

Spectral Analysis for Periodic Solutions of the Cahn–Hilliard Equation on \mathbb{R}

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Abstract

We consider the spectrum associated with the linear operator obtained when the Cahn–Hilliard equation on \mathbb{R} is linearized about a stationary periodic solution. Our analysis is particularly motivated by the study of spinodal decomposition, a phenomenon in which the rapid cooling (quenching) of a homogeneously mixed binary alloy causes separation to occur, resolving the mixture into regions of different crystalline structure, separated by steep transition layers. In this context, a natural problem regards the evolution of solutions initialized by small, random (in some sense) perturbations of the pre-quenching homogeneous state. Solutions initialized in this way appear to evolve transiently toward certain unstable periodic solutions, with the rate of evolution described by the spectrum associated with these periodic solutions. In the current paper, we use Evans function methods and a perturbation argument to locate the spectrum associated with such periodic solutions. We also briefly discuss a heuristic method due to J. S. Langer for relating our spectral information to coarsening rates.

1 Introduction

We consider the Cahn–Hilliard equation on \mathbb{R} ,

$$u_t = (-u_{xx} + F'(u))_{xx}, \tag{1.1}$$

where throughout the analysis we will make the following standard assumptions on F :

(H) $F \in C^4(\mathbb{R})$ has a double-well form: there exist real numbers $\alpha_1 < \alpha_2 < \alpha_3 < \alpha_4 < \alpha_5$ so that F is strictly decreasing on $(-\infty, \alpha_1)$ and (α_3, α_5) and strictly increasing on (α_1, α_3) and $(\alpha_5, +\infty)$, and additionally F is concave up on $(-\infty, \alpha_2) \cup (\alpha_4, +\infty)$ and concave down on (α_2, α_4) . The interval (α_2, α_4) is typically referred to as the *spinodal region*.

We observe at the outset that for each F satisfying assumptions (H), there exists a unique pair of values u_1 and u_2 (the *binodal* values) so that

$$F'(u_1) = \frac{F(u_2) - F(u_1)}{u_2 - u_1} = F'(u_2) \quad (1.2)$$

and such that the line passing through $(u_1, F(u_1))$ and $(u_2, F(u_2))$ lies entirely on or below F . Also, we note that for any linear function $G(u) = Au + B$ we can replace $F(u)$ in (1.1) with $H(u) = F(u) - G(u)$ without changing our equation in any way. If we choose

$$G(u) = \frac{F(u_2) - F(u_1)}{u_2 - u_1}(u - u_h) + F(u_h),$$

where u_h (the natural homogeneous configuration) is the unique value for which both $F''(u_h) < 0$ and

$$F(u_h) = \frac{F(u_2) - F(u_1)}{u_2 - u_1},$$

then $H(u)$ has a local maximum $H(u_h) = 0$ and equivalent local minima at the binodal values $H(u_1) = H(u_2)$. Finally, upon replacing u with $u + u_h$ we can shift H so that the local maximum is located at $u = 0$. Following [10], we will refer to a double-well function $F(u)$ for which the local maximum is $F(0) = 0$ and the local minima (though not necessarily the local minimizers) are equivalent as *standard form*. In addition we will assume in the current analysis that once F has been put into standard form it is an even function. Our primary example will be

$$F(u) = \frac{1}{4}\alpha u^4 - \frac{1}{2}\beta u^2, \quad (1.3)$$

which clearly satisfy our general assumptions for all $\alpha, \beta > 0$.

For equation (1.1) under assumptions (H), there exist precisely three types of bounded non-constant stationary solutions $\bar{u}(x)$: periodic solutions, pulse-type *reversal* solutions for which $\bar{u}(\pm\infty) = u_{\pm}$, $u_- = u_+$, and monotonic transition waves (the *kink* solutions) for which $\bar{u}(\pm\infty) = u_{\pm}$, $u_- \neq u_+$; in particular, the asymptotic endstates of the kink solutions are the binodal values (see [10] Theorems 1.1, 1.3, and 1.4). As discussed in [8, 10] these solutions can be categorized according to stability as follows: the transition waves are all both spectrally and nonlinearly stable, while the reversal solutions are linearly unstable with a positive real eigenvalue (nonlinear instability has not, to my knowledge, been analyzed). Periodic solutions appear, at least in some cases, to be linearly stable with respect to perturbations that have the same period as the wave, but it is shown in [10] that a broad class of such solutions are linearly unstable to general perturbations. The goal of the current paper is to employ Evans function methods and a perturbation argument to more accurately locate the spectrum associated with such periodic solutions. We note that our analysis has direct application to the calculation of coarsening rates for evolution in the spinodal decomposition process, and we briefly discuss such an applications in Section 4.

Our analysis is particularly motivated by the study of spinodal decomposition, a phenomenon in which the rapid cooling of a homogeneously mixed binary alloy causes separation to occur, resolving the mixture into regions of different crystalline structure, separated by steep transition layers, in which one component concentration rises above its high-temperature concentration, while the other component concentration falls below its high-temperature concentration. More precisely, this phase separation is typically considered to take place in two stages: First, a relatively fast process occurs during which the homogeneous mixture quickly begins to separate (this is the stage typically referred to as spinodal decomposition), followed by a second *coarsening* process (sometimes referred to as *ripening*) during which the regions continue to broaden on a relatively slower timescale, and the maximum difference in the concentrations of the two components continues to increase.

In this context u typically denotes the concentration of one component of the binary alloy (or a convenient affine transformation of this concentration), and the Cahn–Hilliard equation arises from the phenomenologically derived conservation law

$$u_t + \nabla \cdot \left\{ -M(u) \nabla \frac{\delta E}{\delta u} \right\} = 0, \quad (1.4)$$

where $M(u)$ (taken constant in our analysis) denotes the molecular mobility associated with concentration u (somewhat analogous to thermal conductivity), and E denotes the total free energy functional associated with concentration u . The Cahn–Hilliard equation as considered here arises from these considerations and a form of $E(u)$ proposed in 1958 by Cahn and Hilliard, who were considering particularly the interfacial energy between components of a binary compound [2]. Taking $F(u)$ to denote the bulk free energy density associated with a homogeneously arranged alloy with concentration u , Cahn and Hilliard posed the energy functional

$$E(u) = \int_{\Omega} F(u) + \frac{\epsilon}{2} |\nabla u|^2 dx, \quad (1.5)$$

where in the setting of [2] Ω denotes a bounded open subset of \mathbb{R}^3 , and the term $\frac{\epsilon}{2} |\nabla u|^2$ is an interfacial energy correction that arises (as Cahn and Hilliard view it) through Taylor expansion of a general bulk free energy $\mathcal{F} = \mathcal{F}(u, \nabla u, \text{Hess}(u), \dots)$ and the assumption of isotropy. (In fact, the functional $E(u)$ was proposed earlier by van der Waals in [17] as an appropriate energy for a two-phase system, but the work of Cahn and Hilliard seems to be independent of this.) While ϵ is taken as constant in the current analysis, it may not be constant in general.

Combining (1.4) with (1.5), we obtain the general Cahn–Hilliard equation

$$u_t = \nabla \cdot \left\{ M(u) \nabla \left(-\epsilon(u) \Delta u - \frac{\epsilon'(u)}{2} |\nabla u|^2 + F'(u) \right) \right\}, \quad (1.6)$$

where in this calculation we have allowed ϵ to depend on u to clarify the form in which it generally would appear in the Cahn–Hilliard equation. (This equation first appeared in

Cahn’s paper [1].) In order to obtain the form (1.1), we have taken both M and ϵ to be constant, and additionally have scaled both time t and F . If we set

$$\tilde{u}(t, x) = u\left(\frac{t}{\epsilon M}, x\right), \quad (1.7)$$

and

$$\tilde{F}(u) = \frac{1}{\epsilon} F(u), \quad (1.8)$$

we find that \tilde{u} solves an equation of form (1.1) (in space dimension one) with F replaced by \tilde{F} .

In the case of relatively high temperatures, F generally has a quadratic form, expressing the expectation that free energy is minimized by configurations that maximize entropy, and such configurations correspond with values of u for which the components of the alloy are homogeneously mixed. On the other hand, as temperature drops, free energy (Helmholtz free energy $\mathcal{F} = U - ST$, where U denotes internal energy, S denotes entropy, and T denotes temperature) increases at a rate proportional to entropy, and F can take on the double-well form of assumption (H). In this way, the original high-temperature configuration, identified by a constant concentration $u = u_h$, can become unstable at the lower temperature, and consequently small perturbations from u_h do not dissipate, but rather grow at a locally exponential rate. The natural object of study in this context is as follows: Describe the time evolution of solutions of (1.1) initialized by a small perturbation from the constant state $u = u_h$. The important role of stationary solutions in this evolution was suggested by Langer in [11], where he sets out three hypotheses that we quote here: “1. A decomposing alloy, at least during the late stages of coarsening, spends most of its time in configurations which are nearly stationary solutions of the generalized diffusion equation [i.e., our (1.1)]. 2. The rate of decay of one of these almost stationary configurations is determined primarily by thermal fluctuations. Random inhomogeneities in the initial configuration may have some early effect on the location of the emerging zones; but these inhomogeneities should not have much to do with the late rate of coarsening. These hypotheses suggest that: 3. The rate of coarsening may be determined by using fluctuation theory to compute the rate of decay of exactly stationary configurations.”

Regarding the early stages of spinodal decomposition, which Langer did not address, we note that C. Grant has shown that in the case $d = 1$ and on a finite domain, a broad class of initial perturbations from the constant state u_h indeed evolve toward an unstable periodic stationary solution, whose period is selected by u_h . The period is given below as X_s and referred to as the *spinodal period*. See [3, 4].

In preparation for our discussion of the role of leading eigenvalues in determining coarsening rates, we review some elementary observations regarding the existence and structure of stationary periodic solutions to (1.1). According to Theorem 1.5 of [10] we have that if F is an *even* double-well function in standard form and u_2 is the upper binodal value for F , then for every amplitude $u_* \in (0, u_2)$ there exists precisely one (up to translation) periodic stationary solution with minimum $-u_*$ and maximum u_* . More precisely, this solution,

denoted here $\bar{u}(x; u_*)$, satisfies

$$-\bar{u}_{xx} + F'(\bar{u}) = 0 \Rightarrow \bar{u}_x^2 = 2(F(\bar{u}) - F(u_*)).$$

If we select the shift so that $\bar{u}(0; u_*) = 0$, we find the integral relation

$$\int_0^{\bar{u}(x; u_*)} \frac{dy}{\sqrt{2(F(y) - F(u_*))}} = x, \quad (1.9)$$

from which we see immediately (by symmetry) that $\bar{u}(x; u_*)$ has period

$$X(u_*) = 4 \int_0^{u_*} \frac{dy}{\sqrt{2(F(y) - F(u_*))}}, \quad (1.10)$$

with also (by direct calculation)

$$X'(u_*) = \frac{2\sqrt{2}}{\sqrt{-F(u_*)}} - \sqrt{2} \int_0^{u_*} \frac{F'(y) - F'(u_*)}{(F(y) - F(u_*))^{3/2}} dy. \quad (1.11)$$

In the event that $F'''(y) \geq 0$ for $y \in [0, u_*]$, and $F'''(y)$ is not identically 0, we have the expected coarsening $X'(u_*) > 0$; that is, the period increases with increasing amplitude. We record here that it is easily shown that the period does not approach 0 as $u_* \rightarrow 0$, but rather approaches a minimum value

$$X_{\min} = \frac{2\pi}{\sqrt{-F''(0)}} \quad (1.12)$$

(see the proof of Part (ii) of Lemma 3.2 for details).

In the case that F is given by (1.3), equation (1.9) specifies \bar{u} in terms of a Jacobi elliptic function,

$$\bar{u}(x; u_*) = u_* \operatorname{sn}\left(\frac{\sqrt{-2F(u_*)}}{u_*} x; k\right), \quad (1.13)$$

where $\operatorname{sn}(y; k)$ denotes the Jacobi elliptic function, defined so that

$$\operatorname{sn}(y; k) = \sin \phi; \quad \text{where} \quad y = \int_0^\phi \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}},$$

where in our case

$$k^2 = -\frac{\beta u_*^4}{4F(u_*)}. \quad (1.14)$$

The period in this case is

$$X(u_*) = \frac{4u_*}{\sqrt{-2F(u_*)}} K(k), \quad (1.15)$$

where K denotes the complete elliptic integral

$$K(k) = \int_0^1 \frac{ds}{\sqrt{(1-s^2)(1-k^2s^2)}}.$$

In practice (i.e., for the explicit calculations discussed in this paper), we take values for these functions from the MATLAB built-in functions *ellipj.m* and *ellipke.m*.

If we linearize (1.1) about $\bar{u}(x)$ (setting $u = \bar{u} + v$), we obtain the linear perturbation equation

$$v_t = (-v_{xx} + F''(\bar{u})v)_{xx}, \quad (1.16)$$

with associated eigenvalue problem

$$L\phi := (-\phi_{xx} + F''(\bar{u})\phi)_{xx} = \lambda\phi. \quad (1.17)$$

In this framework the onset of spinodal decomposition is often analyzed as follows. The high-temperature homogeneous configuration has been standardized to $u_h = 0$, and upon linearization about this constant solution we obtain from (1.17) the eigenvalue problem

$$-\phi^{(4)} + F''(0)\phi'' = \lambda\phi. \quad (1.18)$$

In this constant coefficient case, the spectrum consists entirely of $L^\infty(\mathbb{R})$ -eigenvalues, and the eigenfunctions have the form $\phi(x) = e^{i\xi x}$. Upon substitution of ϕ into (1.18) we obtain the dispersion relation

$$\lambda(\xi) = -\xi^4 - F''(0)\xi^2, \quad (1.19)$$

which is maximized by $\xi_s = \pm\sqrt{-F''(0)/2}$, with corresponding leading eigenvalue $\lambda_s = F''(0)^2/4$. The period selected by ξ_s is

$$X_s = 2\pi\sqrt{-\frac{2}{F''(0)}}, \quad (1.20)$$

(the *spinodal period*), which suggests (as discussed above) that when (1.1) is solved with $u(0, x)$ taken as a small, random, perturbation from $u_h = 0$ the solution will move relatively quickly (relative to the rate of later dynamics) toward the periodic stationary solution $\bar{u}_s(x)$ with period X_s . Indeed, this agrees both with numerical investigations (see, for example, [12]), and with the analytic work of Grant, discussed above [3, 4].

If we consider the spinodal decomposition process in Langer's framework, we note that at each time t we expect u to be near a periodic stationary solution $\bar{u}^t(x)$. In this way, we expect the rate of evolution to depend on the leading eigenvalue associated with the stationary periodic solution $\bar{u}^t(x)$, and it is precisely these leading eigenvalues that we analyze in the current analysis. We see, however, that if we want to take advantage of this spectral information, we need to understand the manner in which u is perturbed away from \bar{u}^t at time t , and in principle this perturbation should arise from physical rather than mathematical

considerations. Langer’s analysis [11] addresses precisely this issue: he derives the Cahn–Hilliard equation from a more primitive statistical model, and this allows him to reference back to his statistical model and capture information about the physical perturbations we expect. We note here particularly that in this way Langer is bringing in something additional to the Cahn–Hilliard equation, and so the predicted evolution is no longer strictly governed by the equation itself, but rather by more fundamental considerations. On the other hand the phenomenological physical constants that appear in Langer’s statistical model are inherited (in Langer’s derivation) by the Cahn–Hilliard equation, and so we expect the evolution described by Langer’s statistical model to accurately correspond with the evolution governed by the Cahn–Hilliard equation.

Langer’s development is discussed in more detail in Section 4, but we can finish the current physical discussion by referring to the main observation that arises from his work and from the application on \mathbb{R} in Section 4. If we assume that the time evolution proceeds as Langer suggests, then at each time t we can associate the solution of (1.1) with a particular stationary periodic solution $\bar{u}^t(x)$, and so the coarseness can be measured as the period $X(t)$ of this wave. In this framework, we argue heuristically in Section 4 that $X(t)$ evolves, at least during the later stages of coarsening, according to the ODE

$$\frac{dX}{dt} = \lambda_{\max}(X)X, \quad X(0) = X_0, \quad (1.21)$$

where the values $\lambda_{\max}(X)$ are precisely the leading eigenvalues that we are concerned with in the current paper; precisely, $\lambda_{\max}(X)$ denotes the leading eigenvalue associated with the stationary solution given by (1.9) with period X . This model is derived under the assumption of late-stage coarsening (i.e., for solutions already assumed close to the asymptotic kink solution), and so it is natural to take a relatively large period for X_0 . In Section 4 we solve (1.21) for a choice of F and show that the resulting coarsening rate is logarithmic as expected.

Following the development of [10] (and more broadly the references [5, 6, 7, 13, 14, 15, 16]), we proceed by searching for eigenfunctions with the particular form $\phi(x) = e^{i\xi x}p(x)$, where $\xi \in \mathbb{R}$ and $p(x)$ has period X . Upon substitution of this ansatz into (1.17) we arrive at an eigenvalue problem for p on a bounded domain $x \in [0, X]$,

$$L_\xi p = \lambda p; \quad p^{(k)}(0) = p^{(k)}(X), \quad k = 0, 1, 2, 3, \quad (1.22)$$

where

$$L_\xi := e^{-i\xi x} L e^{i\xi x}.$$

We now construct solutions of (1.22) in terms of a basis for solutions of (1.17) $\{\phi_j\}_{j=1}^4$, initialized by $\phi_j^{k-1}(0; \lambda) = \delta_j^k$ for $k = 1, 3, 4$, with $(b\phi_j)'(0; \lambda) = \delta_j^2$, where $b(x) = F''(\bar{u}(x))$ and δ_j^k denotes a Kronecker delta. In particular, we create a basis of solutions for (1.22) $\{p_j\}_{j=1}^4$ through the relations $p_j(x; \lambda) = e^{-i\xi x} \phi_j(x; \lambda)$. Looking for solutions of (1.22)

$$p(x) = \sum_{j=1}^4 V_j(\lambda) p_j(x; \lambda),$$

we conclude that there exists a solution to (1.22) if and only if there exists $\xi \in \mathbb{R}$ so that $e^{i\xi X}$ is an eigenvalue of the matrix eigenvalue problem

$$M(\lambda; X)V = e^{i\xi X}V; \quad V = (V_1, V_2, V_3, V_4)^{\text{tr}} \quad (1.23)$$

where $M(\lambda; X)$ is the monodromy or Floquet matrix

$$M(\lambda; X) = \begin{pmatrix} \phi_1(X; \lambda) & \phi_2(X; \lambda) & \phi_3(X; \lambda) & \phi_4(X; \lambda) \\ (b\phi_1)'(X; \lambda) & (b\phi_2)'(X; \lambda) & (b\phi_3)'(X; \lambda) & (b\phi_4)'(X; \lambda) \\ \phi_1''(X; \lambda) & \phi_2''(X; \lambda) & \phi_3''(X; \lambda) & \phi_4''(X; \lambda) \\ \phi_1'''(X; \lambda) & \phi_2'''(X; \lambda) & \phi_3'''(X; \lambda) & \phi_4'''(X; \lambda) \end{pmatrix}. \quad (1.24)$$

(The form of terms in the second row is taken for computational convenience.) Accordingly, we define the Evans function for periodic waves as

$$D(\lambda, \xi) := \det(M(\lambda, X) - e^{i\xi X}I). \quad (1.25)$$

It is clear from the discussion leading up to (1.25) that for periodic waves, L has an eigenvalue λ whenever there exists $\xi \in \mathbb{R}$ so that $D(\lambda, \xi) = 0$.

In order to state our main result, we make the following definitions. First, let F be an even double-well function in standard form, and let $\bar{u}(x)$ denote the periodic solution specified by (1.9). Observing that \bar{u}_x solves the ODE

$$-\phi'' + b(x)\phi = 0, \quad (1.26)$$

where $b(x) := F''(\bar{u}(x))$, we use reduction of order to specify a second, linearly independent solution

$$\psi(x) = \begin{cases} \bar{u}'(x) \int_0^x \frac{dy}{\bar{u}'(y)^2} & 0 \leq x \leq \frac{X}{4} \\ \bar{u}'(x) \int_{X/2}^x \frac{dy}{\bar{u}'(y)^2} + \frac{X'(u_*)}{2F'(u_*)} \bar{u}'(x) & \frac{X}{4} \leq x \leq \frac{3X}{4} \\ -\bar{u}'(x) \int_x^X \frac{dy}{\bar{u}'(y)^2} + \frac{X'(u_*)}{F'(u_*)} \bar{u}'(x) & \frac{3X}{4} \leq x \leq X \end{cases}. \quad (1.27)$$

We now define

$$\begin{aligned} \Psi(x) &:= \int_0^x \psi(y) dy \\ \Phi_3(x) &:= \int_0^x \phi_3(y; 0) dy \\ U(x) &:= \int_0^x \bar{u}(y) dy, \end{aligned}$$

and for notational brevity we will take the convention that for any function $f(x)$

$$\mathcal{I}[f] := \int_0^X f(x) dx. \quad (1.28)$$

We are now in a position to state the main result of the analysis.

Theorem 1.1. *Suppose F is an even double-well function in standard form, and let $\bar{u}(x)$ denote a periodic solution of (1.1) with minimum $-u_*$ and maximum $+u_*$, where $u_* \in (0, u_2)$, and u_2 is the upper binodal value described following (H). Then there exists a value $r > 0$ such that for $|\xi| < r$ the curve*

$$\lambda(\xi) = a_2\xi^2 + a_4\xi^4 + \mathbf{O}(|\xi|^6), \quad (1.29)$$

lies entirely in the spectrum of L , $\sigma(L)$, where L is as in (1.17). The coefficients a_2 and a_4 are defined as follows: if $X = X(u_)$ denotes the period of $\bar{u}(x)$ then*

$$\begin{aligned} a_2 &= \frac{X}{\Phi_3(X)}, \\ a_4 &= -a_2^2 \frac{A}{B}, \end{aligned} \quad (1.30)$$

where

$$\begin{aligned} A &= -X\mathcal{I}[\Psi]^2\mathcal{I}[\bar{u}^2] - 2X^2\mathcal{I}[\Psi]\mathcal{I}[\bar{u}\Phi_3] + \frac{X'(u_*)X^2}{F'(u_*)\Phi_3(X)}\mathcal{I}[\bar{u}\Phi_3]^2 \\ &\quad + \frac{B}{X} \left\{ -2\mathcal{I}[x\Phi_3] + 2\mathcal{I}[U\Psi] + X\mathcal{I}[\Phi_3] + \frac{X\mathcal{I}[\Phi_3^2] - \mathcal{I}[\Phi_3]^2}{\Phi_3(X)} + \frac{X^2\Phi_3(X)}{12} \right\} \\ B &= -X^3\Phi_3(X) - \frac{X'(u_*)}{F'(u_*)}X^2\mathcal{I}[\bar{u}^2]. \end{aligned}$$

Moreover, we have

$$\lim_{u_* \rightarrow 0} a_2(X(u_*)) = -F''(0),$$

and we can express $\Phi_3(X)$ either as

$$\Phi_3(X) = 4 \int_0^{\frac{X}{4}} \frac{u_*^2 - \bar{u}(x)^2}{\bar{u}'(x)^2} dx - \frac{X'(u_*)}{F'(u_*)}u_*^2,$$

or equivalently

$$\Phi_3(X) = \sqrt{2} \int_0^{u_*} \frac{u_*^2 - x^2}{(F(x) - F(u_*))^{3/2}} dx - \frac{X'(u_*)}{F'(u_*)}u_*^2.$$

We now conclude the introduction with a heuristic discussion of the application of Theorem 1.1. If we regard the higher order terms as negligible, then we find that the leading eigenvalue along this curve is approximately

$$\lambda_{\max}(X) = -\frac{a_2^2}{4a_4} = \frac{B}{4A}. \quad (1.31)$$

It is, of course, to be stressed that λ_{\max} may easily fall outside the range in which Theorem 1.1 guarantees our expansion (1.29). On the other hand, we recall that in the case $\bar{u}(x) =$

$u_h = 0$, which can be regarded as the periodic solution with minimum period (and hence with maximum leading eigenvalue), we have

$$\lambda(\xi) = -F''(0)\xi^2 - \xi^4,$$

and so our observation that $a_2 \rightarrow -F''(0)$ as $u_* \rightarrow 0$ suggests that our perturbation approximation for λ_{\max} may give reasonable values for large leading eigenvalues as well. Indeed, we find in practice (see, e.g., Figure 1) that (1.31) gives a reasonable approximation of the leading eigenvalue for all amplitudes u_* .

As an example case, we consider (1.1) with

$$F(u) = 250u^4 - 500u^2 \tag{1.32}$$

(the large coefficients arise naturally when an equation of the form

$$u_t = (-\epsilon^2 u_{xx} + F'(u))_{xx},$$

for ϵ small, is rescaled into form (1.1)). In Figure 1 we plot the leading eigenvalues associated with F for all amplitudes $u_* \in [0, 1]$, computed in two different ways: (1) by perturbation using (1.31); and (2) by computation. In both cases the calculations are carried out using MATLAB. For the perturbation analysis, we use the MATLAB built-in functions *ellipj.m* and *ellipke.m* for the Jacobi elliptic integrals, and we carry out the integrations with *quad.m* and a small choice of tolerance. For the computationally obtained eigenvalues, we evolve the $\{\phi_j\}_{j=1}^4$ up to X and numerically evaluate the zeros of the monodromy matrix. We note that this latter procedure is not accurate in the case of arbitrarily small eigenvalues, because errors incurred in the evolution of the $\{\phi_j\}_{j=1}^4$ can become larger than the eigenvalues. The perturbation approach becomes better in this regime, and so we can regard it as most useful for small eigenvalues. On the other hand, the perturbation approach is much faster in all regimes.

2 Analysis of the Evans Function

In this section we analyze the Evans function described in (1.25); precisely, we consider

$$D(\lambda, \xi) = \det \begin{pmatrix} [\phi_1] - [e^{i\xi x}] & [\phi_2] & [\phi_3] & [\phi_4] \\ [(b\phi_1)'] & [(b\phi_2)'] - [e^{i\xi x}] & [(b\phi_3)'] & [(b\phi_4)'] \\ [\phi_1''] & [\phi_2''] & [\phi_3''] - [e^{i\xi x}] & [\phi_4''] \\ [\phi_1'''] & [\phi_2'''] & [\phi_3'''] & [\phi_4'''] - [e^{i\xi x}] \end{pmatrix},$$

where $[\phi_k] := \phi_k(X; \lambda) - \phi_k(0; \lambda)$, and we recall the notation $b(x) = F''(\bar{u}(x))$. As an initial simplification, we note that upon integration of (1.17) we obtain the general relationship

$$[\phi_k'''] = b(0)[\phi_k'] - \lambda \mathcal{I}[\phi_k], \tag{2.1}$$

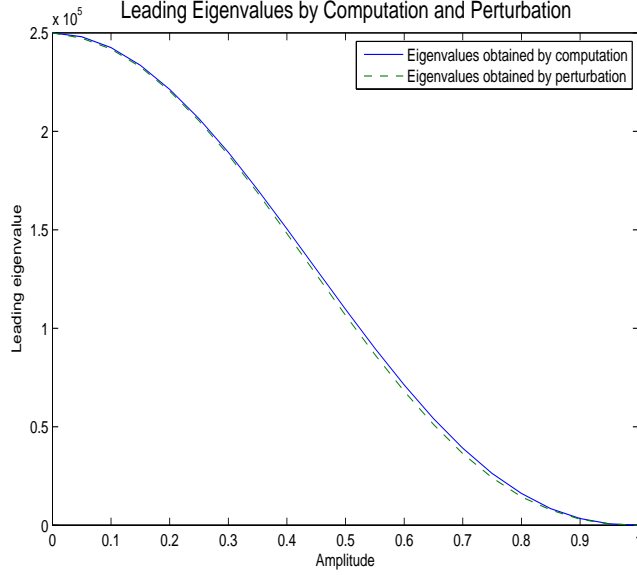


Figure 1: Comparison of leading eigenvalues obtained by perturbation and computation.

where we have observed

$$b'(0) = F'''(\bar{u}(0))\bar{u}'(0) = F'''(0)\bar{u}'(0) = 0,$$

because $F'''(0) = 0$, according to our assumptions on F (in particular, because F''' is odd and $C^1(\mathbb{R})$).

Upon substitution of (2.1) into $D(\lambda, \xi)$ and performing one row operation, we find that $D(\lambda, \xi)$ is the determinant of the matrix

$$\begin{pmatrix} [\phi_1] - [e^{i\xi x}] & [\phi_2] & [\phi_3] & [\phi_4] \\ b(0)[\phi'_1] & b(0)[\phi'_2] - [e^{i\xi x}] & b(0)[\phi'_3] & b(0)[\phi'_4] \\ [\phi''_1] & [\phi''_2] & [\phi''_3] - [e^{i\xi x}] & [\phi''_4] \\ -\lambda\mathcal{I}[\phi_1] & -\lambda\mathcal{I}[\phi_2] + [e^{i\xi x}] & -\lambda\mathcal{I}[\phi_3] & -\lambda\mathcal{I}[\phi_4] - [e^{i\xi x}] \end{pmatrix}. \quad (2.2)$$

In developing our expansion, we will find power series expansions of $D(0, \xi)$, $D_\lambda(0, \xi)$, $D_{\lambda\lambda}(0, \xi)$, and $D_{\lambda\lambda\lambda}(0, \xi)$ in ξ . In order to carry this out, we need to understand the ϕ_k evaluated at $\lambda = 0$. To streamline notation, we will set

$$\varphi_k(x) := \phi_k(x; 0). \quad (2.3)$$

Upon setting $\lambda = 0$ in (1.17) and integrating twice, we obtain

$$\begin{aligned}
\varphi_1'' - b(x)\varphi_1 &= -b(0); & \varphi_1(0) &= 1, b(0)\varphi_1'(0) = 0 \\
\varphi_2'' - b(x)\varphi_2 &= -x; & \varphi_2(0) &= 0, b(0)\varphi_2'(0) = 1 \\
\varphi_3'' - b(x)\varphi_3 &= 1; & \varphi_3(0) &= 0, b(0)\varphi_3'(0) = 0 \\
\varphi_4'' - b(x)\varphi_4 &= x; & \varphi_4(0) &= 0, b(0)\varphi_4'(0) = 0.
\end{aligned} \tag{2.4}$$

It will also be convenient to observe the combinations

$$\begin{aligned}
\frac{\bar{u}'(x)}{\bar{u}'(0)} &= \varphi_1(x) + b(0)\varphi_3(x) \\
\frac{\bar{u}'(0)}{b(0)}\psi(x) &= \varphi_2(x) + \varphi_4(x)
\end{aligned} \tag{2.5}$$

It will additionally be convenient to define

$$\begin{aligned}
z_k(x) &:= (\partial_\lambda \phi_k)(x; 0) \\
w_k(x) &:= (\partial_\lambda^2 \phi_k)(x; 0) \\
h(x) &:= \bar{u}'(0)(z_1(x) + b(0)z_3(x)) \\
p(x) &:= \bar{u}'(0)(w_1(x) + b(0)w_2(x)) \\
q(x) &:= \frac{b(0)}{\bar{u}'(0)}(z_2(x) + z_4(x)).
\end{aligned} \tag{2.6}$$

We also note the associated equations:

$$\begin{aligned}
z_k'' - b(x)z_k &= -\int_0^x \Phi_k(y)dy; & z_k(0) &= 0, z_k'(0) = 0 \\
w_k'' - b(x)w_k &= -2\int_0^x \int_0^y z_k(\xi)d\xi dy; & w_k(0) &= 0, w_k'(0) = 0 \\
h'' - b(x)h &= -U(x); & h(0) &= 0, h'(0) = 0.
\end{aligned} \tag{2.7}$$

We will solve each of the ODE in (2.4) and (2.5) in terms of two linearly independent solutions of

$$\varphi'' - b(x)\varphi = 0.$$

As noted in the introduction, one such solution is $\bar{u}'(x)$, while a second linearly independent solution is $\psi(x)$, as given in (1.27). In the following lemma, we collect several identities obtained by direct calculation.

Lemma 2.1. *Suppose $F \in C^4(\mathbb{R})$ is an even double-well function in standard form, $\bar{u}(x)$ is the periodic solution of (1.1) given by (1.9), and the $\{\varphi_k\}_{k=1}^4$, $\{z_k\}_{k=1}^4$, h , q , and p are as defined just above. Then we have the following identities:*

(i) *Integral identities*

$$\begin{aligned}\mathcal{I}[\bar{u}] &= \mathcal{I}[\psi] = 0; & \mathcal{I}[U\psi] &= -\frac{X'(u_*)}{2F'(u_*)}\mathcal{I}[\bar{u}^2]; & \mathcal{I}[h] &= \mathcal{I}[\bar{u}\Phi_3] \\ \Phi_2(X) &= -\Phi_4(X) = -\mathcal{I}[x\varphi_3] = \frac{1}{b(0)}\mathcal{I}[x\varphi_1]; & \mathcal{I}[(X-x)\varphi_k] &= \mathcal{I}[\Phi_k] \\ \Phi_3(X) &= \mathcal{I}[\psi\bar{u}] = -\frac{X'(u_*)}{F'(u_*)}u_*^2 + \sqrt{2}\int_0^{u_*}\frac{u_*^2-x^2}{(F(x)-F(u_*))^{3/2}}dx \\ \mathcal{I}[x\varphi_4] &= X^2\Phi_3(X) + 2\mathcal{I}[U\Psi] - 2\mathcal{I}[x\Phi_3]; & \mathcal{I}[z_3] &= \mathcal{I}[\Phi_3^2] - \Phi_3(X)\mathcal{I}[\Phi_3]\end{aligned}$$

(ii) *Jump identities*

$$\begin{aligned}\varphi_3(x) &= \bar{u}(x)\psi(x) - \bar{u}'(x)\Psi(x) \Rightarrow [\varphi_3] = 0; & [\varphi_4] &= \bar{u}'(0)\mathcal{I}[\Psi] \\ [\varphi_1] &= 0; [q] = -\bar{u}'(0)\mathcal{I}[\Psi^2] + \psi(X)\mathcal{I}[\bar{u}\Psi]; \\ [h] &= \frac{X'(u_*)\bar{u}'(0)}{2F'(u_*)}\mathcal{I}[\bar{u}^2]; & [\psi] &= \frac{X'(u_*)}{F'(u_*)}\bar{u}'(0),\end{aligned}$$

(iii) *Derivative jump identities, $k = 1, 2, 3, 4$*

$$\begin{aligned}[\varphi'_1] &= [\varphi'_3] = 0 \\ [h'] &= \frac{1}{\bar{u}'(0)}\mathcal{I}[\bar{u}^2]; & [q'] &= \frac{X'(u_*)}{2\bar{u}'(0)F'(u_*)}\mathcal{I}[\bar{u}^2]; & [z'_k] &= \frac{1}{\bar{u}'(0)}\mathcal{I}[\bar{u}\Phi_k]\end{aligned}$$

(iv) *Second derivative jump identities, $k = 1, 2, 3, 4$*

$$\begin{aligned}[\varphi''_1] &= [\varphi''_3] = 0; \\ [\varphi''_2] &= b(0)[\varphi_2] - X; & [\varphi''_4] &= b(0)[\varphi_4] + X \\ [h''] &= b(0)[h]; & [z''_k] &= b(0)[z_k] - \mathcal{I}[(X-x)\varphi_k]\end{aligned}$$

Proof. In all cases the proof is by direct calculation, beginning with the observation by variation of parameters that the general ODE

$$\phi'' - b(x)\phi = f(x); \quad \phi(0) = \phi_0, \phi'(0) = \omega_0,$$

is solved by

$$\phi(x) = \frac{\phi_0}{\bar{u}'(0)}\bar{u}'(x) + \omega_0\bar{u}'(0)\psi(x) - \bar{u}'(x)\int_0^x\psi(y)f(y)dy + \psi(x)\int_0^x\bar{u}'(y)f(y)dy.$$

Using this identity, we can solve a second order ODE for each of the $\{\varphi_k\}_{k=1}^4$, $\{z_k\}_{k=1}^4$, h , q , and p , and the expressions in Lemma 2.1 correspond with evaluation of these identities. We omit the details. \square

As stated above, we now proceed by expanding each of $D(0, \xi)$, $D_\lambda(0, \xi)$, $D_{\lambda\lambda}(0, \xi)$, and $D_{\lambda\lambda\lambda}(0, \xi)$ in powers of ξ . Expansions are given respectively in Lemmas 2.2, 2.3, 2.4, and 2.5.

Lemma 2.2. *Under the assumptions of Lemma 2.1, we have*

$$D(0, \xi) = (e^{i\xi X} - 1)^4.$$

Proof. Upon setting $\lambda = 0$ in (2.2), we obtain

$$\begin{aligned} D(0, \xi) &= \det \begin{pmatrix} [\varphi_1] - [e^{i\xi x}] & [\varphi_2] & [\varphi_3] & [\varphi_4] \\ b(0)[\varphi'_1] & b(0)[\varphi'_2] - [e^{i\xi x}] & b(0)[\varphi'_3] & b(0)[\varphi'_4] \\ [\varphi''_1] & [\varphi''_2] & [\varphi''_3] - [e^{i\xi x}] & [\varphi''_4] \\ 0 & [e^{i\xi x}] & 0 & -[e^{i\xi x}] \end{pmatrix} \\ &= [e^{i\xi X}] \det \begin{pmatrix} [\varphi_1] - [e^{i\xi x}] & [\varphi_3] & [w] \\ b(0)[\varphi'_1] & b(0)[\varphi'_3] & b(0)[w'] - [e^{i\xi x}] \\ [\varphi''_1] & [\varphi''_3] - [e^{i\xi X}] & [w''] \end{pmatrix} \\ &= [e^{i\xi X}] \det \begin{pmatrix} -[e^{i\xi x}] & 0 & [w] \\ 0 & 0 & -[e^{i\xi x}] \\ 0 & -[e^{i\xi X}] & b(0)[w] \end{pmatrix}, \end{aligned}$$

where in the final equality we have used several relations in Lemma 2.1. The claim is now immediate. \square

Lemma 2.3. *Under the assumptions of Lemma 2.1, we have*

$$\begin{aligned} (\partial_\lambda D)(0, \xi) &= [e^{i\xi x}]^2 \left\{ X\Phi_3(X) - \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] \right\} \\ &\quad + [e^{i\xi x}]^3 \left\{ \mathcal{I}[x\varphi_3] - [z_1] - \bar{u}'(0)[q'] - [z_3''] \right\}. \end{aligned}$$

Proof. We differentiate (2.2) and evaluate the result at $\lambda = 0$ to find

$$\begin{aligned} (\partial_\lambda D)(0, \xi) &= \det \begin{pmatrix} [z_1] & [\varphi_2] & 0 & [\varphi_4] \\ b(0)[z'_1] & b(0)[\varphi'_2] - [e^{i\xi x}] & 0 & b(0)[\varphi'_4] \\ [z''_1] & [\varphi''_2] & -[e^{i\xi x}] & [\varphi''_4] \\ -\Phi_1(X) & [e^{i\xi x}] & 0 & -[e^{i\xi x}] \end{pmatrix} \\ &\quad + \det \begin{pmatrix} -[e^{i\xi x}] & [z_2] & 0 & [\varphi_4] \\ 0 & b(0)[z'_2] & 0 & b(0)[\varphi'_4] \\ 0 & [z''_2] & -[e^{i\xi x}] & [\varphi''_4] \\ 0 & -\Phi_2(X) & 0 & -[e^{i\xi x}] \end{pmatrix} \\ &\quad + \det \begin{pmatrix} -[e^{i\xi x}] & [\varphi_2] & [z_3] & [\varphi_4] \\ 0 & b(0)[\varphi'_2] - [e^{i\xi x}] & b(0)[z'_3] & b(0)[\varphi'_4] \\ 0 & [\varphi''_2] & [z''_3] & [\varphi''_4] \\ 0 & [e^{i\xi x}] & -\Phi_3(X) & -[e^{i\xi x}] \end{pmatrix} \\ &\quad + \det \begin{pmatrix} -[e^{i\xi x}] & [\varphi_2] & 0 & [z_4] \\ 0 & b(0)[\varphi'_2] - [e^{i\xi x}] & 0 & b(0)[z'_4] \\ 0 & [\varphi''_2] & -[e^{i\xi x}] & [z''_4] \\ 0 & [e^{i\xi x}] & 0 & -\Phi_4(X) \end{pmatrix}. \end{aligned}$$

For notational convenience, we temporarily label these four summands respectively A, B, C, and D.

We have, by direct calculation, the combinations

$$B + D = [e^{i\xi x}]^3 \left[\Phi_4(X) - \bar{u}'(0)[q'] \right],$$

and

$$A + C = [e^{i\xi X}]^2 \left[X\Phi_3(X) - \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] \right] - [e^{i\xi X}]^3 \left[z_3'' + z_1 \right],$$

and summing these gives the claim. \square

The following two lemmas are proved by differentiating (2.2) two and three times with respect to λ and evaluating each of the resulting determinants at $\lambda = 0$. In both cases the calculations are tedious but straightforward, and we omit the details.

Lemma 2.4. *Under the assumptions of Lemma 2.1, we have*

$$(\partial_\lambda^2 D)(0, \xi) = \alpha_0 + \alpha_1 [e^{i\xi x}] + \alpha_2 [e^{i\xi x}]^2 + \mathbf{O}(|[e^{i\xi x}]|^3),$$

where

$$\begin{aligned} \alpha_0 &= -2X \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] \Phi_3(X); \\ \alpha_1 &= 2\alpha_0; \\ \alpha_2 &= -\bar{u}'(0)[\psi][p'] + 2X\mathcal{I}[z_3] + \frac{2}{\bar{u}'(0)}([\varphi_4]\mathcal{I}[h] - 2X\Phi_3(X)[h]) \\ &\quad + 2([h][q'] - [q][h']) + 2(\Phi_3(X)\mathcal{I}[x\varphi_4] - \Phi_4(X)\mathcal{I}[x\varphi_3]) \\ &\quad - 2\bar{u}'(0)[z_3']\mathcal{I}[x\psi] \end{aligned}$$

In particular,

$$(\partial_\lambda^2 D)(0, 0) = \alpha_0; \quad (\partial_\lambda^2 \partial_\xi D)(0, 0) = iX\alpha_1; \quad (\partial_\lambda^2 \partial_\xi^2 D)(0, 0) = -X^2(\alpha_1 + 2\alpha_2).$$

Lemma 2.5. *Under the assumptions of Lemma 2.1, we have*

$$\begin{aligned} (\partial_\lambda^3 D)(0, 0) &= -3X[\psi]\bar{u}'(0)\Phi_3(X)[p'] - 6[h']\Phi_3(X)([\varphi_4]\mathcal{I}[\Psi] - [\psi]\mathcal{I}[(X-x)\varphi_4]) \\ &\quad + 6X\Phi_3(X)([h][q'] - [q][h']) + 6[\psi][h']\Phi_2(X)\mathcal{I}[(X-x)\varphi_3] \\ &\quad + 6X[\psi](\mathcal{I}[h][z_3'] - [h']\mathcal{I}[z_3]). \end{aligned}$$

3 Perturbation Analysis

For notational convenience we write

$$\begin{aligned} D(\lambda, \xi) &\approx A_1\lambda^2 + A_2\lambda^3 + A_3\lambda^2\xi + A_4\lambda\xi^2 + A_5\lambda^2\xi^2 \\ &\quad + A_6\lambda\xi^3 + A_7\xi^4 + A_8\lambda\xi^4 + A_9\xi^5 + A_{10}\xi^6, \end{aligned} \tag{3.1}$$

where the remaining terms are either zero or of higher order when we search for roots of the form

$$\lambda_{\max}(\xi) = a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + \mathbf{O}(\xi^5). \quad (3.2)$$

(It has been shown in [10] that there are no zero or first order terms in such an expansion.) We clearly have the relations:

$$\begin{aligned} A_1 &= \frac{1}{2}\partial_\lambda^2 D(0, 0); & A_2 &= \frac{1}{6}\partial_\lambda^3 D(0, 0); & A_3 &= \frac{1}{2}\partial_\lambda^2 \partial_\xi D(0, 0); & A_4 &= \frac{1}{2}\partial_\lambda \partial_\xi^2 D(0, 0); \\ A_5 &= \frac{1}{4}\partial_\lambda^2 \partial_\xi^2 D(0, 0); & A_6 &= \frac{1}{6}\partial_\lambda \partial_\xi^3 D(0, 0); & A_7 &= \frac{1}{4!}\partial_\xi^4 D(0, 0); \\ A_8 &= \frac{1}{4!}\partial_\lambda \partial_\xi^4 D(0, 0); & A_9 &= \frac{1}{5!}\partial_\xi^5 D(0, 0); & A_{10} &= \frac{1}{6!}\partial_\xi^6 D(0, 0). \end{aligned} \quad (3.3)$$

Before proceeding with the perturbation expansion, we record some useful observations regarding the coefficients $\{A_k\}_{k=1}^{10}$. The following lemma is proved by combining Lemmas 2.1–2.5. We omit the details.

Lemma 3.1. *Under the assumptions of Lemma 2.1 we have the following identities:*

$$\begin{aligned} A_1 &= -X \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] \Phi_3(X); & A_3 &= 2iX A_1 \\ A_2 &= -\frac{1}{2} \frac{X'(u_*)}{F'(u_*)} \bar{u}'(0)^2 \Phi_3(X) [p'] - \frac{1}{\bar{u}'(0)} \mathcal{I}[\bar{u}^2] \left([\varphi_4] \mathcal{I}[\psi] - [\psi] \mathcal{I}[(X-x)\varphi_4] \right) \\ &\quad + X \Phi_3(X) \left([h][q'] - [q][h'] \right) + \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] \Phi_2(X) \mathcal{I}[(X-x)\varphi_3] \\ &\quad + X \frac{X'(u_*)}{F'(u_*)} \bar{u}'(0) \left(\mathcal{I}[h][z'_3] - [h] \mathcal{I}[z_3] \right) \\ A_4 &= \left(\frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] - X \Phi_3(X) \right) X^2; & A_6 &= 2iX A_4; & A_8 &= -\frac{25}{12} X^2 A_4 \\ A_5 &= -\frac{1}{2} \frac{X'(u_*)}{F'(u_*)} \bar{u}'(0)^2 [p'] + X \mathcal{I}[z_3] + \frac{1}{\bar{u}'(0)} \left([\varphi_4] \mathcal{I}[h] - 2X \Phi_3(X) [h] \right) \\ &\quad + \left([h][q'] - [q][h'] \right) + \left(\Phi_3(X) \mathcal{I}[x\varphi_4] - \Phi_4(X) \mathcal{I}[x\varphi_3] \right) - \bar{u}'(0) [z'_3] \mathcal{I}[x\psi] \\ A_7 &= X^4; & A_9 &= 2iX A_7; & A_{10} &= -\frac{13}{6} X^6. \end{aligned}$$

Upon substitution of (3.2) into the equation $D(\lambda, \xi) = 0$, we obtain the requirements

$$\begin{aligned} A_1 a_2^2 + A_4 a_2 + A_7 &= 0 \\ 2A_1 a_2 a_3 + A_3 a_2^2 + A_4 a_3 + A_6 a_2 + A_9 &= 0 \\ A_1 a_3^2 + 2A_1 a_2 a_4 + A_2 a_2^3 + 2A_3 a_2 a_3 + A_4 a_4 + A_5 a_2^2 + A_6 a_3 + A_{10} &= 0. \end{aligned} \quad (3.4)$$

Clearly, from the first equation in (3.4)

$$a_2 = \frac{-A_4 \pm \sqrt{A_4^2 - 4A_1A_7}}{2A_1}.$$

We compute

$$\begin{aligned} A_4^2 - 4A_1A_7 &= \left(X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] - X^3 \Phi_3(X) \right)^2 + 4X^5 \frac{X'(u_*)}{F'(u_*)} \Phi_3(X) \mathcal{I}[\bar{u}^2] \\ &= \left(X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] + X^3 \Phi_3(X) \right)^2, \end{aligned}$$

Using an expression for $\Phi_3(X)$ from Lemma 2.1 we can write

$$X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] + X^3 \Phi_3(X) = X^2 \frac{X'(u_*)}{F'(u_*)} \int_0^X \bar{u}(x)^2 - u_*^2 dx + \sqrt{2} \int_0^{u_*} \frac{u_*^2 - x^2}{(F(x) - F(u_*))^{3/2}} dx,$$

and since $X'(u_*) > 0$ and $F'(u_*) < 0$ it's clear that this expression is positive. We have, then,

$$A_1 a_2 = \frac{1}{2} \left(X^3 \Phi_3(X) - X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] \pm \left(X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] + X^3 \Phi_3(X) \right) \right).$$

In this way we have two possible choices for $A_1 a_2$,

$$-X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2]; \quad \text{and} \quad X^3 \Phi_3(X),$$

both positive. The corresponding choices for a_2 are

$$a_2^\# = \frac{X}{\Phi_3(X)}; \quad a_2^b = -\frac{X^2 F'(u_*)}{X'(u_*) \mathcal{I}[\bar{u}^2]}.$$

We next consider the second equation in (3.4). First, using Lemma 3.1 we compute

$$A_3 a_2^2 + A_6 a_2 + A_9 = 2iX(A_1 a_2^2 + A_4 a_2 + A_7) = 0,$$

where the second equality is the first relation in (3.4). We are left with

$$(2A_1 a_2 + A_4) a_3 = 0,$$

and by direct calculation we find

$$2A_1 a_2 + A_4 = \pm \left(X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] + X^3 \Phi_3(X) \right),$$

where $+$ is associated with a_2^b and $-$ with a_2^\sharp . If we use our expression for $\Phi_3(X)$ from Lemma 2.1 we find

$$\begin{aligned} & X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] + X^3 \Phi_3(X) \\ &= X^2 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] + X^3 \left[-\frac{X'(u_*)}{F'(u_*)} u_*^2 + \sqrt{2} \int_0^{u_*} \frac{u_*^2 - x^2}{(F(x) - F(u_*))^{3/2}} dx \right] \\ &= X^2 \frac{X'(u_*)}{F'(u_*)} \int_0^X \bar{u}(x)^2 - u_*^2 dx + \sqrt{2} X^3 \int_0^{u_*} \frac{u_*^2 - x^2}{(F(x) - F(u_*))^{3/2}} dx, \end{aligned} \quad (3.5)$$

and since $\bar{u}(x) \leq u_*$ for all $x \in [0, X]$ it's clear that both summands are positive (recall that $X'(u_*) > 0$ and $F'(u_*) < 0$). We conclude that

$$2A_1 a_2 + A_4 \neq 0 \quad (3.6)$$

and so $a_3 = 0$.

Before proceeding to the third equation in (3.4) we record two observations regarding the choice of a_2 . First, to set a baseline for these observations, notice that if (1.1) is linearized about the constant solution $u_h = 0$ we obtain the eigenvalue equation

$$(-\phi_{xx} + F''(0))_{xx} = \lambda \phi,$$

with eigenvalues

$$\lambda(\xi) = -F''(0)\xi^2 - \xi^4.$$

In this way we would like to take our expansion $\lambda(\xi) = a_2 \xi^2 + a_4 \xi^4$ so that

$$\begin{aligned} \lim_{u_* \rightarrow 0} a_2(u_*) &= -F''(0) \\ \lim_{u_* \rightarrow 0} a_4(u_*) &= -1. \end{aligned}$$

Lemma 3.2. *Let the assumptions of Lemma 2.1 hold. Then*

$$\lim_{u_* \rightarrow 0} a_2^\sharp(u_*) = -F''(0).$$

Remark 3.1. *In particular, this lemma asserts that the choice a_2^\sharp is a convenient choice in the sense that it is likely to give a good approximation of the leading eigenvalue even in the case of large λ . (See the discussion following the statement of Theorem 1.1.) We can check by numerically evaluating the integrals involved with a_2^b that we seem to have*

$$\lim_{u_* \rightarrow 0} a_2^b(u_*) = +\infty,$$

so a_2^b is not a good choice for the case of large λ .

We also observe that we expect the maximum value obtained by the curve $\lambda^\sharp(\xi)$ —associated with the perturbation expansion based on a_2^\sharp —to be the same as the maximum value obtained by the curve $\lambda^\flat(\xi)$. To see why this should be the case, note first that if we denote the eigenvalues of the monodromy matrix $\{r_j\}_{j=1}^4$ then

$$\det M(\lambda; X) = r_1 r_2 r_3 r_4 = 1.$$

Generally speaking, r_1 and r_2 can be chosen to correspond with the curve $\lambda^\sharp(\xi)$, while r_3 and r_4 can be chosen to correspond with the curve $\lambda^\flat(\xi)$. More precisely, $r_1 = e^{i\xi X}$ will be an eigenvalue of the monodromy matrix precisely when $\lambda^\sharp(\xi)$ is an eigenvalue of L , and $r_3 = e^{i\xi X}$ will be an eigenvalue of the monodromy matrix precisely when $\lambda^\flat(\xi)$ is an eigenvalue of L . In the event that r_1 has a non-zero imaginary part, we can take r_2 to be its complex conjugate, so that $r_1 r_2 = 1$. In this way, $r_3 r_4 = 1$. But if r_3 has non-zero imaginary part then r_4 is its complex conjugate, and so $|r_3| = 1$. This argument suggests that for any given λ , either r_1 and r_3 both have unit modulus, or neither has unit modulus. In this way, λ is either obtained by both $\lambda^\sharp(\xi)$ and $\lambda^\flat(\xi)$ (typically at different values of ξ) or is not obtained by either.

Though we won't rigorously verify these observations here, we note that similar and more sophisticated observations have been verified in [15, 16] in the case of the Euler–Bernoulli equation.

Proof of Lemma 3.2. We first recall that

$$X(u_*) = 4 \int_0^{u_*} \frac{dx}{\sqrt{2(F(x) - F(u_*))}}.$$

We note that to order $F(x) \approx \frac{1}{2}F''(0)x^2$, so

$$\begin{aligned} \lim_{u_* \rightarrow 0} X(u_*) &= \frac{4}{\sqrt{-F''(0)}} \lim_{u_* \rightarrow 0} \int_0^{u_*} \frac{dx}{\sqrt{u_*^2 - x^2}} \\ &= \frac{4}{\sqrt{-F''(0)}} \lim_{u_* \rightarrow 0} \left\{ \sin^{-1} \frac{x}{u_*} \Big|_0^{u_*} \right\} = \frac{2\pi}{\sqrt{-F''(0)}}. \end{aligned} \tag{3.7}$$

Next, we recall that

$$X'(u_*) = \frac{2\sqrt{2}}{\sqrt{-F(u_*)}} - \sqrt{2} \int_0^{u_*} \frac{F'(x) - F'(u_*)}{(F(x) - F(u_*))^{3/2}} dx,$$

and compute directly (using Part (i) of Lemma 2.1)

$$\begin{aligned} \Phi_3(X) &= -\frac{X'(u_*)}{F'(u_*)} u_*^2 + \sqrt{2} \int_0^{u_*} \frac{u_*^2 - x^2}{(F(x) - F(u_*))^{3/2}} dx \\ &= -\frac{2\sqrt{2}}{F'(u_*)\sqrt{-F(u_*)}} u_*^2 + \sqrt{2} \int_0^{u_*} \frac{\frac{u_*^2}{F'(u_*)} F'(x) - x^2}{(F(x) - F(u_*))^{3/2}} dx. \end{aligned}$$

Using $F'(x) \approx F''(0)x$ (and again $F(x) \approx \frac{1}{2}F''(0)x^2$), we compute

$$\begin{aligned} \lim_{u_* \rightarrow 0} \int_0^{u_*} \frac{\frac{u_*^2}{F'(u_*)}F'(x) - x^2}{(F(x) - F(u_*))^{3/2}} dx &= \left(\frac{2}{-F''(0)}\right)^{3/2} \lim_{u_* \rightarrow 0} \int_0^{u_*} \frac{xu_* - x^2}{(x^2 - u_*^2)^{3/2}} dx \\ &= \left(\frac{2}{-F''(0)}\right)^{3/2} \lim_{u_* \rightarrow 0} \left\{ \tan^{-1} \frac{x}{\sqrt{u_*^2 - x^2}} + \frac{u_* - x}{\sqrt{u_*^2 - x^2}} \Big|_0^{u_*} \right\} \\ &= \left(\frac{2}{-F''(0)}\right)^{3/2} \left(\frac{\pi}{2} - 1\right). \end{aligned}$$

We conclude

$$\lim_{u_* \rightarrow 0} \Phi_3(X) = \frac{4}{(-F''(0))^{3/2}} + \frac{4}{(-F''(0))^{3/2}} \left(\frac{\pi}{2} - 1\right) = \frac{2}{(-F''(0))^{3/2}} \pi,$$

Combining this last calculation with (3.7) gives the claim. \square

Finally, we solve the third equation in (3.4) for a_4 ,

$$a_4 = -\frac{A_2 a_2^3 + A_5 a_2^2 + A_8 a_2 + A_{10}}{2A_1 a_2 + A_4},$$

noting from the previous considerations that we are not dividing by 0. We already have a relatively convenient form for the denominator, $2A_1 a_2 + A_4$, so we turn now to deriving an expression for the numerator, $A_2 a_2^3 + A_5 a_2^2 + A_8 a_2 + A_{10}$.

For notational brevity we set

$$B := X^2 + \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2] a_2, \quad (3.8)$$

where in principle a_2 could denote either a_2^\sharp or a_2^\flat . We now combine Lemmas 2.3, 2.4, and 2.5 with relations (3.3) to compute (factoring out a_2^2)

$$\begin{aligned} &A_2 a_2 + A_5 + \frac{A_8}{a_2} + \frac{A_{10}}{a_2^2} \\ &= \left[-\frac{1}{2} X[\psi][p'] + X([h][q'] - [q][h']) \right] (\Phi_3(X) a_2 - X) \\ &+ B \left[\mathcal{I}[\Phi_3^2] - X \mathcal{I}[\Phi_3^2] - 2\Phi_3(X) \mathcal{I}[U\Psi] + 2\Phi_3(X) \mathcal{I}[x\Phi_3] - X\Phi_3(X) \mathcal{I}[\Phi_3] \right] \\ &+ a_2 \left[X \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}\Phi_3]^2 - \mathcal{I}[\bar{u}^2] \Phi_3(X) \mathcal{I}[\Psi]^2 \right] \\ &+ 2X^3 \frac{X'(u_*)}{F'(u_*)} \Phi_3(X) \mathcal{I}[\bar{u}^2] - 2X^2 \mathcal{I}[\bar{u}\Phi_3] \mathcal{I}[\Psi] \\ &+ \left(\frac{25X^5 \Phi_3(X)}{12a_2} - \frac{13X^6}{6a_2^2} \right) - \frac{25}{12a_2} X^4 \frac{X'(u_*)}{F'(u_*)} \mathcal{I}[\bar{u}^2]. \end{aligned}$$

The expression stated in Theorem 1.1 results from substituting a_2^\sharp into this last expression (note that the first line vanishes with this choice of a_2).

Proof of Theorem 1.1. First, it's clear from our construction of $D(\lambda, \xi)$ and the analyticity of the $\{\phi_j\}_{j=1}^4$ in λ that $D(\lambda, \xi)$ is analytic on $\mathbb{C} \times \mathbb{C}$. This justifies our general Taylor expansion

$$D(\lambda, \xi) = \sum_{\alpha} \frac{\partial^\alpha D(0, 0)}{\alpha!} \lambda^{\alpha_1} \xi^{\alpha_2}, \quad (3.9)$$

for $|(\lambda, \xi)|$ sufficiently small. In this way our perturbation argument will be valid, with the values a_2 and a_4 we obtained, if we can establish that the roots of $D(\lambda, \xi)$ can be obtained as an expansion in ξ .

To this end, we first observe that $D_\lambda(0, 0) = 0$ (see Lemma 2.3), so that the Implicit Function Theorem cannot be directly applied to $D(\lambda, \xi)$. In order to apply the Implicit Function Theorem, we clearly must select a particular solution branch, $\lambda^\sharp(\xi)$ or $\lambda^b(\xi)$. We proceed with $\lambda^\sharp(\xi)$, noting that the exact same calculation is valid with \sharp is replaced everywhere by b . Working similarly as in [9], we define the new variable

$$\rho = \frac{\lambda - a_2 \xi^2}{\xi^2}.$$

We set

$$G(\rho, \xi) := \frac{D(a_2^\sharp \xi^2 + \rho \xi^2, \xi)}{\xi^4},$$

so that, according to (3.1)

$$G(\rho, \xi) = A_1(a_2^\sharp + \rho)^2 + A_4(a_2^\sharp + \rho) + A_7 + \mathbf{O}(\xi),$$

so that $G(0, 0) = A_1(a_2^\sharp)^2 + A_4 a_2^\sharp + A_7 = 0$ (by the first equation in (3.4)). Likewise,

$$G_\rho(\rho, \xi) = \frac{D_\lambda(a_2^\sharp \xi^2 + \rho \xi^2, \xi)}{\xi^2} = 2A_1(a_2^\sharp + \rho) + A_4 + \mathbf{O}(\xi),$$

so that $G_\rho(0, 0) = 2A_1 a_2^\sharp + A_4 \neq 0$, as shown in (3.6). According, then, to the Implicit Function Theorem $G(\rho, \xi)$ has a unique locally C^∞ solution

$$\rho(\xi) = b_1 \xi + b_2 \xi^2 + b_3 \xi^3 + \mathbf{O}(\xi^4).$$

Accordingly, $D(\lambda, \xi)$ is solved by

$$\lambda(\xi) = a_2^\sharp \xi^2 + \xi^2 \rho = a_2^\sharp \xi^2 + b_1 \xi^3 + b_2 \xi^4 + b_3 \xi^5 + \mathbf{O}(\xi^6).$$

Last, we observe that the expansion will have no terms involving odd powers of ξ . We know from our preceding calculations and our perturbation analysis that there are precisely two eigenvalue curves (i.e., $\lambda^\sharp(\xi)$ and $\lambda^b(\xi)$) with the general form

$$\lambda(\xi) = a_2 \xi^2 + \mathbf{O}(\xi^4), \quad (3.10)$$

where we recall that it has already been shown directly that $a_3 = 0$ for such curves. Suppose, for example, that $\lambda^\sharp(\xi)$ is not an even function. Nonetheless, $\sigma(\xi) := \lambda^\sharp(-\xi)$ is certainly a curve of eigenvalues of form (3.10) (i.e., if $e^{i\xi X}$ is an eigenvalue of the monodromy matrix then so is its complex conjugate $e^{-i\xi X}$), and so it must be the case that

$$\lambda^\flat(\xi) = \lambda^\sharp(-\xi).$$

But this would require $a_2^\sharp = a_2^\flat$, which cannot be true (as is clear from (3.5)). This contradiction establishes that $\lambda^\sharp(\xi)$ must be even, and clearly we have the same result for $\lambda^\flat(\xi)$. \square

4 The Langer Model and Coarsening Rates

In this section we will briefly review the coarsening framework Langer developed in [11], then apply it in the current setting.

Following Langer, we assume the alloy under investigation is composed of two metals, A and B , and that it is contained in a bounded d -dimensional set Ω . We specify N lattice sites in the interior of Ω , each separated from its nearest neighbors by a distance we denote a , and we assume that at each lattice site there is either one atom of species B , in which case we record the composition at that site as $+1$, or one atom of species A , in which case we record the composition at that site as -1 . We will discuss the model in two regimes, a continuum regime and a discrete regime. Since it will be important in this discussion to carefully distinguish between scalar and vector variables, we will use a bold font to distinguish a vector.

Continuum description. For the continuum regime, we let $\mathbf{x} \in \mathbb{R}^d$ denote a position in d -dimensional space, and we define $\zeta(\mathbf{x})$ to be an average composition taken over the ν lattice sites nearest \mathbf{x} . More precisely, for some appropriate positive integer ν we set

$$\zeta(\mathbf{x}) := \frac{\text{Number of B atoms} - \text{Number of A atoms}}{\nu},$$

where the atoms are always taken from the ν nearest neighbors around \mathbf{x} . Strictly speaking, ζ will not generally be continuous, but we will work with a smooth approximation of ζ that we will again denote ζ .

Discrete description. For the discrete regime, we subdivide our set Ω into N/ν microregions, each consisting of ν atoms. We now define a vector $\boldsymbol{\eta}$, with components η_α , $\alpha = 1, 2, \dots, N/\nu$, calculated as the average composition over microregion α . In particular, if we let $\{\mathbf{x}_\alpha\}_{\alpha=1}^{N/\nu}$ denote the N/ν microregion centers, we can relate the continuum and discrete descriptions by

$$\eta_\alpha = \zeta(\mathbf{x}_\alpha). \quad (4.1)$$

Here C is a constant depending on relevant physical parameters such as Boltzmann's constant and system temperature, physicality that we have chosen to suppress for this discussion.

Working in the discrete setting, we denote by $\rho = \rho(t, \boldsymbol{\eta})$ the probability distribution function over the states $\boldsymbol{\eta} \in \mathbb{R}^{N/\nu}$, normalized so that

$$\int_{\mathbb{R}^{(N/\nu)}} \rho(t, \boldsymbol{\eta}) d\boldsymbol{\eta} = 1.$$

Suppose now $\boldsymbol{\eta}_s$ denotes a stationary solution in the discrete framework. Langer develops an asymptotic approximation for $\rho(t, \boldsymbol{\eta}_s)$,

$$\rho(t, \boldsymbol{\eta}_s) \approx C e^{-t/\tau}, \quad (4.2)$$

where

$$\frac{1}{\tau} := \sum_{\{n: \omega_n < 0\}} |\omega_n|, \quad (4.3)$$

and the ω_n are eigenvalues of the finite difference discrete approximation to the eigenvalue problem (1.17).

Working in the context of a particular—but in some sense canonical—example Langer argues that τ^{-1} can reasonably be viewed as the rate at which transition layers are being eliminated by the coalescence of neighboring pockets of A -rich or B -rich regions. From this point of view, if we let M denote the number of such regions, Langer's model is

$$\frac{dM}{dt} \cong -\frac{1}{\tau(M)}. \quad (4.4)$$

If we let l denote the distance between transitions, then (4.4) becomes (using that the physical length of the system is $L = lM$)

$$\frac{dl}{dt} = \frac{l^2}{L\tau(l)}. \quad (4.5)$$

In this way, we see that if we can compute $\tau(l)$ we will have an ODE that describes the coarsening of the alloy under consideration.

In what follows, we suggest a slight modification to (4.4). In this development we regard $M = M(t)$ as the state of the system at time t in the following sense: $M(t)$ denotes the number of regions that are either A -rich or B -rich at time t . We note that $M(t)$ is a stochastic variable, and we assume that at time $t = 0$ the system is certainly in state $M(0) = M_0$, and that the probability that the system is still in state M_0 at time t is proportional to $e^{-\frac{t}{\tau}}$. That is, we assume

$$\Pr\{M(t) = M_0\} = e^{-\frac{t}{\tau}}.$$

Next, we observe that, except at the endstates, when an A -rich or B -rich region dissolves, the system goes from state M_0 to state $M_0 - 2$; i.e., by our counting scheme two regions are lost in each annihilation. Let \mathcal{T} denote the first time the system arrives in state $M_0 - 2$. Then

$$\Pr\{\mathcal{T} \leq t\} = 1 - e^{-\frac{t}{\tau}},$$

and so \mathcal{T} is exponentially distributed with $E[\mathcal{T}] = \tau$. In this way, we expect that in an averaging sense

$$M(\tau) - M(0) \approx -2,$$

and so upon dividing by τ and regarding τ as suitably small,

$$\frac{dM}{dt} \approx -\frac{2}{\tau}. \quad (4.6)$$

In developing our *coarsening ODE* below we will work with (4.6) rather than (4.4).

While Langer's analysis was carried out entirely in the context of a bounded domain, it extends quite naturally to the case of unbounded domains, under consideration here. To this end, consider the bounded interval $[-L, L]$, and a periodic solution on this interval with period X . If L is large and M , as in the previous section, denotes the number of enriched regions, then we have the approximate relation

$$X = \frac{4L}{M}. \quad (4.7)$$

(I.e., a full period is typically the width of two enriched regions.) We have, then,

$$\frac{dX}{dt} = -\frac{4L}{M^2} \frac{dM}{dt} = -\frac{4L}{M^2} \left(-\frac{2}{\tau} \right) = \frac{2}{\tau M} X,$$

where in the last equality we've used (4.7).

Now,

$$\frac{1}{\tau} = \sum_{\{n:\omega_n < 0\}} -\omega_n,$$

and as $L \rightarrow \infty$ the positive eigenvalues $-\omega_n$ become more numerous, approaching a continuum band associated with the case \mathbb{R} . More precisely, we expect to have a positive eigenvalue associated with each of the M regions (one for each transition), and the average value of these eigenvalues approaches $\lambda_{\max}(X)/2$ as they fill in the continuum band $[0, \lambda_{\max}(X)]$. In this way we have

$$\frac{1}{\tau} \approx M \frac{\lambda_{\max}(X)}{2}.$$

We see that

$$\frac{dX}{dt} = \lambda_{\max}(X) X, \quad (4.8)$$

which is our coarsening ODE on \mathbb{R} .

As a case study we consider equation (1.1) with

$$F(u) = 250u^4 - 500u^2.$$

The leading eigenvalues in this case are plotted as a function of amplitude in Figure 1. Using (1.10) we can obtain leading eigenvalues as a function of period, and upon substitution of

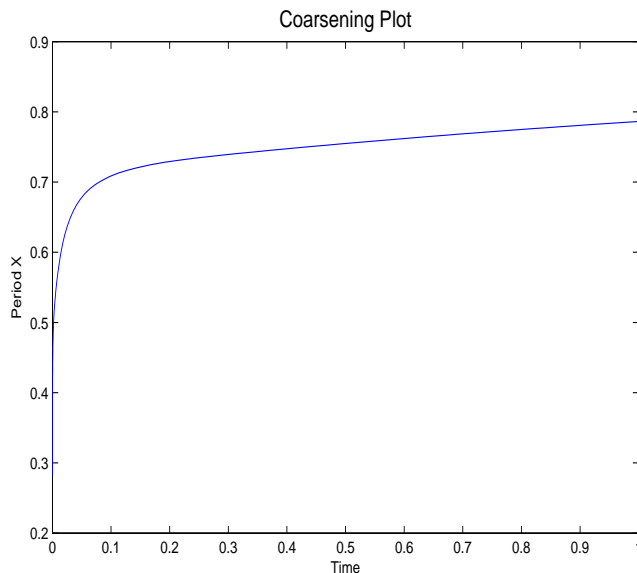


Figure 2: Comparison of leading eigenvalues obtained by perturbation and computation.

these values into $\lambda_{\max}(X)$ we can solve (4.8). The solution is plotted in Figure 4. In Figure 4 we take as our initial period the spinodal period X_s , given in (1.20). For our current choice of F , $X_s = .2810$. To be clear, we do not expect (4.8) to be a good model for such an early stage of coarsening, but the figure we obtain still captures the expected logarithmic rate. We stress that accurately integrating the Cahn–Hilliard equation to large times is computationally intensive, and so it is particularly in these late-time regimes when our results are most useful.

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