Clines and Material Interfaces with Nonlocal Interaction

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To Ivar Stakgold on the occasion of his 70th birthday.[1]

Abstract

A natural nonlocal analog of the inhomogeneous nonlinear diffusion equation $u_t = \nabla \cdot A(x)\nabla u - f(u,x)$ is the equation $u_t = \int_\Omega J(x, y - x)[u(y) - u(x)]dy - f(u,x)$, where $J > 0$. Under natural conditions on J and f, we establish here the existence of a spatially nonuniform stationary solution on the real line, satisfying given boundary conditions at $\pm\infty$, and representing a transition between two uniform states. Under additional conditions, it is unique and stable to a large range of perturbations. Because of the inhomogeneity of J and f, the solution may not be translated. Applications arise in the theories of grain boundaries and population clines.

1 Introduction

The results of this paper have bearing on continuum theories of clines in an inhomogeneous biological environment and to Allen-Cahn type theories of interfaces in inhomogeneous materials. In the first case, nonlocal migrational behavior is allowed, and in the latter, nonlocal interaction among states at different spatial locations. Our setting is one-dimensional, but when extended to higher dimensions, the results will also provide an integrodifferential analog of boundary value problems for semilinear elliptic equations (work in progress).

We begin with a description of the Allen-Cahn theory. Their original theory [3, 4, 5] was based on an order parameter $u(x,t)$ describing

[1] in Nonlinear Problems in Applied Mathematics, T. S. Angell, L. Pamela Cook, R. E. Kleinman, and W. E. Olmstead, eds., 134-149, SIAM Publications, 1996.

the relevant properties of a solid material evolving according to gradient dynamics for a free energy functional

$$E[u] = \int_\Omega \left[\frac{1}{2}|\nabla u|^2 + W(u)\right] dx. \tag{1}$$

The second term represents the bulk free energy of the system (in their paper, it was a double well function, but in the present case it will typically have a single well for each fixed x). The first term is a penalty exacted on any spatial nonuniformity, and of course represents a local interaction in this continuum model.

The L_2-gradient dynamics for this functional yields the following evolution equation for u:

$$\tau u_t = \Delta u - f(u) \tag{2}$$

for a positive relaxation constant τ, where $f(u) = W'(u)$.

We now make the interaction (first) part of E (1) nonlocal, replacing it by $\frac{1}{4}\int\int J(x-y)(u(x)-u(y))^2 dxdy$, where J is an even nonnegative L_1 function. Then the gradient evolution (2) is replaced by

$$\tau u_t = J * u - Ku - f(u), \tag{3}$$

where $K = \int_\Omega J(x)dx$ and $*$ denotes convolution.

Nonlocal evolutions akin to this one have been proposed and studied before; see [14, 15, 16, 17, 18, 2, 11, 12, 19]. This specific equation was studied in [2, 9, 6].

If a basic inhomogeneity is imposed on the medium, so that its properties are described not merely by the values of u but also by the spatial position x [6], then in the above, the kernel J is a function $J(x, y-x)$, and $f = f(u,x)$. The evolution problem then is

$$\tau u_t = J_x * u - K(x)u - f(u,x), \tag{4}$$

where we define $K(x) = \int_\Omega J(x, y-x)dy$ and $J_x * u = \int_\Omega J(x, y-x)u(y)dy$.

In all of the following, we assume

A1.

$J(x,s)$ is smooth and decreases rapidly enough as $s \to \infty$,
$J(x,s) \geq 0$,
$J(x,s) = J(x,-s)$,
$K(x) > 0$.

We specialize to the case when Ω is the real line and for some $a > 0$ the functions $J(x,s)$ and $f(u,x)$ are independent of x for $x < -a$ as well as for $x > a$. Thus the medium has a different character on the two sides of the x-interval $|x| < a$. The case $a = 0$, wherein the medium is discontinuous, is allowed, as indicated in the last section. We suppose there is a stable equilibrium of the kinetic equation $\tau u_t = -f(u, x)$ for each fixed x in these two regions, denoted for definiteness by $u = 1 \ \ (x > a)$ and $u = 0 \ \ (x < -a)$. Our purpose is to investigate the possible stationary states $u(x)$ representing a spatial transition from the state $u = 0$ to $u = 1$.

In the context of a simple model of crystalline solids, such a transition may represent an order parameter profile at the boundary between two adjoining materials with different properties but which share an order parameter field. Our prototypical example has $f(u, x) = W_u(u, x)$, where

$$(5) \quad W(u, x) = \frac{1}{2}u^2 - \theta(x)u, \quad \theta(x) = 0 \text{ for } x < -a, \quad \theta(x) = 1 \text{ for } x > a.$$

Thus in the material on the left, W has a unique minimum at $u = 0$, and on the right it is at $u = 1$. However, our main theorem is stated in more general terms.

Inhomogeneities can also be imposed on the original Allen-Cahn model, and stationary profiles sought. This has been done, but in a population dynamical framework [7, 8, 10]. Then the transition solution may represent a cline or a spatial gradient in the population distribution of some species near the junction of two distinct habitats.

The spatial interaction described by the first two terms on the right of (4) would, in the population dynamical context, represent the tendency of the population to uniformize simply by random migration of its individuals. For example, at a local maximum of the population density, the sum of these terms would be negative, tending to drive the density downward at that point. As distinct from the model (2), the migration will generally be nonlocal in the sense that an individual can make "quick trips" over finite distances.

In this note, we establish the existence of spatially nonuniform stationary solutions of (4), typically of the form of monotone solutions which approach 0 as $x \to -\infty$ and 1 as $x \to \infty$. Their uniqueness and asymptotic stability relative to a wide class of perturbations will also be proved.

2 Comparison principles for the evolution problem

The equation (4) enjoys comparison principles very much like those in operation for (2). Some of them have been used in the context of similar equations (see most of the papers cited above following (3)). Their derivations follow along standard lines, but we review them here for reference and completeness.

We denote the right side of (4) by the (nonlinear) operator Mu. For simplicity, we set $\tau = 1$. We take Ω to be the real line R.

Prop. 1 *Let f be continuous in x and continuously differentiable in u, uniformly for $x \in R$, and let $f(0,x) \leq 0$. Let $u(x,t)$, for $0 \leq t \leq T$, be a bounded continuous solution of*

$$u_t \geq Mu, \tag{6}$$

$$u(x,0) \geq 0,$$

continuously differentiable in t. Then $u(x,t) \geq 0$ for all $t \in [0,T]$.

Proof

For some $\alpha,\ \beta,\ \epsilon > 0$ let $v(x,t) = u(x,t)e^{-\alpha t} + \epsilon(\beta t + x^2)$. Assume that v attains a negative value somewhere in the strip $\{(x,t) :\ t \in (0,T]\}$. Then it must attain a minimum at some finite point (x_0, t_0) in the strip, because of the term in x^2. At that point, $J_x * v - Kv > 0$ by A1. We note that

$$J_x * x^2 - Kx^2 = \int_{-\infty}^{\infty} J(x,s)s^2 ds,$$

and we choose β to be larger than this number. The inequality (6) gives a corresponding inequality for v_t. For α large enough, this last inequality implies that $v_t(x_0, t_0) > 0$, which contradicts our assumption that v has a minimum there. Hence $v(x,t) \geq 0$, and since this is true for all positive ϵ, the conclusion follows.

Prop. 2 *Let f and u satisfy the regularity conditions of Prop. 2.1. Let $u(x,t)$ be a bounded continuous solution of (4) in the above strip, with $Mu(x,0) \geq 0$. Then $u_t \geq 0$ in the strip. The same result holds with the inequalities reversed.*

Proof As for example in [1], one lets $v(x,t) = u(x,t) - u(x,0)$ and shows by Prop. 2.1 that it is nonnegative, so $u(x,t) \geq u(x,0)$. Then for any positive δ, one sets $w(x,t) = u(x,t+\delta) - u(x,t)$ and shows it to be nonnegative, since it is so initially. Thus $u(x,t+\delta) - u(x,t) \geq 0$. Dividing by δ and passing to the limit, one obtains the conclusion.

Prop. 3 *Let $U_0(x)$, $U_1(x)$ be bounded continuous functions satisfying $MU_0 \geq 0 \geq MU_1$, $U_0 \leq U_1$. Then there exists a stationary solution $U(x)$ of (4) satisfying $U_0(x) \leq U(x) \leq U_1(x)$ for all x.*

Proof Let $u_0(x,t)$ be the evolving solution of (4) with initial data U_0. By Prop. 2.2, it is monotone in t, and it can be shown with Prop. 2.1 that $u_0(x,t) \le U_1(x)$ always. Therefore $u_0(x,t)$ approaches a limit $U(x)$ pointwise. By the monotone convergence, $J_x * u_0(x,t) \to J_x * U(x)$. On a subsequence t_k depending on x, $u_t(x,t_k) \to 0$. Thus U satisfies (4).

3 Existence, uniqueness, and stability

In the following, we assume that f satisfies the hypothesis (for an example, see (5))

A2. The function $f(u,x)$ is piecewise differentiable in x, differentiable in u uniformly for $x \in R$, and for some $a > 0$ satisfies

$$\begin{array}{rl} f(u,x) < 0 & \text{for } 0 < u < 1, \quad x > a; \\ f(u,x) > 0 & \text{for } 0 < u < 1, \quad x < -a; \\ f(0,x) \le 0 \le f(1,x) & \text{for all } x; \\ f(0,x) = 0 & \text{for } x < -a; \\ f(1,x) = 0 & \text{for } x > a; \\ f(0,x) < 0 & \text{for some } x; \quad f(1,x) > 0 \text{ for some } x. \end{array}$$

For some results, we also require

A3. The function $f(u,x)$ is differentiable in x as well as u. It and the function J satisfy

$$\begin{array}{l} \partial f(u,x)/\partial x \le 0, \\ s\partial J(x,s)/\partial x \ge 0, \\ \partial f(u,x)/\partial x < 0 \text{ for } |x| < a, \ u \in (0,1). \end{array}$$

Theorem 1 *Under assumptions A1 and A2, there exists a nonconstant solution $u(x)$ of*

$$J_x * u - Ku - f(u,x) = 0 \tag{7}$$

with values between 0 and 1. If in addition A3 holds, then the solution is monotone in x and satisfies

$$u(\infty) = 1, \quad u(-\infty) = 0. \tag{8}$$

If $J(x,s)$ is independent of the first variable x, then the solution is unique and asymptotically stable within the class of functions lying between any two of its translates.

Proof According to A2, the functions $U_0 = 0$, $U_1 = 1$ satisfy the hypotheses of Prop. 2.3, so we have the existence of a stationary solution $u(x)$. Moreover, U_0 and U_1 are not exact solutions (by A2), so u lies strictly between them, for at least some values of x. (It can be shown that this is true for all x.) The assumption A2 ensures that there is no constant solution between those two values, so the solutions constructed are not constant. This completes the proof of the existence statement.

Now assume A3. Let $u^*(x,t)$ satisfy (4) with $u^*(x,0)=0$, and let $u(x)=\lim_{t\to\infty}u^*(x,t)$. First, we shall show that $u^*(x,t)$ is monotone increasing in x for all t. Take $\tau=1$ for simplicity. Differentiating (4), we find that the derivative $p(x,t)=u^*_x(x,t)$ satisfies

$$p_t = J_x * p - Kp - f_u(u,x)p + h(x,t), \tag{9}$$

where

$$h(x,t)=\int J_1(x,y-x)[u(y,t)-u(x,t)]dy - f_x(x,u)$$

and $J_1(x,s)=\partial J(x,s)/\partial x$.

We have $p(x,0)=0$ and wish to show that p remains nonnegative. We adapt the proof of Prop. 2.1, setting $v(x,t)=p(x,t)e^{-\alpha t}+\epsilon(\beta t+x^2)$. Assume that v does not remain nonnegative. Then there will be a greatest value $t_0\geq 0$ of t such that $v(x,t)\geq 0$ for $0\leq t\leq t_0$, and a sequence of values $t_k{\downarrow}t_0$ such that $v(x,t_k)<0$ for each k and some x depending on k. For simplicity, we take $t_0=0$, as the proof is similar if it is positive.

Because p is a bounded function of x for each t, we know that $v(x,t_k)>0$ for large $|x|$, so there is a value x_k at which a negative minimum is achieved, for fixed $t=t_k$. By possibly decreasing some or all of the values t_k, we may in fact ensure that

$$v_t(x_k,t_k)\leq 0. \tag{10}$$

We calculate

$$\begin{aligned} v_t &= (J_x * p - Kp - f_u(u,x)p + h(x,t))e^{\alpha t} - \alpha p e^{-\alpha t} + \epsilon\beta \\ &= J_x * v - Kv - (f_u(u,x)+\alpha)v - \\ &\quad -\epsilon\{J_x*(\beta t+x^2) - K(\beta t+x^2) - (\alpha+f_u)(\beta t+x^2)\} + he^{-\alpha t} + \epsilon\beta. \end{aligned}$$

At any of the points (x_k,t_k), we have $v<0$, $J_x*v-Kv>0$. Choose α and β so large that $\alpha+f_u(...)>0$ and $\beta > J_x*x^2-Kx^2\equiv\beta_0$, as in Prop. 2.1. We then have

$$v_t(x_k,t_k) > \epsilon(\beta-\beta_0) + h(x_k,t_k)e^{-\alpha t}. \tag{11}$$

Because of our assumptions A3, we know that $h(x,0)\geq 0$ (in case $t_0>0$, the second inequality in A3 is needed at this point), so that by continuity we can ensure that this function is larger than an arbitrarily small negative number by choosing $t = t_k$ sufficiently small. Therefore ¿From (11), $v_t(x_k, t_k) > 0$, which contradicts (10).

Therefore v remains positive, and since ϵ is arbitrary, p does as well, so that $u^*(x,t)$ is monotone increasing in x (as well as in t). Hence the limit function $u(x)$ is monotone. The limits $u(\pm\infty)$ therefore exist. Letting $|x|\to\infty$ in (7), we see that the limits must be zeros of f, which does not depend on x for large $|x|$. By A2, the only possibilities are (8).

For any $\delta > 0$, let $w(x,t)$ be the solution of (4) with initial data $w(x,0) = u(x-\delta)$. The assumption that $f(u,x)$ is nonincreasing in x implies that $Mw(x,0) \geq 0$, so that by Prop. 2.1, $w(x,t)$ lies, for all t, between $u(x-\delta)$ and $u(x)$. Moreover, it is monotone increasing in t so approaches a monotone stationary solution $u_1(x)$ as $t\to\infty$.

Now assume that $J = J(x-y)$ is independent of the first argument. Then $K(x)$ is a constant, which we take to be 1. Since $\int_{-\infty}^{\infty} u'(x)[J * u - u]dx = 0$ (direct verification), we know that

$$\int_{-\infty}^{\infty} f(u(x),x)u'(x)dx = \int_0^1 f(u,x(u))du = 0, \tag{12}$$

where $x(u)$ is the inverse function to $u = u(x)$. Similarly, the same equation holds with the symbol u in the first integral replaced by u_1 and the symbol $x(u)$ in the second replaced by $x_1(u)$, where x_1 is the inverse function generated by $u_1(x)$. However, by its construction $x_1(u) \geq x(u)$. This fact, together with the third part of A3, ensure that

$$\int_0^1 f(u,x(u))du > \int_0^1 f(u,x_1(u))du$$

unless $x(u) = x_1(u)$. Therefore this last equation holds. This in turn implies that the solutions u and u_1 are the same. A similar argument was used in [7].

By a sweeping argument, this establishes uniqueness of monotone solutions $u(x)$ in the class of solutions that lie between $u(x)$ and $u(x-\delta)$. A simple extension yields the same result in the class of functions between $u(x+\delta)$ and $u(x-\delta)$. It also establishes the asymptotic stability of u relative to the class of perturbations bounded in this way. This completes the proof.

4 Clines and discontinuities

In applications to clines, it is important to include functions f typified by

$$f(u,x) = (1 - 2\theta(x))u(1-u),$$

where the function θ is as in (5), and we require $\theta'(x) > 0$ for $|x| < a$. This function f satisfies all the hypotheses in A2 and A3 except the last one in A2. However, our results still hold; in the proof of the theorem, we simply construct the function $U_0 = U_0(x)$ so that it has nontrivial compact support in $\{x > a\}$, is nonnegative, and is sufficiently flat. The function U_1 is changed in a similar manner.

Throughout the paper, we have assumed that $a > 0$, but in fact the results also hold for $a = 0$; this case represents a discontinuity in the underlying medium, such as happens when two homogeneous materials adjoin at the point $x = 0$. To obtain these stationary solutions, one lets $u_a(x)$ be those constructed above, and takes the limit as $a \to 0$. Since all the u_a are monotone, a limit along a subsequence exists everywhere and produces a solution of (7) with $a = 0$.

We have not mentioned the regularity of the solution $u(x)$ of (7), but it may or may not be continuous, even for $a > 0$. Such phenomena are studied in [2].

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