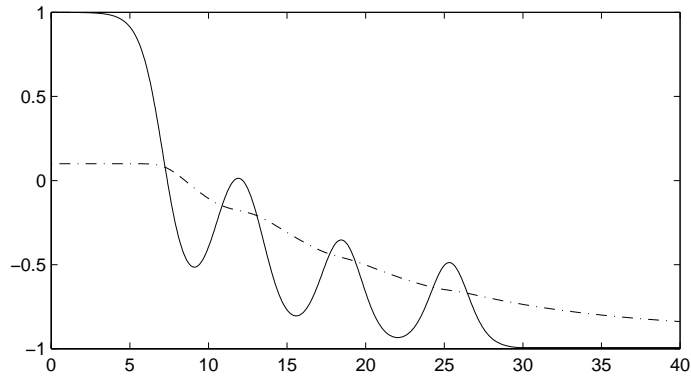

Figure 4: An oscillatory wave, $D = .124$.
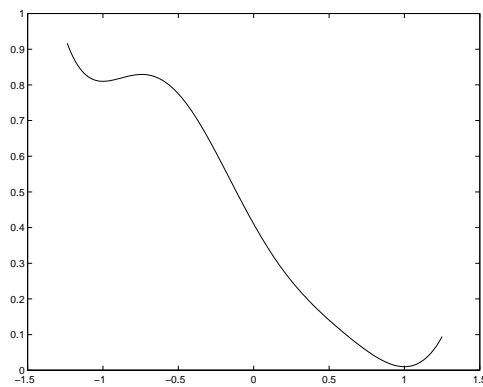
Figure 5: An oscillatory wave, $D = .205$.

Figure 6: A plot of the function $F(\phi; e_\infty)$ for $e_\infty = -\Delta + \frac{1}{2} = -.4$

Figures 2 - 5 show four different wave profiles, each corresponding to a different value of D, but otherwise with the same parameters $\lambda = 2$, $\Delta = .9$, and $V = .02$. The functions g and p were

$$g(\phi) = \frac{1}{4}(1 - \phi^2)^2, \quad p(\phi) = \frac{15}{8}(\phi - \frac{2}{3}\phi^3 + \frac{1}{5}\phi^5)$$

which yield the energy function $F(\phi; e)$ whose graph is given in figure 6.

The results of the numerical study suggest a number of open problems. An fairly exhaustive search of parameter space was conducted, and from this we conjecture the following:

- There is a unique monotone wave, in the sense that exactly one value of D gives such a wave profile. As a consequence, when λ is small, there is a unique value of D giving a solution.

- As λ is increased (equivalently as the wells of the energy s become more uneven), more solutions appear, corresponding to higher values of D and having more oscillations.

- For fixed D and $\Delta > 1$, there is exactly one monotone wave whose velocity increases with Δ.

8   Conclusion

We have given an in-depth analysis of the traveling wave problem for phase field models. To some extent, the questions of existence, uniqueness, monotonicity and non-existence have all been addressed. Quantitative results regarding velocity bounds and non-existence have also been provided.

We have made no attempt to address the dynamics of the waves under consideration. Some work in this direction is presented in [12]. As for the non-monotone solutions, our suspicion is that they are unstable; this is frequently the case for oscillatory traveling waves [20]. The interested reader also may wish to look at some of the numerical experiments in [17] for some unusual dynamical features.

References

[1] R. Almgren and A. Almgren, *Phase field instabilities and adaptive mesh refinement*, TMS/SIAM, 1996, pp. 205–214.

[2] P. W. Bates, P. C. Fife, R. A. Gardner, and C. K. R. T. Jones, *The existence of traveling wave solutions of a generalized phase field model*, Siam J. Math. Anal., 28 (1997), pp. 60–93.

[3] ——, *Phase field models for hypercooled solidification*, Physica D, 104 (1997), pp. 1–31.

[4] H. Berestycki and L. Nirenberg, *Traveling fronts in cylinders*, Ann. Inst. Henri Poincaré, (1992), pp. 497–572.

[5] G. Caginalp and P. Fife, *Dynamics of layered interfaces arising from phase boundaries*, SIAM J. Appl. Math., 48 (1988), pp. 506–518.

[6] G. Caginalp and Y. Nishiura, *Examples of traveling wave solutions for phase field models and convergence to sharp interface models in the singular limit*, Quart. of Appl. Math., 49 (1991), pp. 147–162.

[7] G. Caginalp and W. Xie, *Mathematical models of phase boundaries in alloys: phase field and sharp interface*, Phys. Rev. E, 48 (1993), pp. 1897–1909.

[8] S. J. Chapman, S. D. Howison, and J. R. Ockendon, *Macroscopic models for superconductivity*, SIAM Review, 34 (1992), pp. 529–560.

[9] J. B. Collins and H. Levine, *Diffusion interface model of diffusion limited crystal growth*, Phys. Rev. B, 31 (1985), p. 6118.

[10] P. C. Fife, *Dynamics of Internal Layers and Diffuse interfaces*, SIAM, 1988.

[11] P. C. Fife and J. B. McLeod, *The approach of solutions to nonlinear diffusion equations to traveling front solutions*, Arch. Rat. Mech. Anal., 65 (1977), pp. 335–361.

[12] K. Glasner, *Rapid growth and critical behavior in phase field models of solidification*, (1999). In press.

[13] K. Glasner and R. Almgren, *Dual fronts in phase field models*, (1999). Submitted.

[14] A. Karma and W.-J. Rappel, *Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetics*, Phys. Rev. E., (1996), pp. 3017–3020.

[15] J. S. Langer, *Models of Pattern Formation in First order Phase Transitions*, World Scientific, 1986.

[16] H. Lowen and J. Bechhoefer, *Critical behavior of crystal growth velocity*, Europhys. Lett., 16 (1991), pp. 195–200.

[17] H. Lowen, J. Bechhoefer, and L. Tuckerman, *Crystal growth at long times: Critical behavior at the crossover from diffusion to kinetics limited regimes*, Phys. Rev. A, 45 (1992), pp. 2399–2415.

[18] O. Penrose and P. Fife, *Thermodynamically consistent models for the kinetics of phase transitions*, Physica D, 43 (1990), pp. 44–62.

[19] S. Schofield and D. Oxtoby, *Diffusion disallowed crystal growth. I. Landau-Ginzburg model*, J. Chem. Phys., 94 (1991), pp. 2176– 1286.

[20] A. Vol'Pert, V. Volpert, and V. Volpert, *Traveling Wave Solutions of Parabolic systems*, American Mathematical Society, 1994.

[21] S. Wang, R. Sekerka, A. Wheeler, B. Murray, C. Coriell, R. Braun, and G. McFadden, *Thermodynamically consistent phase-field models for solidification*, Physica D, 69 (1993), pp. 189–200.

[22] A. Wheeler, W. Boettinger, and G. McFadden, *Phase-field model for isothermal transitions in binary alloys*, Physical Review A, 45 (1992), pp. 7424–7439.

[23] ――, *Phase-field model of solute trapping during solidification*, Physical Review E, 47 (1993), pp. 1893–1909.

[24] M. Zukerman, R. Kupferman, O. Shochet, and E. Ben-Jacob, *Concentric decomposition during rapid compact growth*, Physica D, 90 (1996), pp. 293–305.

Karl Glasner
Department of Mathematics, University of Utah
Salt Lake City, Utah 84112-0090 USA
email: glasner@math.utah.edu