Metastable Travelling Wave Solutions of Singularly Perturbed Reaction-Diffusion Equations

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Abstract: This paper determines the asymptotic solution of certain initial-boundary value problems for singularly perturbed reaction-diffusion equations, including the Allen-Cahn and Cahn-Hilliard equations, on bounded one-dimensional spatial domains for $t \geq 0$. Attention is focused on the metastable evolution of a transition layer over an asymptotically exponentially-long time interval.

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1. Introduction

Consider the bistable scalar reaction-diffusion equation

$$\epsilon^2 \left(f(u)u_x\right)_x + h(u) = u_t \tag{1}$$

on the strip $-1 \le x \le 1$, $t \ge 0$ where ϵ is a small positive parameter tending to zero, f is smooth and positive, and h is smooth and such that

$$\begin{cases} h(u_\pm) = 0 & \text{for successive roots } u_- < u_+ \text{ satisfying } h'(u_\pm) < 0 \\ \text{while} & \\ h(u_0) = 0 & \text{for a unique } u_0 \text{ in } (u_-, u_+) \text{ where } h'(u_0) > 0. \end{cases} \tag{2}$$

We will consider (1) subject to the constant (nearly-Dirichlet) boundary conditions

$$u(\pm 1, t) \pm \epsilon c_\pm u_x(\pm 1, t) = u_\pm \text{ for } c_\pm \ge 0 \text{ and } t \ge 0 \tag{3}$$

as well as smooth and compatible initial conditions satisfying $u(x_0, 0) = u_0$ at a unique point x_0 in $(-1, 1)$.

The problem (1)–(3) is a generalization of the Allen-Cahn equation (for which $f(u) \equiv 1$ and $h(u) = 2u(1-u^2)$), that represents the simplest class of models for the phase separation of a binary mixture. The factor $f(u)$ represents the mobility associated with the phase separation (see Fife and Lacey (1994) and the references therein). In Fife and Lacey, the diffusion term in (1) was replaced by $\nabla \cdot (f(u)\nabla u)$ and a motion by curvature result for the interfacial dynamics was obtained. Our goal is to study the long-time evolution of the one-dimensional problem (1)–(3) and some related problems, including the Cahn-Hilliard equation.

The outline of the paper is as follows. In §2 we use an iteration scheme to study a solution of a generalized Allen-Cahn problem (1)–(3) with one internal layer. By resolving certain key exponentially small terms, we derive an asymptotic ordinary differential equation for the time-dependent location of the interface. The results generalize those obtained in Neu (1984), Carr and Pego (1989), Fusco and Hale (1989), and Ward (1994). In §3 we provide an alternative method to derive the result by an extension of that used in Reyna and Ward (1994). It involves a preliminary WKB transformation of (1)–(3) to reduce it to a problem for which the conventional method of matched asymptotic expansions can be used to calculate the solution. In terms of the new variables introduced, there is no need to resolve exponentially small terms. In §4 we show numerical results illustrating metastable behavior. In §5, we use an iteration method to construct a one-layer solution to the Cahn-Hilliard equation with Dirichlet boundary conditions. The analytical results for the metastable dynamics compare very favorably over a very long time interval with results obtained from a full finite difference calculation.

2. An Iteration Scheme for the Generalized Allen-Cahn Equation

Our first goal is to study the long-time evolution of the solution to (1)–(3) using an iteration scheme. We first consider the stationary phase-plane problem

$$(f(\varphi)\varphi_\eta)_\eta + h(\varphi) = 0, \quad -\infty < \eta < \infty, \qquad \varphi(\pm\infty) = u_\pm \tag{4}$$

for $\varphi(\eta)$, which results from performing an $O(1/\epsilon)$ stretching of the x variable and then taking the limit as $\epsilon \to 0$. To eliminate translation invariance on the resulting heteroclinic orbit, we will fix

$$\varphi(0) = u_0. \tag{5}$$

A monotonically-increasing solution to (4)–(5) can be found by multiplying the differential equation by the integrating factor $f(\varphi)\varphi_\eta$ to first obtain

$$(f(\varphi)\varphi_\eta)^2 = H(\varphi) \equiv -2\int_{u_-}^{\varphi} h(s)f(s)\,ds,$$

presuming that H satisfies

$$H(\varphi) > 0 \quad \text{for} \quad u_- < \varphi < u_+ \quad \text{with} \quad H(u_+) = 0. \tag{6}$$

Thus, the unique implicit solution to (4)–(5) is

$$\eta = \int_{u_0}^{\varphi} \frac{f(r)}{\sqrt{H(r)}}\,dr. \tag{7}$$

An approximation to $\varphi(\eta)$ can also be obtained numerically by integrating φ_η backward and forward from $\eta = 0$. Because $h(u)$ has simple zeros at $u_\pm$, the asymptotic behavior of $\varphi(\eta)$ as $\eta \to \pm\infty$ can be obtained by expanding the integrand of (7) about $r = u_\pm$ to show that

$$\begin{cases} \varphi(\eta) = u_\pm \mp L_\pm e^{\mp A_\pm \eta} + O(e^{\mp 2A_\pm \eta}) \\ \text{and} \\ \varphi_\eta(\eta) = L_\pm A_\pm e^{\mp A_\pm \eta} + O(e^{\mp 2A_\pm \eta}) \qquad \text{as } \eta \to \pm\infty \end{cases} \tag{8}$$

for $A_\pm \equiv \sqrt{-h'(u_\pm)/f(u_\pm)} > 0$ and for readily-specified positive constants $L_\pm$. Straightforward arguments (cf. Fife and Hsiao (1988)) show that a sharp transition layer joining u_- and u_+ and tending to the profile φ develops quickly near the x_0 where $u(x_0, 0) = u_0$. The generation and sharpening of such an internal layer in the case of the Allen-Cahn equation will be illustrated below. The asymptotic solution in such an initial time interval could, indeed, be generated using matched expansions (cf. Il'in (1992) which considers analogous viscous shock equations).

Now consider the function

$$\varphi(\eta) \quad \text{for} \quad \eta \equiv (x - x_\epsilon(t))/\epsilon \tag{9}$$

with $x_\epsilon(t)$ as a smooth function, satisfying $|x_\epsilon(t)| < 1$, *to be determined.* Note that the profile $\varphi(\eta)$ (i) has the asymptotic limits u_- as $\epsilon \to 0$ for $-1 \le x < x_0(t)$ and u_+ for $x_0(t) < x \le 1$ as well as monotonic shock-layer behavior near $x_0(t)$, (ii) satisfies the partial differential equation (1) with a residual $-\epsilon^{-1}\varphi_\eta dx_\epsilon/dt$ which is small (at least away from the shock since φ_η/ϵ is asymptotically negligible), and (iii) satisfies the boundary conditions (3) with an asymptotically exponentially-small residual $\varphi(\eta_\pm) \pm c_\pm \varphi_\eta(\eta_\pm) - u_\pm$ at the algebraically-large, time-varying endpoints

$$\eta_\pm \equiv (\pm 1 - x_\epsilon(t))/\epsilon.$$

The solution to (1)–(3), asymptotically described by the travelling wave (9), will be determined as

$$u(x,t) = \varphi(\eta) + v(\eta, t), \tag{10}$$

with the shock location $x_\epsilon(t)$ being such that $x_0(0) = x_0$ and with an asymptotically negligible profile velocity dx_ϵ/dt. We shall not require φ and v to be orthogonal (as is frequently done for analogous inertial manifolds). Our Ansatz (10) forces the correction term v to satisfy the nonlinear differential equation

$$\begin{gathered} f(\varphi+v)v_{\eta\eta} + 2f'(\varphi+v)\varphi_\eta v_\eta + f(\varphi+v)\varphi_{\eta\eta} + f'(\varphi+v)\varphi_\eta^2 \\ + h(\varphi+v) + \frac{1}{\epsilon}\frac{dx_\epsilon}{dt}v_\eta - v_t + f'(\varphi+v)v_\eta^2 = -\frac{1}{\epsilon}\varphi_\eta \frac{dx_\epsilon}{dt} \end{gathered} \tag{11}$$

on the large interval $\eta_- \le \eta \le \eta_+$, together with the boundary conditions

$$v(\eta_\pm, t) \pm c_\pm v_\eta(\eta_\pm, t) = u_\pm - \varphi(\eta_\pm) \mp c_\pm \varphi_\eta(\eta_\pm). \tag{12}$$

Since v_t is expected to be small, (11)–(12) may be considered as a two-point boundary value problem for v as a function of η in which t and $x_\epsilon(t)$ simply remain as parameters. If we more precisely define the shock location $x_\epsilon(t)$ by

$$u(x_\epsilon(t), t) = u_0, \tag{13}$$

note that (5) implies that $v(0,t) = 0$ and that $x_\epsilon(0) = x_0$ is actually independent of ϵ.

Linearizing (1) about φ, we can rewrite (11) as

$$\mathcal{L}\, v \equiv (f(\varphi)v)_{\eta\eta} + h'(\varphi)v = -\frac{1}{\epsilon}\varphi_\eta \frac{dx_\epsilon}{dt} + N(\eta,t;v) \tag{14}$$

where $N \equiv v_t - \frac{1}{\epsilon}\frac{dx_\epsilon}{dt}v_\eta + [f(\varphi)-f(\varphi+v)]v_{\eta\eta} + 2[f'(\varphi)-f'(\varphi+v)]\varphi_\eta v_\eta + [f(\varphi)+f'(\varphi)v - f(\varphi+v)]\varphi_{\eta\eta} + [f'(\varphi)+f''(\varphi)v - f'(\varphi+v)]\varphi_\eta^2 + [h(\varphi)+h'(\varphi)v - h(\varphi+v)] - f'(\varphi+v)v_\eta^2$ vanishes quadratically where $v \equiv 0$. Further, since $\mathcal{L}\,\varphi_\eta = 0$, the linear operator $\mathcal{L}$ is readily inverted (up to an arbitrary multiple of φ_η) when $v(0,t) = 0$. Solutions of (11) must thereby satisfy the integral equation

$$v(\eta,t) = p(\eta)\begin{pmatrix}\mu(t,\epsilon)\\ \epsilon^{-1}dx_\epsilon/dt\end{pmatrix} + V(\eta,t;v) \tag{15}$$

for the known row vector

$$p(\eta) \equiv \varphi_\eta(\eta)\int_0^\eta H(\varphi(\alpha))^{-1}(1 \ - I_0^\alpha)\, d\alpha$$

and the nonlinear integral term

$$V(\eta,t;v) \equiv \varphi_\eta(\eta)\int_0^\eta H(\varphi(\alpha))^{-1}\int_0^\alpha \sqrt{H(\varphi(\beta))}\, N(\beta,t;v)\, d\beta\, d\alpha$$

with

$$I_a^b \equiv \int_{\varphi(a)}^{\varphi(b)} \sqrt{H(r)}\, dr. \tag{16}$$

Both the constant of integration $\mu(t,\epsilon)$ and the shock speed dx_ϵ/dt in the Green's function representation (15) are unknown functions of t. Moreover, the boundary conditions (12) require them to satisfy the constraint

$$\begin{pmatrix}\mu(t,\epsilon)\\ \epsilon^{-1}dx_\epsilon/dt\end{pmatrix} = \mathcal{A}^{-1}(x_\epsilon)K(x_\epsilon,v) \tag{17}$$

provided the 2×2 matrix $\mathcal{A} \equiv \begin{pmatrix}a_+\\ a_-\end{pmatrix}$ for $a_\pm \equiv p(\eta_\pm) \pm c_\pm p_\eta(\eta_\pm)$ is invertible. Here $K(x_\epsilon,v) = \begin{pmatrix}K_+\\ K_-\end{pmatrix}$ with $K_\pm(x_\epsilon,v) \equiv u_\pm - (\varphi(\eta_\pm) \pm c_\pm\varphi_\eta(\eta_\pm)) - (V(\eta_\pm,t;v) \pm c_\pm V_\eta(\eta_\pm,t;v))$ is asymptotically negligible when $v \equiv 0$. We must thereby solve the resulting integral equation

$$v(\eta,t) = p(\eta)\mathcal{A}^{-1}(x_\epsilon)K(x_\epsilon,v) + V(\eta,t;v).$$

For the initial iterate, we will set $v^0 = 0$ in K and V to get the improvement

$$v^1(\eta, t) = p(\eta)\mathcal{A}^{-1}(x_\epsilon)K(x_\epsilon, 0). \tag{18}$$

Using (8), we get the crude approximation

$$K_\pm(x_\epsilon, 0) \sim \pm L_\pm(1 - c_\pm A_\pm)e^{\mp A_\pm \eta_\pm}.$$

Likewise, since the principal contributions to the integrals p and p_η come from near the upper endpoint of integration,

$$a_\pm \sim (1 + A_\pm c_\pm)p(\eta_\pm) \sim \pm(1 \;- I_0^{\pm\infty})\frac{(1 + A_\pm c_\pm)e^{\pm A_\pm \eta_\pm}}{2(A_\pm f(u_\pm))^2 L_\pm}$$

and thereby we obtain the limiting linear system

$$\begin{pmatrix} 1 & -I_0^\infty \\ 1 & -I_0^{-\infty} \end{pmatrix} \begin{pmatrix} \mu_0 \\ \frac{1}{\epsilon}\frac{dx_\epsilon^0}{dt} \end{pmatrix} \sim \begin{pmatrix} \frac{2(1-A_+c_+)}{1+A_+c_+}(L_+A_+f(u_+))^2 e^{-2A_+\eta_+} \\ \frac{2(1-A_-c_-)}{1+A_-c_-}(L_-A_-f(u_-))^2 e^{2A_-\eta_-} \end{pmatrix}$$

corresponding to (17). This implies that

$$\begin{aligned} \mu_0 \sim \frac{2}{I_{-\infty}^\infty}\Bigg[& I_{-\infty}^0\left(\frac{1 - A_+c_+}{1 + A_+c_+}\right)(L_+A_+f(u_+))^2 e^{-2A_+\eta_+} \\ &+ I_0^\infty\left(\frac{1 - A_-c_-}{1 + A_-c_-}\right)(L_-A_-f(u_-))^2 e^{2A_-\eta_-}\Bigg] \end{aligned} \tag{19}$$

and

$$\begin{aligned} \frac{dx_\epsilon^0}{dt} \sim \frac{2\epsilon}{I_{-\infty}^\infty}\Bigg[&\left(\frac{1 - A_-c_-}{1 + A_-c_-}\right)(L_-A_-f(u_-))^2 e^{2A_-\eta_-} \\ &- \left(\frac{1 - A_+c_+}{1 + A_+c_+}\right)(L_+A_+f(u_+))^2 e^{-2A_+\eta_+}\Bigg] \end{aligned} \tag{20}$$

and provides the improved asymptotically negligible estimate $v^1(\eta, t) \sim p(\eta)\begin{pmatrix} \mu_0(t, \epsilon) \\ \epsilon^{-1}dx_\epsilon^0/dt \end{pmatrix}$.

As important, however, is that (20) describes the asymptotic evolution of the slowly-moving profile (9) (presuming the crude approximations used so far are adequate). To see this, substitute for $\eta_\pm$ in (20) in terms of the approximation for x_ϵ to provide the limiting differential equation

$$\frac{dx_\epsilon^0}{dt} \sim \epsilon\left(B_- e^{-2A_-/\epsilon}e^{-2A_- x_\epsilon^0/\epsilon} - B_+ e^{-2A_+/\epsilon}e^{2A_+ x_\epsilon^0/\epsilon}\right) \tag{21}$$

where the coefficients $B_\pm$, respectively, have the signs of $1 - c_\pm A_\pm$. When $B_+ B_- > 0$, the approximate differential equation (21) has the unique rest point

$$x_\epsilon^0(\infty) \sim [(A_+ - A_-) + \epsilon \log(B_-/B_+)/2]/(A_+ + A_-) \tag{22}$$

within $(-1, 1)$ so we can conveniently rewrite (21) as

$$\frac{dx_\epsilon^0}{dt} \sim \epsilon k \left[e^{-2A_-(x_\epsilon^0 - x_\epsilon^0(\infty))/\epsilon} - e^{2A_+(x_\epsilon^0 - x_\epsilon^0(\infty))/\epsilon} \right] \tag{23}$$

where $k \equiv B_\pm e^{-2A_\pm(1 \mp x_\epsilon^0(\infty))/\epsilon}$ is asymptotically exponentially small. Further analysis (cf. Laforgue and O'Malley (1995a, 1995b) and O'Malley and Ward (1996)) could be done to relate k to the size of the principal eigenvalue of the linearized steady-state problem. When $k > 0$ (i.e., for nearly Dirichlet boundary conditions satisfying both $c_\pm A_\pm < 1$), it follows that x_ϵ^0 will move monotonically, but very sluggishly, to the stable interior rest point. For $k < 0$, however, the rest point loses stability, so the shock layer is forced to move very slowly toward an endpoint. (This, then, shows a big difference between Dirichlet and Neumann boundary conditions.) When $B_+ B_- < 0$, motion is monotonic toward the endpoint closest to the initial shock. In all cases, the initial value for the differential equation (23) is naturally the location x_0 where $u(x_0, 0) = u_0$. Because one term in the bracket of (23) is asymptotically large and the other asymptotically small (until, e.g., $x_\epsilon^0(t) - x_\epsilon^0(\infty) = O(\epsilon)$), $x_\epsilon^0(t)$ can be readily approximated for all times, thereby providing the limiting solution $\varphi((x - x_\epsilon^0(t))/\epsilon)$ for $t > 0$.

Better approximations result from a more careful analysis. If we denote $\mathcal{A}^{-1}(x_\epsilon)$ by $\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$, (17) implies that

$$\frac{dx_\epsilon}{dt} = W(x_\epsilon; v) \equiv \epsilon b_2(x_\epsilon) K(x_\epsilon, v).$$

Let x_ϵ^0 be the solution of the initial value problem with $v = 0$ implicitly given by $t = \int_{x_0}^{x_\epsilon^0} dz/W(z, 0)$. Then, it follows that x_ϵ satisfies the integral equation

$$x_\epsilon(t) = x_\epsilon^0(t) + \int_0^t \left[W(x_\epsilon(s); v) - W(x_\epsilon^0(s); 0) \right] ds, \tag{24}$$

coupled to

$$v(\eta, t) = p(\eta) \mathcal{A}^{-1}(x_\epsilon) K(x_\epsilon, v) + V(\eta, t; v). \tag{25}$$

The full problem is thus solved by using the natural successive approximations scheme for (24)–(25) and the Ansatz (10).

We note that the approximate solution

$$\varphi((x - x_\epsilon(t))/\epsilon)$$

obtained is not, *strictly*, a travelling wave solution (cf. Fusco et al. (1996) and Volpert et al. (1994)) since $x_\epsilon(t)$ is not linear in t. Instead, this approximation is asymptotically stationary since the profile moves only exponentially slowly in time. The basic approach can, nonetheless, provide an effective basis for a numerical method for this and more general problems, including ones with convection terms, a number of moving shocks, and more space dimensions (cf., e.g., Estep (1994), Garbey (1994), and Ward (1994)).

3. A WKB Method for the Generalized Allen-Cahn Equation

We now present a WKB-type method to rederive the results (21) and (22) concerning the transition layer. The crucial step will be to introduce a change of variables that transforms (1)–(3) into a problem where the conventional method of matched asymptotic expansions can be applied.

We first introduce a new unknown $z(x,t)$ by setting

$$u(x,t) = \varphi\left(z(x,t)/\epsilon\right) , \tag{26}$$

where φ is the stationary monotonic wave profile defined in (4). Then, equation (1) transforms exactly to

$$\epsilon z_{xx} + A(z/\epsilon)(1 - z_x^2) = \frac{z_t}{\epsilon f(\varphi(z/\epsilon))} \tag{27}$$

where the smooth function

$$A(\eta) \equiv \frac{h(\varphi(\eta))}{\sqrt{H(\varphi(\eta))}} = -\frac{d}{d\eta}(\log \sqrt{H(\varphi(\eta))}) \tag{28}$$

satisfies

$$A(\eta) = \pm A_\pm + O(e^{\mp A_\pm \eta}) \text{ as } \eta \to \pm\infty, \tag{29}$$

due to the analogous asymptotic behavior of φ, as well as the sign condition

$$\eta A(\eta) > 0 \text{ for all } \eta \neq 0.$$

The boundary conditions (3) transform to

$$z_x(\pm 1, t) = \pm\frac{u_\pm - \varphi(z(\pm 1,t)/\epsilon)}{c_\pm \varphi_\eta(z(\pm 1,t)/\epsilon)} = \frac{1}{c_\pm A_\pm} + O(e^{\mp A_\pm z(\pm 1,t)/\epsilon}) \tag{30}$$

(anticipating that $\pm z(\pm 1, t)$ will be positive and not $O(\epsilon)$).

Wherever $z(x, t) \gg O(\epsilon)$, the properties of A imply that, to within exponential accuracy, we can replace $A(z/\epsilon)$ in (27) by either A_+ or $-A_-$, depending on the sign of z. We then find that z_x approximately satisfies Burgers equation. This motivates an additional change of variables, of either

$$z_x(x, t) = \coth(w(x, t)/\epsilon) \tag{31}$$

or

$$z_x(x, t) = \tanh(w(x, t)/\epsilon) \tag{32}$$

for a *positive* unknown w. The selection of the hyperbolic cotangent is appropriate in the stable interior layer case when both $c_\pm A_\pm < 1$, because the boundary conditions (30) then imply that $z_x(\pm 1, t) > 1$, while the tanh selection is used in the unstable interior layer case when both $c_\pm A_\pm > 1$. We shall not attempt to use the WKB procedure when $(c_+A_+ - 1)(c_-A_- - 1) < 0$ (when there is no steady state solution with an interior layer) or when the product is zero (and higher order approximations are needed). Substituting the new unknown into (27) and (30) provides a first-order system for z and w, either

$$\begin{cases} z_x = \coth(w/\epsilon) \\ w_x = -A(z/\epsilon) - \frac{z_t \sinh^2(w/\epsilon)}{\epsilon f(\varphi(z/\epsilon))} \end{cases} \tag{33}$$

or

$$\begin{cases} z_x = \tanh(w/\epsilon) \\ w_x = -A(z/\epsilon) + \frac{z_t \cosh^2(w/\epsilon)}{\epsilon f(\varphi(z/\epsilon))}, \end{cases} \tag{34}$$

subject to the boundary conditions

$$w(\pm 1, t) = \frac{\epsilon}{2} \log \left| \frac{1 + z_x(\pm 1, t)}{1 - z_x(\pm 1, t)} \right| \sim \frac{\epsilon}{2} \log \left| \frac{1 + c_\pm A_\pm}{1 - c_\pm A_\pm} \right| \equiv \epsilon w_\pm. \tag{35}$$

This WKB transformation to problem (32) or (33) is an *exact* reformulation of the metastable problem (1)–(3). To study it, we shall use the conventional matching method for singular perturbation problems, without additional exponential asymptotics.

3.1 The Equilibrium Problem

The equilibrium solution of the transformed problem must satisfy

$$w_x = -A(z/\epsilon). \tag{36}$$

We are seeking a solution with one interior layer of the form $\varphi[(x - x_e)/\epsilon]$ for some x_e. Indeed, since (31) and (32) imply that $z_x \sim 1$ unless $w(x) = O(\epsilon)$, we expect z to satisfy

$$z(x) \sim x - x_e \tag{37}$$

away from $O(\epsilon)$ regions near the endpoints ± 1.

Using (29), (36) implies that w will have the piecewise linear outer limit

$$w(x) \sim \begin{cases} A_-(1+x) + \epsilon w_- & \text{for } -1 \le x < x_e \\ A_+(1-x) + \epsilon w_+ & \text{for } x_e < x \le 1 \end{cases} \tag{38}$$

away from an $O(\epsilon)$ neighborhood of x_e where $z = O(\epsilon)$. Continuity of the asymptotic limit for w at x_e then forces the determination

$$x_e \sim (A_+ - A_-)/(A_+ + A_-), \tag{39}$$

in agreement with the limit of (22).

To obtain the $O(\epsilon)$ correction to (39), we insert a corner layer near x_e that smoothes the discontinuity in the outer approximation to w_x. Introducing

$$\eta = (x - x_e)/\epsilon,$$

$z(x) \sim \epsilon\eta$ so (36) becomes

$$w_\eta = -\epsilon A(z/\epsilon) \sim -\epsilon A(\eta). \tag{40}$$

Using (27) and integrating provides

$$w \sim \epsilon \log\left\{\alpha f(\varphi(\eta))\varphi_\eta(\eta)\right\} \tag{41}$$

for a positive constant of integration α. The limits

$$w \sim \epsilon\left[\log\left\{\alpha f(u_\pm)L_\pm A_\pm\right\} \mp A_\pm \eta\right] \tag{42}$$

of this inner solution as $\eta \to \pm\infty$ are matched with the corresponding outer limits

$$w \sim A_\pm(1 \mp x_e) + \epsilon[w_\pm \mp A_\pm \eta] \tag{43}$$

obtained by expanding (38) as a function of η. This determines α and provides

$$x_e \sim \left[(A_+ - A_-) + \epsilon(w_+ - w_- + \log\left(\frac{L_- A_- f(u_-)}{L_+ A_+ f(u_+)}\right))\right] / (A_+ + A_-) \tag{44}$$

as found in (22).

In summary, the WKB transformed problem determines the equilibrium value x_e for a one-layer solution to within $O(\epsilon)$ terms without the need for any exponential asymptotics. The leading term in x_e was obtained from the simple requirement that w be continuous and the $O(\epsilon)$ term was obtained using a conventional corner layer analysis. Equilibrium solutions with multiple interior layers can be calculated in a similar manner. This analysis suggests that the numerical computation of equilibrium solutions for (1) using the transformed problem should be very well-conditioned.

3.2 The Time-Dependent Problem

We now use the WKB formulation to find the solution of (1)–(3) in the form $u(x,t) = \varphi(z(x,t)/\epsilon)$ with $z(x,t) \sim x - x_\epsilon(t)$ away from boundary layers near $x = \pm 1$. Thus, $z(x_\epsilon(t),t) = 0$ defines the internal layer's asymptotic trajectory. Since metastable motion is quasi-stationary, the analysis does not differ greatly from the equilibrium situation.

We first assume that the time interval is such that $x_\epsilon(t)$ is within $O(\epsilon)$ of the equilibrium location x_e (i.e. $x_\epsilon(t) - x_e = O(\epsilon)$). As shown in §2, this should persist for an exponentially long time interval. In this case, the outer approximation

$$w(x,t) \sim \begin{cases} A_-(1+x) + \epsilon w_- & \text{for } -1 \le x < x_\epsilon(t) \\ A_+(1-x) + \epsilon w_+ & \text{for } x_\epsilon(t) < x \le 1 \end{cases} \tag{45}$$

provided that the last term on the right side of (33) or (34) are $o(1)$ in the outer region, which is defined away from an $O(\epsilon)$ neighborhood of $x_\epsilon(t)$. Therefore, we require the consistency condition

$$\epsilon^{-1} \frac{dx_\epsilon}{dt} e^{2w/\epsilon} \ll 1 \tag{46}$$

to hold as $\epsilon \to 0$ in the region $x - x_\epsilon(t) \gg O(\epsilon)$, thereby possibly restricting the time interval.

We now insert a corner layer near $x_\epsilon(t)$ in which the three terms in either (33) or (34) balance. Using the stretched variable $\eta \equiv (x - x_\epsilon(t))/\epsilon$, the equation in the interior region is either

$$w_\eta \sim -\epsilon A(\eta) - \frac{z_t \sinh^2(w/\epsilon)}{f(\varphi(\eta))} \quad \text{if } c_\pm A_\pm < 1,$$

or

$$w_\eta \sim -\epsilon A(\eta) + \frac{z_t \cosh^2(w/\epsilon)}{f(\varphi(\eta))} \quad \text{if } c_\pm A_\pm > 1.$$

Since $w > 0$ and $w = O(1)$ near $x_\epsilon(t)$, we approximate these equations as

$$w_\eta + \epsilon A(\eta) \sim \frac{(-1)^\gamma}{4f(\varphi(\eta))} \frac{dx_\epsilon}{dt} e^{2w/\epsilon} \tag{47}$$

where $\gamma = 0$ when $c_\pm A_\pm < 1$ and $\gamma = 1$ when $c_\pm A_\pm > 1$. Multiplying (47) by $-2\epsilon^{-1}H(\varphi(\eta))e^{-2w/\epsilon}$ allows us to integrate to obtain

$$w \sim \frac{\epsilon}{2}\log\left(\frac{H(\varphi(\eta))}{\alpha(t) - (-1)^\gamma(2\epsilon)^{-1}I_0^\eta \, dx_\epsilon/dt}\right) \tag{48}$$

for a constant of integration $\alpha(t)$. Here I_0^η is as defined in (16). Matching the inner limits

$$w \sim \frac{\epsilon}{2}\left[\log\left(\frac{(f(u_\pm)L_\pm A_\pm)^2}{\alpha(t) - (-1)^\gamma(2\epsilon)^{-1}I_0^{\pm\infty}dx_\epsilon/dt}\right) \mp 2A_\pm\eta\right]$$

as $\eta \to \pm\infty$ with the outer limits $w \sim A_\pm(1 \mp x_\epsilon) + \epsilon[w_\pm \mp A_\pm\eta]$ provides $\alpha(t)$ and the differential equation for $x_\epsilon(t)$:

$$\frac{(-1)^\gamma}{2\epsilon}I_{-\infty}^{\infty}\frac{dx_\epsilon}{dt} \sim \left(f(u_-)L_-A_-e^{-w_- - A_-(1+x_\epsilon)/\epsilon}\right)^2 - \left(f(u_+)L_+A_+e^{-w_+ - A_+(1-x_\epsilon)/\epsilon}\right)^2 . \tag{49}$$

Using (35) for $w_\pm$ and the definition of γ, one readily verifies that this is the same limiting differential equation as obtained in (20) by the method of §2. As a check on the analysis, note that the consistency condition (46) is satisfied.

The analysis needed to determine the differential equation for $x_\epsilon(t)$ is essentially the same when $x_\epsilon(t) - x_e \gg O(\epsilon)$. For instance, suppose that $x_\epsilon(t) > x_e$ where x_e is the equilibrium value. Then, we get the two outer regions where $w_x = \mp A_\pm$ together with a plateau region over an $O(1)$ subinterval around x_e where $w_x = 0$ and the two terms on the right of the w_x equation in either (33) or (34) are of the same asymptotic order. Thus, the limiting outer solution for w has a tent-like profile

$$w(x,t) \sim \begin{cases} A_-(1+x) + \epsilon w_- & \text{for } -1 \le x < x_l(t)\,, \\ A_+\left(1 - x_\epsilon(t)\right) + \epsilon w_+ & \text{for } x_l(t) < x < x_\epsilon(t)\,, \\ A_+(1-x) + \epsilon w_+ & \text{for } x_\epsilon(t) < x \le 1 \end{cases} \tag{50}$$

where continuity of the asymptotic limit determines

$$x_l(t) \sim x_e - \frac{A_+}{A_-}(x_\epsilon(t) - x_e)\,. \tag{51}$$

To derive a differential equation for $x_\epsilon(t)$ we insert a corner layer for w near $x = x_\epsilon(t)$ in which the three terms in (33) or (34) balance. The analysis then parallels the derivation (46)–(48) and leads to the one-sided differential equation

$$\frac{(-1)^\gamma}{2\epsilon}I_{-\infty}^{\infty}\frac{dx_\epsilon}{dt} \sim -\left(f(u_+)L_+A_+e^{-w_+}\right)^2 e^{-2A_+(1-x_\epsilon)/\epsilon} \tag{52}$$

which is asymptotically valid for $x_\epsilon(t) > x_e$. A similar analysis can be done for the case where $x_\epsilon(t) < x_e$, with a w plateau from $x_\epsilon(t)$ to $x_r(t) \sim x_e + \frac{A_-}{A_+}(x_e - x_\epsilon(t))$, and the resulting limiting differential equation

$$\frac{(-1)^\gamma}{2\epsilon} I_{-\infty}^{\infty} \frac{dx_\epsilon}{dt} \sim \left(f(u_-)L_-A_-e^{-w_-}\right)^2 e^{-2A_-(1+x_\epsilon)/\epsilon}. \tag{53}$$

In summary, two key features of the WKB transformed problem (33) or (34) are that the time-scale of the motion multiplies the z_t term and that exponentially small terms do not need to be resolved spatially. This allows an efficient, and relatively routine, discretization of (33)–(35) to numerically compute metastable behavior. Such a discretization was given in Reyna and Ward (1994) for a related viscous shock problem. A limitation of the WKB-type transformation is that it requires the underlying evolution equation in the original u variable to obey a maximum principle. Thus, this transformation is not immediately applicable to the Cahn-Hilliard equation. For that equation, however, an iteration scheme such as that used in §2 can be applied.

4. The Allen-Cahn and Cahn-Hilliard Equations

The special case of the Allen-Cahn (or Nagumo or Ginzburg-Landau) equation

$$\epsilon^2 u_{xx} + 2u(1-u^2) = u_t\,, \tag{54}$$

arises in many important applications (cf. Caginalp (1986), Murray (1989), or Ward (1994)). In particular, it is often used to model the simultaneous presence of solid and liquid regions of a material kept at its melting temperature, with $u = \pm 1$ respectively representing the liquid/solid phase. This model is a gradient-flow for the free-energy

$$\mathcal{E}(u) = \int_{-1}^{1} \left(\epsilon^2 u_x^2 + (1-u^2)^2\right)\, dx \tag{55}$$

where ϵ represents the small interaction length and the symmetric field

$$u(x,\infty) = \tanh(x/\epsilon)$$

features an $O(\epsilon)$ interfacial layer about $x = 0$. Formation of a sharp transition at the point x_0, where $u(x_0, 0) = 0$, with a subsequent ("metastable") drift toward the steady state, is illustrated in Figures 1 and 2. As we have shown, the steady state will be unstable when the usual homogeneous Neumann boundary conditions are used (cf. Carr and Pego (1989) and Fusco and Hale (1989)) and one phase will then ultimately dominate throughout the interior spatial domain. Solutions with a sequence of transition layers are, of course, also of interest (cf. Schatzman (1996)).

Experts suggest that a more satisfactory physical description of a phase transition can be obtained through the fourth-order, mass-conserving Cahn-Hilliard model, represented through the Neumann problem

$$(\epsilon^2 u_{xx} + 2u(1-u^2))_{xx} + u_t = 0, \tag{56}$$

$$u_x(\pm 1, t) = 0, \quad u_{xxx}(\pm 1, t) = 0. \tag{57}$$

Reyna and Ward (1994)'s treatment of the Allen-Cahn equation, constrained so that it conserves mass, represents a significant intermediate step between the Allen-Cahn and Cahn-Hilliard models. In Reyna and Ward (1995b), some aspects of the metastable dynamics were studied for (56)–(57).

In §5 we will study a case which is also intermediate between the two standard models. With the Cahn-Hilliard equation (56), we shall associate the Dirichlet boundary conditions

$$u(\pm 1, t) = \pm 1, \quad u_{xx}(\pm 1, t) = 0. \tag{58}$$

In doing so, we lose the mass-conservation property, but obtain a steady-state corresponding to Allen-Cahn, i.e., the profile

$$\varphi\left(\frac{x - x_e}{\epsilon}\right) = \tanh\left(\frac{x - x_e}{\epsilon}\right)$$

provides a stationary solution for any constant x_e. The slow motion of the metastable profile is shown in Figure 3 for a rather large value of ϵ.

5. A More General Fourth-Order Equation

Let's now consider the boundary-value problem

$$\begin{cases} u_t + (\epsilon^2 u_{xx} + Q(u))_{xx} = 0, & |x| \le 1, \quad t > 0 \\ u(\pm 1, t) = \pm s, & u_{xx}(\pm 1, t) = 0 \end{cases} \tag{59}$$

where $Q(u)$ is a smooth *odd* function satisfying $Q(s) = 0$ and $Q'(s) = -\nu^2$ for unique positive values s and ν. The corresponding stationary heteroclinic orbit $\varphi(\eta)$ is an odd monotonic function defined by

$$\varphi_{\eta\eta} + Q(\varphi) = 0, \quad \varphi(0) = 0, \quad \varphi(\infty) = s \tag{60}$$

on $-\infty < \eta < \infty$. Solving for φ_η provides the implicit solution

$$\eta = \int_0^\varphi (2 \int_r^s Q(p)\, dp)^{-1/2} dr$$

which decays exponentially to satisfy

$$\varphi(\eta) = s - ae^{-\nu\eta} + O(e^{-2\nu\eta}) \quad \text{as } \eta \to \infty \tag{61}$$

for a positive constant a determined by Q. In particular, for the Cahn-Hilliard equation, $Q(u) = 2(u - u^3)$, $\varphi(\eta) = \tanh \eta$, $s = 1$, and $\nu = a = 2$. For simplicity, we shall impose the initial condition

$$u(x, 0) = \varphi((x - x_\epsilon(0))/\epsilon) \tag{62}$$

for some interior zero $x_\epsilon(0)$, noting that this function satisfies the given differential equation exactly and satisfies the endconditions at $x = \pm 1$ up to the asymptotically negligible errors $\pm s - \varphi((\pm 1 - x_\epsilon(0))/\epsilon)$ and $-\varphi_{\eta\eta}((\pm 1 - x_\epsilon(0))/\epsilon)$. For other initial values, we'd anticipate having an initial time interval in which the asymptotic solution tends to the profile φ. For simplicity, we will consider only single-layer situations.

Now, let's seek an asymptotic solution of the initial-boundary value problem (59)–(62) using the Ansatz

$$u(x, t) = \varphi(\eta) + v(\eta, t) \tag{63}$$

for the stretched transition layer variable

$$\eta = (x - x_\epsilon(t))/\epsilon \tag{64}$$

on the algebraically-large interval $\eta_- \leq \eta \leq \eta_+$ for $\eta_\pm \equiv (\pm 1 - x_\epsilon)/\epsilon$ where

$$u(x_\epsilon(t), t) = 0 \tag{65}$$

defines the shock location $\eta = 0$ for the profile $\varphi(\eta)$ at any $t \geq 0$.. Expecting v to be asymptotically negligible, the limiting solution will then satisfy $u(x, t) = \varphi\left((x - x_\epsilon(t))/\epsilon\right) + O(\epsilon^N)$ throughout the domain (for every $N > 0$), so we will have

$$u(x, t) \sim \begin{cases} -s, & x < x_\epsilon(t) \\ s, & x > x_\epsilon(t). \end{cases}$$

It's clearly most important to determine how the location $x_\epsilon(t)$ varies with t.

Let's now artificially introduce

$$K(x, t) \equiv \epsilon^2 u_{xx}(x, t) + Q(u(x, t)), \tag{66}$$

so (59) becomes equivalent to

$$K_{xx} = -u_t = \frac{1}{\epsilon} \frac{dx_\epsilon}{dt}(\varphi_\eta + v_\eta) - v_t$$

and $K(\pm 1, t) = 0$. Integrating twice with respect to x from -1 implies that $K_x = k + \frac{dx_\epsilon}{dt}(\varphi + v) - \int_{-1}^{x} v_t((y - x_\epsilon)/\epsilon, t)\, dy$ for some integration constant $k(t, \epsilon)$ and $K(x, t) = k(1+x) + \frac{dx_\epsilon}{dt} \int_{-1}^{x} [\varphi((y - x_\epsilon)/\epsilon) + v((y - x_\epsilon)/\epsilon, t)]\, dy - \int_{-1}^{x} (x - y) v_t((y - x_\epsilon)/\epsilon, t)\, dy$. Since $K(1, t) = 0$,

$$K(x,t) = \frac{dx_\epsilon}{dt} A_{x_\epsilon}(x) + B_{x_\epsilon}(x, t; v)$$

where

$$A_{x_\epsilon}(x) \equiv \frac{1}{2}\left[(1-x)\int_{-1}^{x} \varphi((y - x_\epsilon)/\epsilon)\, dy - (1+x)\int_{x}^{1} \varphi((y - x_\epsilon)/\epsilon)\, dy\right]$$

and

$$B_{x_\epsilon}(x, t; v) \equiv \frac{1}{2}\left[(1-x)\int_{-1}^{x}\left[\frac{dx_\epsilon}{dt} v((y - x_\epsilon)/\epsilon, t) + (1+y) v_t((y - x_\epsilon)/\epsilon, t)\right] dy \right.$$

$$\left. - (1+x)\int_{x}^{1}\left[\frac{dx_\epsilon}{dt} v((y - x_\epsilon)/\epsilon, t) - (1-y) v_t((y - x_\epsilon)/\epsilon, t)\right] dy\right].$$

Note that B_{x_ϵ} vanishes when $v \equiv 0$.

The representation (63) implies that (66) can be rewritten as $K(x,t) = -Q(\varphi) + v_{\eta\eta} + Q(\varphi + v)$, so linearizing u about $\varphi(\eta)$ implies that v will satisfy

$$\mathcal{L}v \equiv v_{\eta\eta} + Q'(\varphi) v = \frac{dx_\epsilon}{dt} A_{x_\epsilon}(x) + C_{x_\epsilon}(\eta, t; v) \tag{67}$$

as a function of η, parameterized by t, where

$$C_{x_\epsilon}(\eta, t; v) \equiv B_{x_\epsilon}(x, t; v) + Q(\varphi) + Q'(\varphi) v - Q(\varphi + v),$$

which accounts for the nonlinearities of Q and the dependence on v_t, vanishes when $v \equiv 0$. Since the positive even function φ_η satisfies $\mathcal{L}\varphi_\eta = 0$ while $v(0, t) = 0$, variation of parameters implies that

$$v(\eta, t) = D_1(\eta)\lambda + D_2(\eta, x_\epsilon)\frac{dx_\epsilon}{dt} + E_{x_\epsilon}(\eta, t; v) \tag{68}$$

where $\lambda(t, \epsilon)$ is a constant of integration,

$$D_1(\eta) \equiv G(\eta, 0)/\varphi_\eta(0)$$

is an odd solution of $\mathcal{L}D_1 = 0$, and

$$D_2(\eta, x_\epsilon) \equiv \int_0^{\eta} G(\eta, q) A_{x_\epsilon}(x_\epsilon + \epsilon q)\, dq, \quad \text{and} \quad E_{x_\epsilon}(\eta, t; v) \equiv \int_0^{\eta} G(\eta, q) C_{x_\epsilon}(q, t; v)\, dq$$

for the Green's function

$$G(\eta, q) \equiv \varphi_\eta(\eta)\varphi_\eta(q) \int_q^\eta \varphi_\eta^{-2}(r)\, dr.$$

The prescribed boundary values for u at $x = \pm 1$ determine asymptotically negligible boundary values $v(\eta_\pm, t)$. *Presuming* the matrix

$$D(x_\epsilon) \equiv \begin{pmatrix} D_1(\eta_-) & D_2(\eta_-, x_\epsilon) \\ D_1(\eta_+) & D_2(\eta_+, x_\epsilon) \end{pmatrix} \tag{69}$$

remains *nonsingular*, we can uniquely determine the unknowns λ and dx_ϵ/dt as

$$\begin{pmatrix} \lambda \\ \frac{dx_\epsilon}{dt} \end{pmatrix} = D^{-1}(x_\epsilon) \begin{pmatrix} v(\eta_-, t) - E_{x_\epsilon}(\eta_-, t; v) \\ v(\eta_+, t) - E_{x_\epsilon}(\eta_+, t; v) \end{pmatrix}, \tag{70}$$

so $v(\eta, t)$ must exactly satisfy the nonlinear integral equation

$$v(\eta, t) = F(\eta, t; x_\epsilon, v) \equiv (D_1(\eta) \quad D_2(\eta, x_\epsilon))D^{-1}(x_\epsilon) \begin{pmatrix} -s - \varphi(\eta_-) - E_{x_\epsilon}(\eta_-, t; v) \\ s - \varphi(\eta_+) - E_{x_\epsilon}(\eta_+, t; v) \end{pmatrix}. \tag{71}$$

In terms of v, (70) implies that x_ϵ will exactly satisfy

$$\frac{dx_\epsilon}{dt} = W(x_\epsilon, t; v) \equiv (\det D(x_\epsilon))^{-1} \,(D_1(\eta_+) \quad D_1(\eta_-)) \begin{pmatrix} s + \varphi(\eta_-) + E_{x_\epsilon}(\eta_-, t; v) \\ s - \varphi(\eta_+) - E_{x_\epsilon}(\eta_+, t; v) \end{pmatrix}. \tag{72}$$

Thus,

$$x_\epsilon(t) = x_\epsilon(0) + \int_0^t W(x_\epsilon(\tau), \tau; v)\, d\tau. \tag{73}$$

Let $x_\epsilon^0(t)$ be defined implicitly from the initial value problem for $\frac{dx_\epsilon}{dt} = Z(x_\epsilon) \equiv W(x_\epsilon, t; 0)$ as

$$t = \int_{x_\epsilon(0)}^{x_\epsilon^0} dz/Z(z).$$

Then, we can find the desired solution (63) by using the coupled iteration scheme

$$\begin{cases} v^{j+1}(\eta, t) = F(\eta, t; x_\epsilon^j, v^j) \\ x_\epsilon^{j+1}(t) = x_\epsilon(0) + \int_0^t W(x_\epsilon^j(\tau), \tau; v^{j+1})\, d\tau \end{cases} \tag{74}$$

for $j = 0, 1, 2, \ldots$, beginning with $v^0(\eta, t) \equiv 0$ and x_ϵ^0.

If we simply omit the asymptotically negligible E_{x_ϵ} terms in (72), we can obtain $x_\epsilon(t)$ approximately as a solution of

$$\frac{dx_\epsilon}{dt} \sim \det(D(x_\epsilon))^{-1} H(x_\epsilon)$$

where

$$H(x_\epsilon) \equiv D_1((-1-x_\epsilon)/\epsilon)(s-\varphi((1-x_\epsilon)/\epsilon)) + D_1((1-x_\epsilon)/\epsilon)(s+\varphi((-1-x_\epsilon)/\epsilon).$$

Thus, any rest point $x_\epsilon(\infty)$ must satisfy $H(x_\epsilon(\infty)) = 0$. Since $H(0) = 0$ while $H'(x) < 0$ everywhere, the unique rest point occurs at the origin, as symmetry would suggest. Moreover, its stability will be determined by the sign of $\det(D(0))$. To show the sluggishness of the transition layer motion, we might directly estimate dx_ϵ/dt.

Instead, let us be more traditional and return to the nonhomogeneous boundary value problem for v and consider the inner product

$$(\mathcal{L}v, z) = \int_{\eta_-}^{\eta_+} \mathcal{L}v(p)\, z(p)\, dp$$

where $z(\eta)$ is a nullvector of $\mathcal{L}$ satisfying $\mathcal{L}z = 0$ and $z(\eta_\pm) = 0$. Since $\int_{\eta_-}^{\eta_+} v_{\eta\eta}(p)\, z(p)\, dp = -vz_\eta|_{\eta_-}^{\eta_+} + \int_{\eta_-}^{\eta_+} v(p)\, z_{\eta\eta}(p)\, dp$, $\mathcal{L}z = 0$ provides the *solvability condition*

$$\int_{\eta_-}^{\eta_+} \mathcal{L}v(p)\, z(p)\, dp = -vz_\eta|_{\eta_-}^{\eta_+}. \tag{75}$$

Taking φ_η as the outer limit for z, adding endpoint layers at $x = \pm 1$ defines

$$\begin{aligned} z(\eta) &\sim \varphi_\eta(\eta) - \varphi_\eta(\eta_-)e^{-\nu(1+x)/\epsilon} - \varphi_\eta(\eta_+)e^{-\nu(1-x)/\epsilon} \\ &\sim \varphi_\eta((x-x_\epsilon)/\epsilon) - 2a\nu e^{-2\nu/\epsilon}\cosh((x+x_\epsilon)\nu/\epsilon). \end{aligned}$$

Then, the boundary term $-vz_\eta|_{\eta_-}^{\eta_+}$ in (75) has the asymptotically-negligible limit $4a^2\nu^2 e^{-2\nu/\epsilon}\sinh(2\nu x_\epsilon/\epsilon)$ provided $|x_\epsilon| < 1$. Presuming the first term on the right side of (67) dominates, we will also get

$$\int_{\eta_-}^{\eta_+} \mathcal{L}v(p)\, z(p)\, dp \sim \frac{1}{\epsilon}\frac{dx_\epsilon}{dt}\int_{-1}^{1} A_{x_\epsilon}(y)\, \varphi_\eta((y-x_\epsilon)/\epsilon)\, dy$$

since the boundary layer contributions are exponentially-smaller than that of the outer solution for z. Integrating by parts, then, we get the limiting solvability condition

$$\frac{dx_\epsilon}{dt}\left[\frac{1}{2}\left(\int_{-1}^{1}\varphi((y-x_\epsilon)/\epsilon)\, dy\right)^2 - \int_{-1}^{1}\varphi^2((y-x_\epsilon)/\epsilon)\, dy\right] \sim 4a^2\nu^2 e^{-2\nu/\epsilon}\sinh(2\nu x_\epsilon/\epsilon).$$

Further, $\int_{-1}^{1}\varphi((y-x_\epsilon)/\epsilon)\, dy \sim -2sx_\epsilon$ and $\int_{-1}^{1}\varphi^2((y-x_\epsilon)/\epsilon)\, dy \sim 2(s^2 - \epsilon c)$ for $c \equiv \int_0^\infty (s^2 - \varphi^2(z))\, dz$. Thus, we finally obtain

$$\frac{dx_\epsilon}{dt} \sim \frac{-2a^2\nu^2 e^{-2\nu/\epsilon}}{s^2(1-x_\epsilon^2) - \epsilon c}\sinh(2\nu x_\epsilon/\epsilon) \tag{76}$$

as an approximate equation of motion. For the Cahn-Hilliard equation, we get

$$\frac{dx_\epsilon}{dt} = O(e^{-4(1-|x_\epsilon|)/\epsilon}).$$

Using the prescribed initial value $x_\epsilon(0)$, we separate variables in (76) to get the approximation

$$2a^2\nu^2 e^{-2\nu/\epsilon} t \sim \int_{x_\epsilon}^{x_\epsilon(0)} \left[\frac{s^2(1-r^2)-\epsilon c}{\sinh(2\nu r/\epsilon)}\right] dr \tag{77}$$

for the transition layer location $x_\epsilon(t)$ for all $t \geq 0$. More careful estimates could also be used to obtain higher-order approximations. It's clear, however, that it will take an asymptotically exponentially long time to reach the stable steady state. Numerical results for $x_\epsilon(t)$ for the rather large value of ϵ used in Figure 3, are shown in Figure 4.

To validate the result in (76) *over a very long time interval*, we now use a high order finite-difference scheme to discretize the Cahn-Hilliard type equation (59). This numerical method is based on a central finite difference scheme for the spatial discretization coupled with a third order backward differentiation scheme for the time discretization. The spatial discretization uses a centered fourth-order scheme for the highest derivative term and a sixth-order scheme for the lower order terms. More precisely, we introduce the following undivided difference operators acting on a vector $\mathbf{u} = (\ldots, u_{i-1}, u_i, u_{i+1}, \ldots)$:

$$(D_+\mathbf{u})_i = u_{i+1} - u_i \quad , \quad (D_-\mathbf{u})_i = u_i - u_{i-1} \quad \text{and} \quad (D_0\mathbf{u})_i = u_{i+1} - u_{i-1}.$$

Thus, the fourth order derivative is approximated using a fourth order centered discretization

$$\frac{\partial^4 u}{\partial x^4} = \frac{1}{h^4}(D_+D_-)^2\left(1 - \frac{1}{6}D_+D_-\right)\mathbf{u} + O(h^4)$$

while the second order term is discretized using a higher order scheme that doesn't widen the stencil of the complete discretization:

$$\frac{\partial^2 Q(u)}{\partial x^2} = \frac{1}{h^2}D_+D_-\left(1 - \frac{1}{12}D_+D_- + \frac{1}{90}(D_+D_-)^2\right)Q(\mathbf{u}) + O(h^6)$$

where $Q(\mathbf{u}) = (\ldots, Q(u_{i-1}), Q(u_i), Q(u_{i+1}), \ldots)$. Note that for smooth solutions, the formal truncation error of these discretizations is $O\left(\epsilon^2 h^4 + h^6\right)$.

For the time integration, we use an adaptive strategy based on the third order backward differentiation method. This discretization allows large time integration steps while still keeping numerical stability. The adaptive strategy, which is necessary to deal with the sudden changes in the time scales that can occur, monitors the second derivative with respect to time by considering

$$C_n = \max_i\left(\frac{u_i^{n+1} - u_i^n}{t_{n+1} - t_n} - \frac{u_i^n - u_i^{n-1}}{t_n - t_{n-1}}\right)$$

with $u_i^n \approx u(x_i, t_n)$, keeping its value in the range $0.003 \leq C_n \leq 0.010$. This guarantees a time interpolant with derivative no larger than a constant times the value of the numerical derivative. In the implementation, we eliminate already computed time steps when the adaptive strategy results in a new time step smaller than half of the previous stepsize.

At each time step, we solve a system of nonlinear equations using Newton's method. The Jacobian for the Newton's iteration is evaluated analytically and inverted numerically using Linpack subroutines for banded matrices. In order to insure numerical accuracy and to overcome the exponential ill-conditioning of the Jacobian, all computations are performed using 30 digit representation (IEEE quadruple precision). We take $n = 1000$ meshpoints.

Let's compare the asymptotic and numerical results for $x_\epsilon(t)$ for the Cahn-Hilliard equation when $Q(u) = 2u(1-u^2)$. For this special case $a = \nu = 2$, $s = c = 1$, so the asymptotic differential equation (76) for $x_\epsilon(t)$ reduces to

$$\frac{dx_\epsilon}{dt} \sim -\frac{16e^{-4/\epsilon}}{1 - x_\epsilon^2 - \epsilon}\left(e^{4x_\epsilon/\epsilon} - e^{-4x_\epsilon/\epsilon}\right).$$

We choose $\epsilon = 0.18$, $x_\epsilon(0) = -0.6$, and initial data $u(x, 0) = \tanh\left((x - x_\epsilon(0))/\epsilon\right)$. The numerical results for the zero $x_\epsilon(t)$ of u are compared in Table 1 with corresponding asymptotic results. They agree very closely over many decades in t. In Figure 5 we superpose the asymptotic and numerical results for the interior layer location $x_\epsilon(t)$ and they show very clear agreement over very long time intervals.

t	x_ϵ (asy.)	x_ϵ (num.)
167.509	-0.47591	-0.47504
18063.56	-0.27935	-0.27934
79255.68	-0.21513	-0.21502
244947.95	-0.16574	-0.16554
684199.81	-0.12056	-0.12043
969493.28	-0.10522	-0.10510
1419857.25	-0.08848	-0.08833
4776290.80	-0.03735	-0.03733
7836411.16	-0.01984	-0.01981
9638932.30	-0.01388	-0.01385

Table 1: $x_\epsilon(t)$ for the Cahn-Hilliard equation with $Q(u) = 2(u - u^3)$, $\epsilon = 0.18$, and $x_\epsilon(0) = -0.6$.

Conclusions

The asymptotic solution of these reaction-diffusion equations on bounded intervals has been obtained through an improvement of methods previously applied to a variety of singularly perturbed evolution equations (cf., e.g., Laforgue and O'Malley (1994, 1995a, 1995b, and 1996), Reyna and Ward (1995a), Nefedov (1996), and O'Malley and Ward (1996)). The long-term metastable evolution requires careful consideration of asymptotically exponentially small errors.

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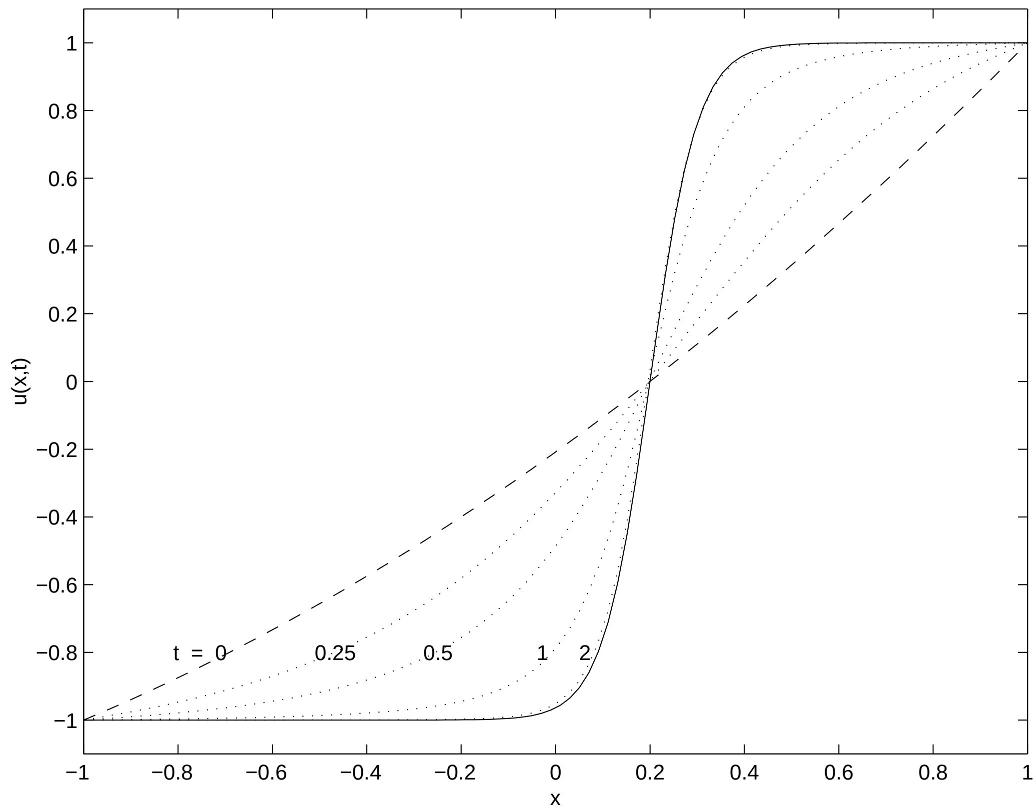

Figure 1: INITIAL FORMATION OF A TRANSITION LAYER. The numerical solution $u(x,t)$ of Allen-Cahn equation (54) with $\epsilon = 0.1$ and Dirichlet boundary conditions, starting with $u(x,0) = (x-0.2)(x+5)/4.8$, is plotted at selected times from $t=0$ to $t=2$. For comparison, the function $\tanh((x-0.2)/\epsilon)$ is also plotted (solid line).

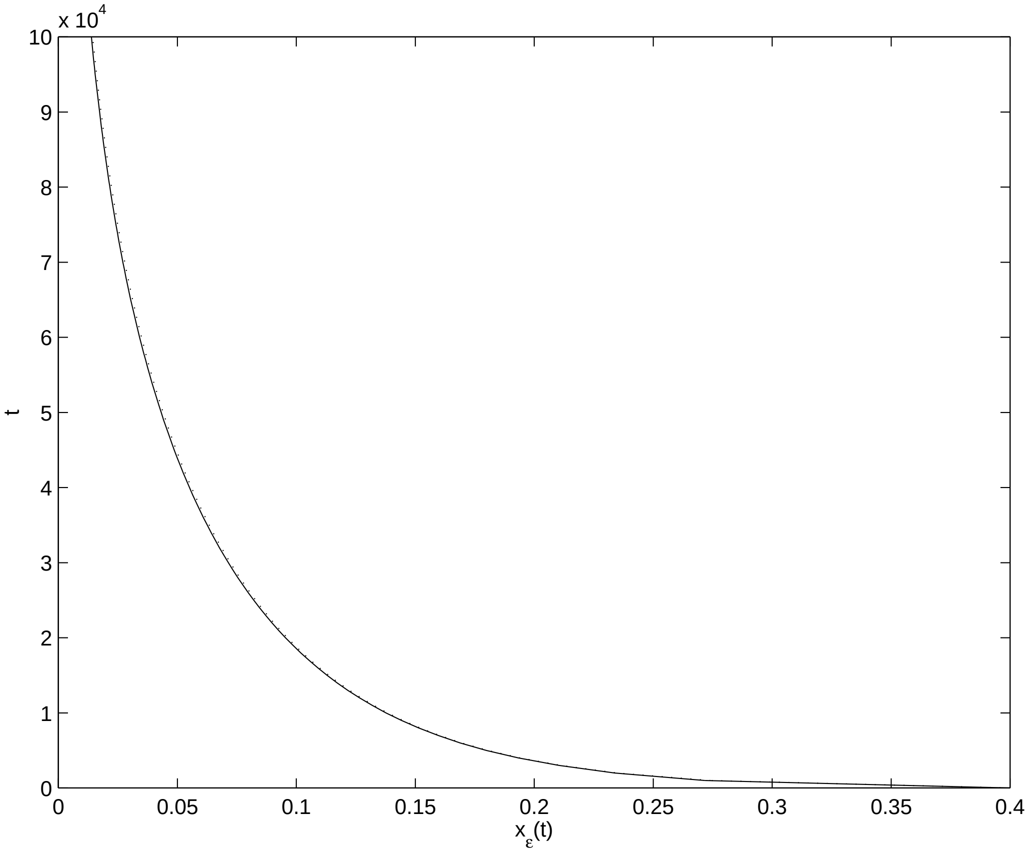

Figure 2: SLOW MOTION OF THE TRANSITION LAYER. Comparison of the interfacial motion obtained from the numerical solution of (54) with $\epsilon = 0.25$, Dirichlet boundary conditions, and initial condition $u(x, 0) = (x - 0.4)(2x + 5)/4.2$, with the analytical solution of (23) such that $x_\epsilon^0(0) = 0.4$.

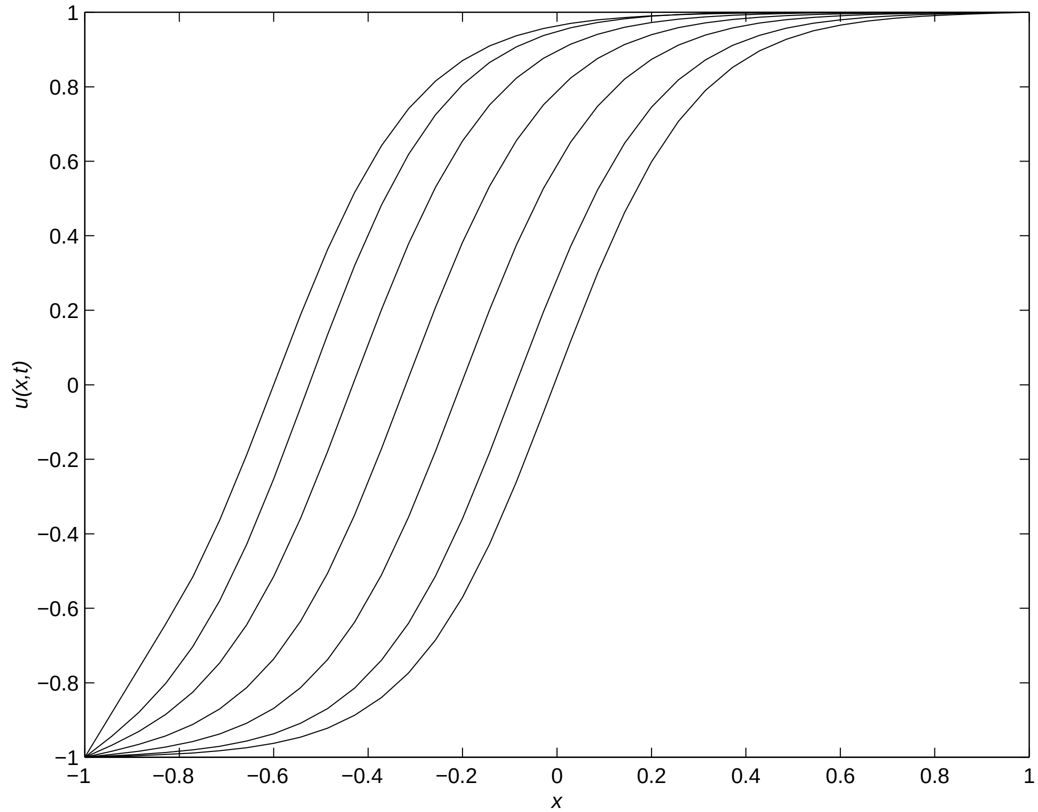

Figure 3: METASTABLE EVOLUTION. Numerical solution of the Cahn-Hilliard equation (56) under Dirichlet boundary conditions (58), with $\epsilon = 0.3$ and $x_\epsilon(0) = -0.6$, at the exponentially increasing times $t = 0$, 1, 5, 25, 125, 625, and 3125 (left to right). The stable steady-state has $x_\epsilon(\infty) = 0$.

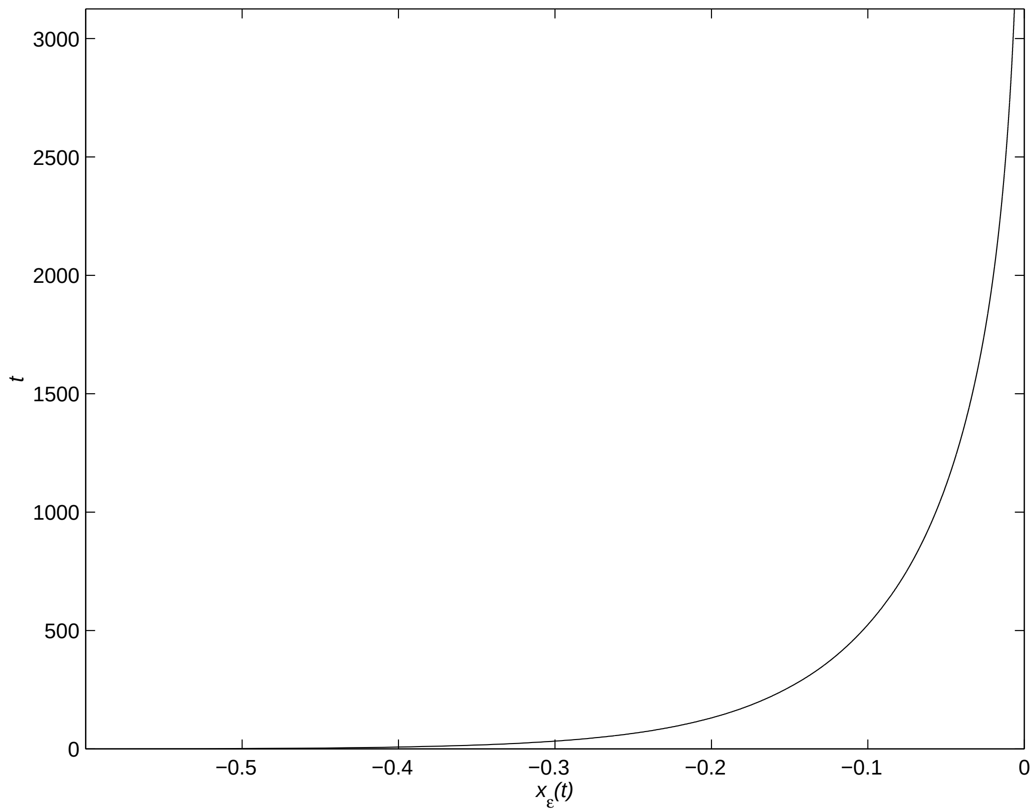

Figure 4: Layer motion obtained from the numerical solution described by Figure 3 for the Cahn-Hilliard equation with $\epsilon = 0.3$ and $x_\epsilon(0) = -0.6$ up to $t = 3125$.

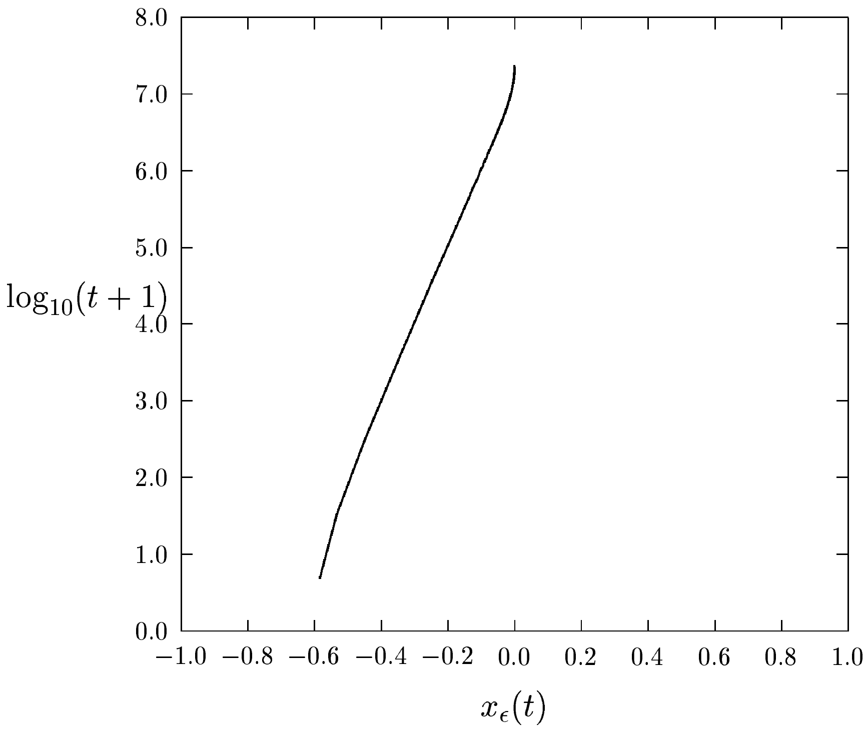

Figure 5: A comparison of the asymptotic and numerical results for $\log_{10}(1+t)$ versus $x_\epsilon(t)$ for the Cahn-Hilliard equation are made. Here $Q(u) = 2(u - u^3)$, $\epsilon = 0.18$ and $x_\epsilon(0) = -0.6$. The solid curve is the asymptotic results and the dashed curve is the full numerical results. The two curves are indistinguishable on this graph.