Well-posedness issues for models of phase transitions with weak interaction

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Abstract

Gradient flows for simple phase field models based on a nonlocal free energy functional (the one used in [1] and elsewhere) of a scalar state variable are investigated. We also consider such functionals with no spatial interaction terms. It is known that in either case the state function may be discontinuous. We allow the discontinuity to migrate and treat its position as a primary ingredient in the dynamics, along with the state variable. This leads to an alternative type of gradient flow. The latter's initial value problem suffers from the lack of uniqueness, and there are multiple traveling waves. One manifestation of this is the possibility of the spontaneous appearance of a new phase at a point, the domain of the new phase then spreading outward. This ill-posedness can be alleviated by the addition, to the free energy functional, of a term concentrated at the discontinuity. Similarly, so doing makes traveling waves unique.

1 Introduction

The main purpose in the first sections of the paper will be to show that even very simple phase-field models do not always provide well-posed initial value problems. Specifically, the examples exhibit nonuniqueness—I prove the local existence of many solutions. Later it is shown what may be added to these models to restore uniqueness. Let me begin by giving a brief background perspective on phase-field models, about which there is now an enormous literature.

These models, as applied to phase transitions in materials, are characterized by one or more phase functions (I take the number to be one) which take on a continuum of values. These functions are intended to be rough microscopic descriptors of the state of the material relevant to its transition between phases. The models usually involve other variables as well. The dynamics of the phase function ϕ is often given in terms of a free energy functional $F[\phi]$ (I am suppressing dependence on the other variables). A linear force/flux relation

$$\phi_t = -C\frac{\delta F}{\delta \phi} \tag{1}$$

is postulated (again, we disregard the effect on this of the other variables). In addition to choosing the functional F, the type of functional derivative $\frac{\delta F}{\delta \phi}$ must be selected. In any case, the latter is a measure of the rate at which F can be changed by changing ϕ. As such, it can be considered a "force", in analogy to the relation between force and potential in classical mechanics. The response ϕ_t is considered a "flux". The relation (1), where C is any positive constant (or function), is called a gradient flow for the functional F.

A precise definition of the phase function ϕ and a detailed knowledge of the microscopic change mechanisms are typically lacking. Without this knowledge, general models based on this framework have been analyzed. The reasonableness of any particular model would depend, among other things, on whether it predicts known results and whether it leads to sensible mathematics.

In this paper I deal only with the latter question. Moreover, I pare down the class of models considered, which involve nonlocal interactions, to its simplest unadorned form.

The nonuniqueness shown in Sections (2–7) provides a negative answer to the question of sensible mathematics for a certain class of flows, and as such is worthwhile information when it comes to constructing phase field models. It is associated with the presence and law of motion of discontinuities in the state variable, coupled with the fact that the value of the state variable is not fixed on either side of these discontinuities.

This nonuniqueness is accompanied by a spontaneous generation phenomenon. A new phase can appear (Section 7) in a manner akin to nucleation, but with no apparent nucleus.

We also look at traveling waves in Section 8 and find that they exist for these same systems, but again are not unique.

The second part of the paper (Sections 9–11) shows that by postulating an additional type of free energy, namely one concentrated at discontinuities, the initial value problem becomes well-posed. I prove the local existence of a unique solution, under natural assumptions on the data, and the existence of a unique traveling wave as well. The paper ends with a discussion in Section 12.

The main focus of this work is on a nonlocal free energy functional which is a natural analog of the real Ginzburg-Landau functional. This functional was shown in [2] to be a continuum limit of a discrete system. Nonlocal free energies have been promoted and studied in the past. In fact nonlocal interactions in continua were already envisaged by van der Waals [17]. The generalized Ginzburg-Landau functional used here was also used in [1] and further studied in other papers such as [2, 3, 8, 6]. Related nonlocal models have appeared in many continuum mechanical connections; among them I cite [16, 4, 9, 10]. Continuum and discrete nonlocal models based on statistical mechanics considerations have been studied extensively; see for example [13, 14, 15, 11, 12].

In [1, 2, 3], the driving force for changes in the state variable was the L_2 gradient of the functional, and that force was applied uniformly in space to induce the motion of the state function. By its very nature, the resulting dynamics, while permitting spatial discontinuities under some conditions, prohibits their motion. The motion of discontinuities would nevertheless provide a way to reduce the total free energy. Among other things, in this paper I suggest a natural way to incorporate this motion into the dynamics.

To reiterate, I argue in the present work that in many cases it may be reasonable to propose that the discontinuities migrate in such a way as to reduce the free energy. The simplest way to do this is to incorporate the motion as part of a gradient flow (force/flux) mechanism. What results is a kinetic law saying that the velocity of this migration is proportional to the jump in free energy density across the discontinuity.

As payment for this law of motion, we have the nonuniqueness referred to above. However, uniqueness may be regained by adding an extra contribution to the free energy functional, namely an "interfacial free energy" based exclusively at the discontinuities. It is taken to be a function of the jump in the state variable. Adding the extra term is conceptually totally different from the migration law indicated above, which is a kinetic phemonenon.

2 A simple free energy-driven mechanism

The free energy density is in this example a smooth double-well function $F(u)$ of a state function $u(x,t)$. It is defined for $u \in [-1,1]$ and has exactly two local minima, at $u = \pm 1$, where $F'(u) = 0$.

The dynamics of u is as follows. If u is continuous at (x,t), then its rate of change at that point is given by

$$u_t = -F'(u), \tag{2}$$

which is (1) in this context. Thus the free energy is reduced locally by a continuous change in the variable u. We shall refer to values of u in the domain of attraction of the equilibrium value $u = -1$ as being in "Phase 1", and those in the domain of attraction of 1 as being in "Phase 2". The first domain is an interval $[-1, -1+b_1)$ and the second one is $(1-b_2, 1]$.

We shall also allow the possibility that u is discontinuous on a curve $x = \xi(t)$ in the (x,t) plane. Only discontinuities which involve a switch from one phase to the other will be considered.

Then the velocity of that discontinuity is prescribed to be proportional to the jump in free energy across it:

$$\dot{\xi}(t) = [F(u)]_{\xi(t)} \tag{3}$$

(dots denote time derivatives). Here and throughout the paper, for evolving pairs (u,ξ) we use the notation $[F(u)]_{\xi(t)} \equiv F(u(\xi^+),t) - F(u(\xi^-),t)$, where $u(\xi^+,t) \equiv \lim_{x\downarrow\xi} u(x,t)$ and $u(\xi^-,t) \equiv \lim_{x\uparrow\xi} u(x,t)$. Again, (3) is the proper interpretation of (1). I shall usually use the practice of setting coefficients such as C in (1) equal to unity.

Dynamical assumptions like (3), in which it is postulated that the speed of a interface is proportional to the jump in free energy across it, are common in materials science modeling; see for example [5].

Except in section 7, we consider problems in which there is only one mobile discontinuity $\xi(t)$, although the analysis could be extended in an obvious manner to problems involving more than one.

Here is a slightly different perspective, which we note for comparison with other models in the paper. The dynamics (2), (3) can also be viewed as a gradient flow for the total free energy

$$E_0[u,\xi](t) = \int_{-\infty}^{\infty} F(u(x,t))\,dx, \tag{4}$$

in the following sense.

The functional $E_0[\phi,\xi]$ is defined for ϕ in the admissibility class $\mathcal{A}(\xi)$ of functions satisfying:

- ϕ is uniformly continuous on each interval $(-\infty,\xi)$ and (ξ,∞), and
- ϕ takes values in $[-1,1]$.

We now let both u and ξ evolve in time t, and calculate

$$\dot{E}_0[u,\xi] = \int_{-\infty}^{\infty} F'(u)\dot{u}\,dx - \dot{\xi}[F(u)]_{\xi(t)}. \tag{5}$$

The right side is a type of scalar product of the pair $(F'(u), -[F(u)]_\xi)$ with the pair $(\dot{u},\dot{\xi})$. Accordingly, a simple gradient flow associated with this expression will be a pair $(u(x,t),\xi(t))$ with $u(\cdot,t) \in \mathcal{A}(\xi(t))$ at each time t satisfying (2) for $x \neq \xi$ and (3) at the discontinuity ξ. (Again, the same expression (5) with any positive constants attached to the two terms on the right would do.) For such pairs, we have

$$\dot{E}_0[u,\xi](t) = -\int_{-\infty}^{\infty} (u_t)^2\, dx - \dot{\xi}^2 \leq 0.$$

Traveling waves will be solutions of the form $u(x,t) = U(x-ct)$, $\xi = \xi(0) - ct$. We may with no loss of generality take $\xi(0) = 0$; then traveling wave solutions $U(z)$, where $z = x - ct$, satisfy

$$-cU'(z) = -f(U(z)), \qquad z \neq 0, \tag{6}$$

$$c = [F(U)]_0. \tag{7}$$

3 The initial value problem for the simple model

The initial value problem is to find a solution of (2) and (3) satisfying prescribed initial data

$$u(x,0) = u_0(x), \quad \xi(0) = \xi_0. \tag{8}$$

We take $\xi_0 = 0$.

For this section, we use a technical but simple construction related to transitions from the interior descending branch of the function F to the ascending one. Assume that $q = \int_{-1}^{1} f(u)\, du > 0$. Then $F(1) = F(-1) + q$. Recall that ± 1 are the only two local minima of F. It follows that there exist intervals $I_- = [a_1, a_2] \subset (-1, 0)$ and $I_+ = [a_3, a_4] \subset (0, 1)$, together with a closed interval $C \subset (0, q)$, all these intervals with positive length, such that for every $c \in C$ and every $U \in I_+$, the equation

$$F(U) - F(W) = c$$

has a unique solution $W \in I_-$ (this relates to (3) with $\dot{\xi} = c$). We call this functional relationship

$$W = P(U, c).$$

Let $\delta > 0$ be small enough that $I_+^\delta = [a_3 + \delta, a_4 - \delta]$ has positive length.

Let $\xi(t)$ be a given continuously differentiable function satisfying

$$\dot{\xi}(t) \in C, \qquad \xi(0) = 0, \tag{9}$$

and let $T > 0$. Let $u_0(x)$ be continuous for $x \neq 0$ and satisfy

$$u_0(x) \text{ in phase 1 for } x < 0,$$

$$u_0(x) \in I_+^\delta, \quad x > 0; \quad u_0(0^-) = P(u_0(0^+), \dot{\xi}(0)). \tag{10}$$

Theorem 1 *Let u_0, $\xi(t)$ satisfy the given conditions (9), (10). Then for small enough T there is a unique solution of (2), (3), (8) existing for $0 \leq t \leq T$.*

Proof: Since $\dot{\xi} > 0$, the function $\xi(t)$ has an inverse $\tau(x)$, so that $\xi(\tau(x)) = x$ for each $x \in [0, \xi(T)] \equiv X_0$. For each x we solve the equation (2) with initial condition $u(x,0) = u_0(x)$. If $x \in X_0$, we integrate up to time $\tau(x)$; otherwise to time T. The bistable nature of F ensures that global solutions exist. For $x \in X_0$, $u(x^-, \tau(x)) = u(x, \tau(x)^+)$ and the condition (3) can be written in the equivalent form $F(u(x,\tau(x)^-)) - F(u(x,\tau(x)^+)) = \dot{\xi}(\tau(x))$. It is further equivalent to

$$u(x, t^+) = P(u(x, t^-), \dot{\xi}(t)) \quad \text{for } t = \tau(x), \tag{11}$$

provided $u(x,t^-)\in I_+$. But since $u_0(x)\in I_+^\delta$, we have that $u(x,\tau(x)^-)\in I_+$ for $x\in X_0$ and small enough T, so that (11) will hold.

To continue, with $x\in X_0$ we integrate (2) for $t\geq\tau(x)$ under the initial condition $u(x,\tau(x)) = u(x,t^+)$, as given by (11). The integration continues up to time T.

For values $x\notin X_0$ we integrate up to time T without interruption. It is easy to show that the solution so constructed is continuous except on the given trajectory $x=\xi(t)$. This completes the proof.

Since the discontinuity's trajectory was given arbitrarily, we conclude that there are many solutions of the initial value problem (8).

Similarly, it can be shown that there exists a discontinuous traveling wave solution for any prescribed velocity c in the interval $(0,q)$. We do not give the construction, as it is a simple problem in ordinary differential equations..

4 A model with spatial interaction

We begin with a C^1 function $J(x)$ which is even, nonnegative, satisfies $\int_{-\infty}^{\infty} J(x)\,dx = 1$, and $J'\in L_1(-\infty,\infty)$. The smooth function $F(u)$ is the one described in Section 2.

We now use an energy functional analogous to (4), but with interaction term:

$$E[u,\xi] = \frac{1}{4}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} J(x-y)(u(x)-u(y))^2 dx\,dy + \int_{-\infty}^{\infty} F(u(x))\,dx. \tag{12}$$

This functional is a variant on the classical scalar Ginzburg-Landau functional; the spatial interaction terms are now nonlocal. It was used in [1] and elsewhere, and derived in [2] as the limit of a lattice model with short-range and long-range interactions. The derivation allows F to have an arbitrarily large barrier between its two minima.

The admissibility class $\mathcal{A}(\xi)$ will be the same as in Section 2.

Again letting both u and the ξ evolve in time t, we have

$$\dot{E} = -\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} J(x-y)u(y)dy - u(x) - F'(u)\right)\dot{u}\,dx - \dot{\xi}[F(u)]_{\xi(t)}. \tag{13}$$

A gradient flow corresponding to this expression will be analogous to that in Section 2, namely a pair $(u(x,t),\xi(t))$ with $u\in\mathcal{A}(\xi(t))$ at each time t satisfying

$$u_t = J*u - u - F'(u), \quad x\neq\xi(t), \tag{14}$$

$$\dot{\xi}(t) = [F(u)]_\xi. \tag{15}$$

Here $J*u$ is convolution over the real line (x-axis), as in (13).

If the right side of (15) is set to zero, we have solutions of (14) whose discontinuity, if it exists, is stationary. This case was included in the theory in [1].

5 What is new about this gradient flow?

The same energy is posited in this definition of gradient flow and the one in [1], in which the right side of (15) is zero. The main difference is that the variation of the discontinuity ξ was not specifically accounted for in the notion of functional derivative (1) in that previous paper. As a consequence, it turns out that in fact discontinuities could not move, whereas of course they can in the new formulation.

From one point of view, it can be seen that we are now allowing for nonuniform kinetic processes, in the sense that the kinetic mechanism driving state changes is very much enhanced at the place where the discontinuity occurs. In the absence of this enhancement, an extensive theory of traveling waves was given in [1] and extended in part to double obstacle problems in [6]. Also, problems in higher dimensions were studied in [8] and [3].

We have four profound consequences resulting from the present formulation: (1) The initial value problem under the present definition does not enjoy uniqueness of solutions. In fact in Theorem 2 below, the trajectory $\xi(t)$ can be prescribed at will beforehand. (2) It is possible for discontinuous traveling waves with nonzero velocity to exist (Section 8). It was found in [1] that under the previous definition, monotone traveling wave profiles must be continuous if $c \neq 0$, although they are sometimes discontinuous at a single point with $c = 0$. (3) Traveling waves are not unique (Section 8). In fact, we show that it is possible for them to exist for any velocity in a certain interval. (4) If the free energy functional contains an additional term (such as that given in Section 9), then the uniqueness of initial value problems and traveling waves reappears (Sections 10 and 11). This term is unrelated to the free energy function F.

As a side remark, note that the nonuniqueness result for traveling waves in this paper is opposite from the following kind of nonuniqueness occurring both in [1] and in the present paper: since discontinuous profiles are solutions in which a range of values of u is skipped over, the function F may be changed at will for u in that range, and the solution remains a solution.

6 The initial value problem

We make the same assumptions on F as in Section 2, and the same definitions of $I_\pm$, C, and the function P. Let $\xi(t)$ and $u_0(x)$ be given with the same properties as in Section 3.

Theorem 2 *Let u_0, $\xi(t)$ satisfy the given conditions (9), (10). Then for small enough T there exists a unique solution of (14), (15), (8) existing for $0 \le t \le T$.*

Preliminaries to the proof: First, we need a convenient integral representation for the solution.

We again use the previous definition of $\tau(x)$, defined for each $x \in X_0 = \{0 < x < \xi(T)\}$. And again (11) will hold for our solutions.

For each fixed x, the equation (14) holds for all t except $t = \tau(x)$ (for $x \in X_0$), where the solution undergoes a jump equal to $P(u(x,t^-), \dot{\xi}(t)) - u(x,t^-)$. We may represent this behavior in a single equation by adding the term $\delta(t-\tau(x))(P(u(x,t^-), \dot{\xi}(t)) - u(x,t^-))$ to the right side of (14). We then integrate the resulting equation with respect to time to obtain

$$u(x,t) = u_0(x) + \int_0^t [J*u(x,s) - u(x,s) - F'(u(x,s))]ds + \chi_{\Omega_-}(x,t)[P(u(x,\tau(x)^-), \dot{\xi}(t)) - u(x,\tau(x)^-)], \tag{16}$$

where χ is the characteristic function of the set in the subscript, namely $\Omega_-(T) = \{(x,t) : x < \xi(t),\ 0 \le t \le T\}$. We make the analogous definition for $\Omega_+(T)$.

Conversely, (14), (15), (8) follow from (16).

We consider functions on the strip $\{0 \le t \le T\}$ which are continuous except on the curve $\{x = \xi(t)\}$, where they have limiting values from both sides, and more specifically consider them in the Banach space

$$Y \equiv C_0(\overline{\Omega_+}) \times C_0(\overline{\Omega_-}), \tag{17}$$

with norm

$$\|u\|_Y = \sup_{\Omega_+\cup\Omega_-} |u(x,t)|. \tag{18}$$

We define the following operators on the space Y:

$$\Psi(u)(x,t) = \int_0^t [J * u(x,s) - u(x,s) - F'(u(x,s))]ds,$$

$$Q(u)(x,t) = \chi_{\Omega_-}(x,t)[P(u(x,\tau(x)^-),\dot{\xi}(t)) - u(x,\tau(x)^-)] + u_0(x). \tag{19}$$

Finally, define the ball in Y

$$B = \{u : \|u - Q(u_0)\|_Y < a\} \tag{20}$$

for some a to be chosen later.

Lemma 1 *The operator Q maps Y into itself.*

Proof: Let $u \in Y$. From the definition (19) it is seen that the restriction of $Q(u)$ to Ω_+ is continuous, and that its restriction to Ω_- is continuous except possibly on the line $\{x = 0,\ t > 0\}$. The reason for including this possibility is that the function u_0 is discontinuous on that line. However, we shall show that the total function $Q(u)$ is continuous there. That fact will suffice to establish the lemma.

So set $t > 0$ and let $x\downarrow 0$. Note that $\lim_{x\downarrow 0}\tau(x) = 0$. Therefore

$$\lim_{x\downarrow 0}[P(u(x,\tau(x)^-),\dot{\xi}(t)) - u(x,\tau(x)^-) + u_0(x)] = P(u(0^+,0),\dot{\xi}(0)) - u(0^+,0) + u_0(0^+).$$

Since the last two terms cancel, we find, using (10) and (19), that

$$\lim_{x\downarrow 0} Q(u(x,t)) = P(u(0^+,0),\dot{\xi}(0)) = u(0^-,0) = \lim_{x\uparrow 0} Q(u(x,t)).$$

Therefore $Q(u)$ is continuous on that line, completing the proof.

The equation (16) may now be written

$$u = \Psi(u) + Q(u). \tag{21}$$

We seek a solution of this equation, i.e. a fixed point for the operator $\Psi + Q$.

Lemma 2

$$u = \Psi(u) + Q(u) \tag{22}$$

if and only if

$$u = \Psi(u) + Q(\Psi(u) + u_0). \tag{23}$$

We need the following preliminary lemma, among other things to show that the last term in (23) is defined.

Lemma 3 *Let f and g be functions of (x,t) whose restrictions to Ω_+ may be extended continuously to $\overline{\Omega_+}$ so as to belong to $C_0(\overline{\Omega_+})$. Assume that f and g have initial values u_0 at $t = 0$, and that their restrictions to Ω_+ take values only in I_+.*

(a) The operator $Q(f)$ has a natural interpretation, and $Q(f) \in Y$. (The same holds for g.)

(b) $Q(f \pm (Q(g) - u_0)) = Q(f)$.

Proof:

Part (a) is obvious from the definitions of Q and Y, since $Q(u)$ sees only the values of u in Ω_+.

Part (b) follows from the observations that $Q(g) - u_0$ vanishes in Ω_+ and that the operator Q sees only the values of its argument in Ω_+. This completes the proof.

Proof of Lemma 2:

If (22) holds, then $u = \Psi(u)+Q(u) = \Psi(u)+Q(\Psi(u)+Q(u)) = \Psi(u)+Q(\Psi(u)+u_0-u_0+Q(u))$. We now apply Lemma 3(b) with $f = \Psi(u) + u_0$ and $g = u$ to obtain that this last expression

$$= \Psi(u) + Q(f + Q(g) - u_0) = \Psi(u) + Q(f) = \Psi(u) + Q(\Psi(u) + u_0),$$

which is (23)

On the other hand if (23) holds, then $\Psi(u) = u - Q(\Psi(u) + u_0)$ and
$u = \Psi(u) + Q(\Psi(u) + u_0) = \Psi(u) + Q(u - Q(\Psi(u) + u_0) + u_0)$
$= \Psi(u)+Q(u-(Q(\Psi(u)+u_0)-u_0)) = \Psi(u)+Q(u)$, which is (22) again by Lemma 3. This finishes the proof.

Proof of Theorem 2.

Our problem (16) therefore reduces to finding a fixed point of the mapping

$$\Phi(u) = \Psi(u) + Q(\Psi(u) + u_0). \tag{24}$$

We shall seek one in the ball B.

First of all, we may guarantee that if $u \in B$, then $\Phi(u) \in B$ by choosing T to be small enough. This is because $\|\Psi(u)\|_Y$ is small for T small, and Q depends continuously on it argument, in the sense of $C_0(\overline{\Omega_+})$.

The parameter a in (20) is to be chosen so small that for all $u \in B$ and $(x,t) \in \Omega_+$, $u(x,t) \in I_+$. This is possible by (10). Thus $P(u(x,t), c)$ is defined for all $(x,t) \in \Omega_+$ and all $c \in C$.

With these stipulations, it is clear that $\Psi(u)$ is a Lipschitz mapping from B into itself, with Lipschitz constant bounded by $L_1 T$ for some L_1, and that $Q(u)$ is also, with some Lipschitz constant L_2. We therefore obtain from (24) that Φ has Lipschitz constant bounded by $L_1 T(1 + L_2)$. The existence of a unique fixed point now follows in the usual way, choosing T small enough, from a contractive mapping argument. This provides the existence and uniqueness of (16), which implies (14), (15), (8).

7 Spontaneous generation of a new phase

It was mentioned before that the gradient flows considered up to this point can easily be generalized to allow for more than one discontinuity. In this section, we consider two of them, moving in opposite directions. The state in the region between the two discontinuities will be in Phase 1, and otherwise it will lie in Phase 2.

Now consider an initial function $u_0(x)$ which is continuous for all x, taking values in I_+^δ. Let $\xi_1(t)$ and $\xi_2(t)$ be two trajectories satisfying $\xi_i(0) = 0$, $\dot{\xi}_1(t) \in C$, and $-\dot{\xi}_2(t) \in C$. Thus both trajectories emanate from the point $x = 0$, one moving to the right and the other to the left.

Theorem 3 *Let $u_0, \xi_1(t), \xi_2(t)$ satisfy the given conditions. Then for small enough T there exists a unique solution of the generalization of (14), (15), (8) to the case of two moving discontinuities, existing for $0 \le t \le T$.*

The proof is very similar to that of Thm. 2, and will not be given.

8 Traveling waves

In this section, we choose a specific function F for simplicity, although the argument can be given in general. Our choice has $F'(u)$ a linear function with slope $m-1>1$ near $u=\pm 1$. The object is to prove the existence but nonuniqueness of traveling wave solutions of (14), (15).

In the following, we refer to a number $m>2$ and a function

$$f(u)=\begin{cases}(m-1)(u-1), & u\in(1-\frac{2}{m}-\epsilon,1),\\ (m-1)(u+1), & u\in(-1,-1+\frac{2}{m}+\epsilon).\end{cases} \tag{25}$$

for some small enough $\epsilon>0$. The smooth function f is left undefined for $u\in(-1+\frac{2}{m}+\epsilon,1-\frac{2}{m}-\epsilon)$, except that

$$q\equiv\int_{-1}^{1}f(u)\,du>0. \tag{26}$$

Thus $f(u)=F'(u)$, where

$$F(u)\equiv\int_{-1}^{u}f(s)\,ds=\begin{cases}\frac{1}{2}(m-1)(u-1)^2+q, & u\in(1-\frac{2}{m}-\epsilon,1),\\ \frac{1}{2}(m-1)(u+1)^2, & u\in(-1,-1+\frac{2}{m}+\epsilon).\end{cases} \tag{27}$$

For $c>0$, we seek a monotone increasing function $U(z)$ on the whole line, continuous except at $z=0$, satisfying

$$-cU'+f(U)=J*U-U, \tag{28}$$

$$c=[F(U)]_0, \tag{29}$$

$$U(\pm\infty)=\pm 1. \tag{30}$$

First, for $L>0$ we seek an appropriate solution on the interval $[-L,L]$.

Let $K_L=\{U(z):U$ nondecreasing, continuous on $[-L,0)\cup(0,L]$, $U(z)\in[1-\frac{2}{m},1]$ for $z>0$, $u(z)\in[-1,-1+\frac{2}{m}]$ for $z<0\}$. Since $\lim_{z\uparrow 0}U(z)$ and $\lim_{z\downarrow 0}U(z)$ exist, we may consider functions in K_L as elements of the Banach space $Y_L=C([-L,0])\times C([0,L])$. Then K_L will be a closed convex subset of Y_L.

Lemma 4 *Let $0<c<q$. Then there exists a solution $U\in K_L$ of (28), (29).*

Proof. We define a mapping Φ from K_L into itself in three steps as follows. Given $\tilde U\in K_L$,

1. Solve

$$-cU'(z)+mU+1-m=J*\tilde U,\quad z\in(0,L], \tag{31}$$

$U(z)\in(1-\frac{2}{m},1]$, $U(L)=1$.

The solution is unique and easily obtained:

$$U(z)=\frac{1}{c}e^{mz/c}\int_z^L e^{-ms/c}[J*\tilde U(s)+m-1]ds+e^{-m(L-z)/c}. \tag{32}$$

It is monotone increasing for the following reason. The monotonicity of $J*\tilde U$ follows from that of $\tilde U$. We have the expression

$$U'(z)=\frac{1}{c}\left\{\int_z^L[J*\tilde U(s)+m-1]\frac{m}{c}e^{-m(s-z)/c}ds-[J*\tilde U(z)+m-1]\right\}+\frac{m}{c}e^{-m(L-z)/c}$$

$$\geq \frac{1}{c}[J * \tilde{U}(z) + m - 1]\left(1 - e^{-m(L-z)/c} - 1\right) + \frac{m}{c}e^{-m(L-z)/c}. \tag{33}$$

But $J * \tilde{U}(z) + m - 1 \leq m$, so we conclude that $U' \geq 0$.

Since $J * \tilde{U} \geq -1$, we have the estimate

$$U(z) \geq U(0) \geq \frac{1}{c}\int_0^L e^{-ms/c}[m-2]ds + e^{-mL/c} = \frac{m-2}{m} + \frac{2}{m}e^{-mL/c} > 1 - \frac{2}{m}. \tag{34}$$

Therefore by (25), the left side of (31) equals $-cU'(z) + f(U) + U$.

2. We show the existence of a unique number $\alpha \in (-1, -1+\frac{2}{m})$ satisfying $F(\alpha) = F(U(0+)) - c$. By (34), $(27)_1$ and the restriction $c < q$, the right side of this equation lies in $(0, \frac{2}{m^2}(m-1)$, which by $(27)_2$ is the range of the function $F(u)$ for $u \in [-1, -1+\frac{2}{m}]$. The function F is monotone in this range, so there is a unique such α.

Our solution on the interval $[-L, 0]$ will have $U(0-) = \alpha$, so that (29) will hold.

3. On that interval, we solve

$$-cU'(z) + mU + m - 1 = J * \tilde{U}, \quad z \in (-L, 0), \quad U(0-) = \alpha \tag{35}$$

(again, the left side equals $-cU' + f(U) + U$).

The solution is

$$U(z) = -\frac{1}{c}e^{mz/c}\int_0^z e^{-ms/c}[J * \tilde{U}(s) + 1 - m]ds + \alpha e^{mz/c}. \tag{36}$$

It can be checked that this function also is monotone increasing with $U(z) \in [-1, -1+\frac{2}{m}]$. Therefore $U \in K_L$. This defines the mapping $u = \Phi(\tilde{u})$.

Because the convolution J is a smoothing operation and solutions of (31) and (35) are at least as smooth as the right sides on the intervals $[0, L]$ and $[-L, 0]$ respectively, the mapping Φ from K_L into itself is compact. There is a fixed point, which must be a solution of (28), (29). This completes the proof of the lemma.

We now define K to be the same as K_L, but with $L = \infty$.

Theorem 4 *Let $c \in (0, q)$. Then there exists a solution $U \in K$ of (28), (29), (30). If $c = 0$, there exists a solution of (28), (30).*

Proof. First, let $c \in (0, q)$. Let U_L be the solutions constructed in the lemma. As $L \to \infty$, they form an equibounded and equicontinuous set on each finite interval $I \in (0, \infty) \cup (\infty, 0)$. A standard argument shows there is a diagonal subsequence converging to a solution of (28), (29). We have only to verify the boundary conditions (30). Let $U_+ = \lim_{z\to\infty} U(z)$; it exists by the monotonicity of $U \leq 1$. Then $\lim_{z\to\infty} J * U = U_+$, and letting $z \to \infty$ in (28) and $(25)_1$, we get $(m-1)(U_+ - 1) = 0$, which implies $U_+ = 1$. The same argument shows $\lim_{z\to-\infty} U(z) = -1$. This completes the proof in this case.

If $c = 0$, we also use a fixed point argument. The explicit expressions (32), (36) simplify. However, step 3 is analogous to step 1 and step 2 is missing. We lose the condition (29) because step 2 is not used. If we consider the limit $c \to 0$ with $c > 0$, the solutions will have a boundary layer near $z = 0$ and approach the solutions with $c = 0$ on closed sets excluding $\{0\}$.

Remark: Since the velocity c was arbitrary, we see that traveling waves are not unique.

9 Inclusion of interfacial free energy

The free energy functional (12) contains energy of interaction between states at different spatial locations as well as bulk energy with density F which does not depend on the state at other points. We now add a third type: energy specifically attached to discontinuous interfaces. The latter will be a function of $u(\xi^+, t)$ and $u(\xi^-, t)$. The easiest case is when it depends only on the jump at the discontinuity, so that the energy will take the form $h([u]_\xi)$. The general case can be handled with more technical difficulty. We have

$$E[u] = \frac{1}{4}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} J(x-y)(u(x)-u(y))^2 dx\, dy + \int_{-\infty}^{\infty} F(u(x))\, dx + h([u]_\xi). \tag{37}$$

Again, the admissibility class $\mathcal{A}$ is that introduced in both of the previous models (see following (4)). We obtain the following analog of (13):

$$\dot{E} = -\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} J(x-y)u(y)dy - u(x) - F'(u)\right)\dot{u}\, dx - \dot{\xi}[F(u)]_{\xi(t)} + h'([u]_{\xi(t)})[\dot{u}]_{\xi(t)}. \tag{38}$$

The natural concept of a gradient flow would now be a pair $(u(x,t), \xi(t))$ with $u \in \mathcal{A}(\xi(t))$ at each time t satisfying (14), (15), and

$$[\dot{u}]_{\xi(t)} = -h'([u]_{\xi(t)}) \tag{39}$$

(again, I am setting all coefficients analogous to C in (1) equal to unity). We shall alter this last equation by applying the constraint that $|u| \le 1$. To explain this, it will be convenient to use the notation $u^\pm(t) = u(\xi(t)^\pm, t)$, $\mu(t) = [u]_{\xi(t)}$.

In all the following, we consider only the case when u^+ is in Phase 2 and u^- is in Phase 1. This implies that $\mu > 0$.

The following constrained problem is applicable when $\dot{\xi}(t) > 0$, which we shall be assuming to be the case for all small enough t.

Suppose the function $u^+(t)$ is given, with $u^+(t) \le 1$ in Phase 2. We stipulate that $u^-(t) \ge -1$ and that when $u^-(t) > -1$, the function $\mu(t)$ satisfy (39), namely

$$\dot{\mu}(t) = -h'(\mu). \tag{40}$$

Finally, if $u^-(t) = -1$ at some value of t and the function would immediately increase above -1 by following the differential equation (40), then it will do so.

In short, the function $\mu(t) = u^+(t) - u^-(t)$ satisfies the following problem with unilateral constraint:

$$\dot{\mu}(t) + h'(\mu) \ge 0, \qquad u^+(t) - \mu(t) + 1 \ge 0, \tag{41}$$

and

$$\left(\dot{\mu}(t) + h'(\mu)\right)\left(u^+(t) - \mu(t) + 1\right) = 0. \tag{42}$$

Given the initial condition $u^-(0) \in [-1, 1]$ and the function $u^+(t) \le 1$ in Phase 2 from $t = 0$ up to $t = t_0$, the problem (41) and (42) determines the function $u^-(t) = u^+(t) - \mu(t)$ uniquely up to that time. We shall denote this functional dependence by

$$u^-(t) = W[u^+, t], \tag{43}$$

where W depends only on the values of u^+ up to time t and not beyond.

This dynamics has a certain unilateral character, because we determine $u^-(t)$ once $u^+(t)$ is given, rather than the other way around. This is natural and appropriate when $\dot{\xi} > 0$ (which will be the case). In fact each iterate used in constructing the exact solution will entail, first, the construction of $u^+(t)$, and then that of $u^-(t)$ by means of (43). On the other hand if $\dot{\xi} < 0$, the opposite order would be appropriate.

We shall see that the inclusion of the last term in (37) and the resulting dynamics (43) brings uniqueness to the initial value and traveling wave problems.

10 Initial value problem with interfacial energy

The equations (14), (15), (43) are now supplemented with initial conditions

$$u(x, 0) = u_0(x), \quad \xi(0) = 0, \tag{44}$$

where we require u_0 to take on values in $[-1, 1]$, and to be continuous except at $x = 0$, where it jumps between phases. In fact, we assume that $u_0(x)$ is in Phase 2 for $x > 0$, Phase 1 for $x < 0$, and

$$[F(u_0)]_0 > 0. \tag{45}$$

Now (43) can be combined with (15) into the single condition

$$\dot{\xi}(t) = F(u^+(t)) - F(W[u^+(\cdot), t]) \equiv R[u^+, t]. \tag{46}$$

where $R[v, t] = F(v(t)) - F(W[v, t])$.

As in Section 3, we shall consider only functions $\xi(t)$ with $\dot{\xi}(t) > 0$ and bounded away from 0, so that there is an inverse function $\tau(x)$: $\xi(\tau(x)) = x$. By (45) and (46), this inequality is satisfied at $t = 0$. We shall restrict the time interval $0 \le t \le T$ to be so small that $\dot{\xi}(t) > 0$ in that interval for all functions ξ in this analysis.

We seek a solution $(u(x, t), \xi(t))$ of (14), (46), (44) in the strip $\Omega = \{0 \le t \le T\}$, and represent it as a fixed point of a certain mapping from a space S of pairs (u, ξ) of functions into itself. The space S will be defined later; for now, we explain how the mapping is constructed. It will be in four steps. First, a technical adjustment: we may have to deal temporarily with the function $F(w)$ for values of the argument w outside of the domain of definition $[-1, 1]$. We simply extend F in a C^2 manner to be quadratic outside that interval. Another needed technicality is the operator $\mathcal{T}$, which truncates to that same interval: $\mathcal{T}u = \min[\max[u, -1], 1]$. The iterates employ the operator $\mathcal{T}$, but the exact solution does not. Let $(\tilde{u}(x, t), \tilde{\xi}(t))$ be a given pair in S.

1. Let $w(x, t)$ satisfy $w = \mathcal{T}w^*$, where

$$w^*_t = -w^* - F'(w^*) + J * \tilde{u}(x, t), \quad w^*(x, 0) = u_0(x), \quad x > 0. \tag{47}$$

   This is an ODE in t for each $x > 0$. By the bistable nature of F', a global solution exists, so that $w(x, t)$ is defined for all points in the half strip $\{x > 0\} \cap \Omega$.

2. Let $\hat{w}(x, t)$ satisfy $\hat{w} = \mathcal{T}\hat{w}^*$, where

$$\hat{w}^*_t = -\hat{w}^* - F'(\hat{w}^*) + J * \tilde{u}(x, t), \quad \begin{cases} \hat{w}^*(x, 0) = u_0(x), \quad x < 0, \\ \hat{w}^*(x, \tilde{\tau}(x)) = W[w(\tilde{\xi}(\cdot), \cdot), \tilde{\tau}(x)], \quad 0 < x < \tilde{\xi}(T), \\ \hat{w}^*(x, T) = W[w(\tilde{\xi}(\cdot), \cdot), T], \quad x \ge \tilde{\xi}(T). \end{cases} \tag{48}$$

Essentially, the initial conditions for $\hat{w}$ are imposed on the Phase-1 side of the interface $\tilde{\xi}$ (except for $x < 0$ or $x > \tilde{\xi}(T)$), and are given there in terms of the values of w on the other side in accordance with (43). By the linear growth of the extended f, the solution $\hat{w}^*$, and hence $\hat{w}$, exist for all points in Ω.

3. Let $\xi(t)$ be defined by the differential equation

$$\dot{\xi}(t) = R[w(\tilde{\xi}(\cdot), \cdot), t] > 0, \quad \xi(0) = 0, \tag{49}$$

and let $\tau(x)$ be its inverse. Here R is given by (46).

Given $\xi(t)$, let $\Omega_+^\xi = \{(x,t) : x > \xi(t), t \in [0,T]\}$, $\Omega_-^\xi = \{(x,t) : x < \xi(t), t \in [0,T]\}$.

4. Finally let

$$u(x,t) = \begin{cases} w(x,t) & \text{in } \Omega_+^\xi, \\ \hat{w}(x,t) & \text{in } \Omega_-^\xi. \end{cases} \tag{50}$$

This defines a map $(u, \xi) = \Phi(\tilde{u}, \tilde{\xi})$. It can be checked that a fixed point is formally a solution of the given initial value problem; however, we must put this construction on a firmer basis. For this we define, for

$$A = 2 \max_{|u| \leq 1} F(u), \tag{51}$$

the function spaces:

$X = \{$functions $v(x)$ on the real line such that v is bounded and uniformly continuous on $(-\infty, -A] \cup [A, \infty)$ and integrable on the interval $(-A, A)\}$, with

$$\|v\|_X = \sup_{|x| \geq A} |v(x)| + \int_{-A}^{A} |v(x)| dx,$$

$Y = C^0(0, T; X)$,
$S = Y \times C^0(0,T)$.

As indicated, we begin with an arbitrary pair $(\tilde{u}, \tilde{\xi}) \in S$, and define functions w, $\hat{w}$, ξ and u.

Lemma 5 *(a)* $J * \tilde{u} \in C^0(\Omega)$,
(b) w *is uniformly continuous on* $\{x > 0\} \cap \Omega$ *and* w_t *is also on the domain where* $|w| < 1$,
(c) $\hat{w}$ *is uniformly continuous and* $\hat{w}_t$ *is also, where* $|w| < 1$,
(d) $\xi \in C^1(0,T)$,
(e) $u \in Y$, *and*
(f) $\|u\|_Y \leq 1 + 2A, \quad |\xi(t)| \leq AT$.

Proof

(a) We write

$$J * \tilde{u} = \int_{-\infty}^{\infty} J(x-y)\tilde{u}(y,t) dy = \int_{|y|>A} \cdots + \int_{|y|<A} \cdots = K_1(x,t) + K_2(x,t).$$

We have the estimates

$$|K_1(x,t)| \leq \sup_{|y|>A} |\tilde{u}(y,t) \leq \|\tilde{u}\|_Y,$$

$$|K_2(x,t)| \leq \max_x J(x) \int_{-A}^{A} |\tilde{u}(x,t)| dx,$$

so that in all, for some constant C

$$\|J * \tilde{u}\|_{C^0(\overline{\Omega})} \leq C\|\tilde{u}\|_Y.$$

To show the uniform continuity of $J * \tilde{u}$, we consider the continuity of each K_i separately in x and t.

$$|K_1(x_1,t) - K_1(x_2,t)| \leq \int_{|y|>A} |J(x_1-y) - J(x_2-y)||\tilde{u}(y,t)|dy,$$

$$|K_2(x_1,t) - K_2(x_2,t)| \leq \sup_{|y|<A} |J(x_1-y) - J(x_2-y)|\|\tilde{u}\|_Y,$$

$$\begin{aligned}|K_1(x,t_1) - K_1(x,t_2)| &\leq \int_{|y|>A} J(x-y)|\tilde{u}(y,t_1) - \tilde{u}(y,t_2)|dy \\ &\leq \sup_{|y|>A} |\tilde{u}(y,t_1) - \tilde{u}(y,t_2)| \\ &\leq \|\tilde{u}(\cdot,t_1) - \tilde{u}(\cdot,t_2)\|_X,\end{aligned}$$

$$\begin{aligned}|K_2(x,t_1) - K_2(x,t_2)| &\leq \max_x J(x) \int_{|y|<A} |\tilde{u}(y,t_1) - \tilde{u}(y,t_2)|dy \\ &\leq C\|\tilde{u}(\cdot,t_1) - \tilde{u}(\cdot,t_2)\|_X.\end{aligned}$$

We only need to remark that all the right sides in these four inequalities approach 0 as $(x_1,t_1) - (x_2,t_2) \to 0$, uniformly in Ω.

(b) and (c) In (47) and (48), the last term on the right of the differential equations has been shown in (a) to be uniformly continuous in (x,t). Moreover the continuity of the function $\tilde{\tau}(x)$ follows from that of $\tilde{\xi}(t)$. Therefore the uniform continuity of w^* and $\hat{w}^*$, hence of w and $\hat{w}$, follow by the continuous dependence of solutions of differential equations on their data. The stated properties of w_t and $\hat{w}_t$ then follow from (47), (48).

(d) Since $W[w^+(\xi(\cdot,\cdot),t]$ is continuous in t, the right side of (49) is continuous in its arguments. The conclusion follows.

(e) Since $u = w$ or $u = \hat{w}$, for each $t_1,\ t_2 \leq T$ we have by (b,c) that $|u(x,t_1) - u(x,t_2)|$ is small of order $|t_1 - t_2|$, except where $\xi(t_1) < x < \xi(t_2)$ or vice versa. In particular, this is true for $|x| > A$. The length of this exceptional interval is bounded by $C|t_1 - t_2|$, where C depends on a bound for $|\dot{\xi}|$. From (46), such a bound for $\dot{\xi}$ is given by $2\max_u F(u) = A$. Therefore $\int_{-A}^{A} |u(x,t_1) - u(x,t_2)|dx \leq C|t_1 - t_2|$. Therefore the restriction of u to the domain $\{|x| < A\}$ is a continuous function from L^1 to $(0,T)$. In all, we have the conclusion.

(f) The inequality for $\|u\|_Y$ follows immediately since $|u| < 1$, and the other from (49), which implies $\dot{\xi} \leq A$.

These results give the basic properties of the mapping Φ, which is seen to map S into itself. We will also need the Lipschitz continuity of Φ. Let $(\tilde{u}_1, \tilde{\xi}_1)$ and $(\tilde{u}_2, \tilde{\xi}_2)$ be two pairs in S, with $w_i,\ \hat{w}_i,\ \xi_i,\ u_i,\ i = 1,2$, the corresponding functions defined in (47)–(50). Let $\eta = \|(\tilde{u_1}, \tilde{\xi_1}) - (\tilde{u_2}, \tilde{\xi_2})\|_S$.

Lemma 6 *(a) For $x > 0$, $|w_1(x,t) - w_2(x,t)| \le CT\eta$.*

(b) For $x < A$, $|\hat{w}_1(x,t) - \hat{w}_2(x,t)| \le CT\eta$.

(c) $|\xi_1(t) - \xi_2(t)| \le CT\eta$.

(d)

$$\|(u,\xi)_1 - (u,\xi)_2\|_S \le CT\eta. \tag{52}$$

Proof

(a), (b) and (c). These follow from the smoothing effect of the convolution; the argument is entirely analogous to the proof of Lemma 5(b,c,d).

(d) First consider points (x,t) where $u_i = w_i$ for $i = 1,2$ or $u_i = \hat{w}_i$ for $i = 1,2$. This includes the regions $x < -A$ and $x > A$. Then parts (a) and (b) tell us $|u_1(x,t) - u_2(x,t)| \le CT\eta$.

The integral $\int_{-A}^{A} |u_1(x,t) - u_2(x,t)| dx$ can be divided into three parts, corresponding to the segment of the interval $(-A, A)$ where $u_i = w_i$, $i = 1,2$, the segment where $u_i = \hat{w}_i$, and the remaining segment where one of the u_i is w_i and the other is $\hat{w}_i$. The length of this latter segment can be estimated by $\sup_t |\xi_1(t) - \xi_2(t)|$, which by part (c) is bounded by $CT\eta$. This latter is then a bound on the contribution to the integral from the third segment. All in all, we have $\int_{-A}^{A} |u_1(x,t) - u_2(x,t)| dx \le CT\eta$.

Putting this together with the estimates from (a), (b), and (c), we obtain the conclusion (52).

With this result, we can now prove the main existence theorem:

Theorem 5 *For small enough T there is a unique classical solution of the initial value problem (14), (15), (39), (44).*

Proof

Iteration may be performed with the map Φ (defined by the four steps), restricted to the ball $B = \{(u,\xi) \in S,\ \|(u,\xi)\|_S \le 1 + 3A\}$. Lemma 5(f) shows that it maps B into itself if $T \le 1$, which we assume. Lemma 6(d) shows that the iterates will converge to a fixed point (u,ξ) of Φ for small enough T. We have merely to show that this fixed point is a classical solution.

Let (u_n, ξ_n) be a sequence of iterates, and let $\{w_n\}$ and $\{\hat{w}_n\}$ be the associated sequences defined by (47) and (48). Lemma 6(a,b) shows that w_n and $\hat{w}_n$ converge uniformly in $\{x > 0\}$ and $\{x < A\}$ respectively to uniformly continuous limits w and $\hat{w}$. And of course $\xi_n \to \xi$ uniformly.

Let $(x_0, t_0) \in \Omega_+^\xi$. We have $u_n(x,t) = w_n(x,t)$ for (x,t) in a neighborhood of (x_0,t_0), for large enough n. Then in such a neighborhood, $u = w$. Therefore u is uniformly continuous in Ω_+^ξ. A similar statement is true in Ω_-^ξ.

By (47) and (48), the time derivatives of w_n^* and $\hat{w}_n^*$, hence u_n, also converge uniformly along a subsequence, so that the limit function u satisfies (14), (44), provided that the defining limits w and $\hat{w}$ have not been subject to the truncation operator $\mathcal{T}$. This will be true if $u(x,t)$ lies in the open interval $(-1,1)$ for every finite (x,t) in Ω with $t > 0$.

We show that now. As a preliminary comment, note that for each t, $u(x,t)$ is not identically 1 or -1 for all x. Therefore $-1 < J * u(x,t) < 1$. First, consider points in Ω_+^ξ. Suppose, for some point (x_0,t_0) in that set, that $u(x_0,t_0) = 1$. Then since $J * u(x_0,t_0) < 1$, the operator on the right of (14) satisfies $-u - F'(u) + J * u < 0$. Therefore immediately $w^*(x_0,t)$, hence $u(x_0,t)$, decreases below the value 1 as t increases beyond t_0. This also shows that in Ω_+^ξ the function u can never approach the value 1 as $t \uparrow t_0$ for some $t_0 > 0$ with $u(x_0,t) < 1$ for $t < t_0$. As a result of this, we conclude that $u(x,t) < 1$ for $(x,t) \in \Omega_+^\xi$ except possibly for $t = 0$. Similarly, $u > -1$ in this set.

Therefore the limit function u satisfies (14) in Ω_+^ξ. A similar argument shows that this equation is also satisfied in Ω_-^ξ.

Finally, the iteration version of (49) implies the convergence of $\dot{\xi}_n$, and the jump condition (46) follows by passing to the limit in (49).

11 Traveling waves again

Traveling waves are solutions which have existed for all time, so that by (40) the discontinuity $[U]_0$ will be fixed at some zero μ_0 of the function $h'(\mu)$. Let us suppose it is unique.

Then the velocity c is determined from $F(U(0^+))$ by (29), namely

$$c = F(U(0^+)) - F(U(0^+) - \mu_0). \tag{53}$$

The existence theory of Section 8 may then be applied if c is in the range permitted there; we obtain uniqueness.

If $\mu_0 = 0$, any discontinuity will have disappeared. The free energy term at the discontinuity will therefore not be present. The theory of such traveling waves is therefore the same as that developed in [1]. In particular, they are unique.

12 Discussion

We have explored simple gradient models of phase-field type for a scalar state function $u(x,t)$ which can also be termed a phase variable. A common point among the examples given here is that the spatial interaction terms are either nonexistent or nonlocal. As a result, the state function can be discontinuous; moreover the value of the state function on either side of a discontinuity is not fixed, but rather is to be determined as part of the solution.

Another common point is that the position of the discontinuity is, along with the state variable, a primary ingredient in the dynamical scenario. The free energy may or may not have a contribution directly associated with the discontinuity. If it does not, the gradient flow is not well posed, the initial value problem suffering from nonuniqueness. This ill-posedness is alleviated if such a contribution exists.

In the former case we have a sort of nucleation phenomenon, in that a new phase may spontaneously arise at any place at any time. A nucleus familiar from other contexts, i.e. small region of disturbance, is not present. Alternatively, one could say that its size has been reduced to zero. This, and also the presence of discontinuous interfaces, are associated with the weak (i.e. nonlocal) nature of the spatial interaction.

Previous studies of the generalization of our convolution model (14) to higher dimensions, such as [8, 7], have pictured phase interfaces as regions in space where the state function u is smooth but has a steep gradient. This phenomenon results from using a parameterized version of J, namely $J_\epsilon(x) = \frac{1}{\epsilon^d} J\left(\frac{x}{\epsilon}\right)$, where d is the dimension. That can be done in the present context as well, and the interface may have a discontinuity as well as a large gradient. However, we have not focussed on the possibility of steep gradients, rather envisaging the discontinuities themselves as being phase interfaces.

In this paper we have restricted attention to one space dimension, which suffices to illustrate the points being made. In [3] the authors showed a phenomenon which may be unexpected at first glance: the fact that stationary solutions of the gradient flow considered there can exist in higher dimensions with the discontinuity set consisting of a quite arbitrary smooth codimension one manifold. One can think of generalizing the gradient flows considered here to problems in higher space dimensions, thus allowing the discontinuities to migrate. The "interface" analogous to ξ would then be a curve, in the 2D case, and in (15), $\dot{\xi}$ would denote the normal velocity. Since such a curve may be irregular, it may be more appropriate to consider in its stead the evolving spatial set when ϕ is in one of the two phases. In any case, the details of such a generalization are not immediately clear.

Finally, we note that the functional (37) has a trivial global minimum $u \equiv u_m$, where u_m is the location of the minimum of F. The focus in this paper has not been on minimizing E, but rather on its gradient dynamics.

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