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The role of multiple microscopic mechanisms in cluster interface evolution

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Abstract

In this paper we discuss mesoscopic models describing pattern formation mechanisms for a prototypical model of surface processes that involves multiple microscopic mechanisms. We focus on a mean field partial differential equation, which contains qualitatively microscopic information on particle–particle interactions and multiple particle dynamics, and we rigorously derive the macroscopic cluster evolution laws and transport structure. We show that the motion by mean curvature is given by $V = \mu\sigma\kappa$, where k is the mean curvature, σ is the surface tension and μ is an effective mobility that depends on the presence of the multiple mechanisms and speeds up the cluster evolution. This is in contrast with the Allen–Cahn equation where $V = \kappa$.

1. Introduction

In this paper we study the effect of multiple microscopic mechanisms such as surface diffusion and adsorption/desorption which are typically involved in surface processes, on macroscopic cluster interface morphology and evolution. Although the starting point of our discussion is the micromechanisms arising in surface processes, in this paper we focus on a simplified mean field partial differential equation associated with the microscopics and rigorously derive the corresponding cluster evolution laws and transport properties. The simplified mean field type equation

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is a combination of Cahn–Hilliard and Allen–Cahn type equations. The former models, as we show later, can describe surface diffusion including particle/particle interactions, while the latter describes a simplified model of adsorption to and desorption from the surface. It is worth mentioning that in the model of discussion, the mobility is completely different from the Allen–Cahn equation and this implies that the diffusion speeds up the mean curvature flow.

Surface processes, such as catalysis, chemical vapor deposition and epitaxial growth, typically involve transport and chemistry of precursors in a gas phase; unconsumed reactants and radicals adsorb onto the surface of a substrate where numerous processes may take place simultaneously, for instance surface diffusion, reactions and desorption back to the gas phase. Surface processes have traditionally been modeled using continuum-type reaction diffusion models [11,15], where the adsorptive layer has been assumed to be spatially uniform. This approach either neglects detailed interactions between particles or treats them phenomenologically, while on the other hand nonequilibrium statistical mechanics theories provide an exact microscocpic description [13].

Next we discuss microscopic mechanisms in surface processes and then connections to mesoscopic e.g. Cahn–Hilliard/Allen–Cahn models.

1.1. Microscopic modeling

The mathematical tools employed in the statistical mechanics models are interacting particle systems, which are Markov processes set on a lattice corresponding to a solid surface; typical examples are the Ising-type systems [12], describing the evolution of an order parameter at each lattice site. Such microscopic models are an important computational tool in numerous applications and are numerically solved using Monte Carlo algorithms [20]. Ising models are defined on the d-dimensional lattice $\mathbb{Z}^d$ as follows. At each lattice site $x \in \mathbb{Z}^d$ an order parameter $\sigma(x)$—referred to as "spin"—is allowed to take the values 0 and 1 describing vacant and occupied sites, respectively. A spin configuration σ is an element of the configuration space $\Sigma = \{0, 1\}^{\mathbb{Z}^d}$ and we write $\sigma = \{\sigma(x)\colon\ x \in \mathbb{Z}^d\}$. The energy H of the system, evaluated at σ, is given by a Hamiltonian

$$H(\sigma) = -\frac{1}{2}\sum_{x \neq y} J(x-y)\sigma(x)\sigma(y) + h\sum_{x}\sigma(x),$$

where h is attributed to an external field and J is a particle/particle interaction energy; J is even, $J(r) = J(-r)$, decays rapidly at infinity and is nonnegative, i.e. the interactions are *attractive*; we may also consider potentials with both attractive and repulsive components. Equilibrium states of the Ising model are described by the Gibbs states, defined at a prescribed temperature T and on a finite domain [12]. The dynamics of microscopic models consist of a sequence of spin flips and spin exchanges and correspond to different physical processes.

1.2. Stochastic microscopic dynamics

Next we briefly describe these detailed micromechanisms in the context of surface processes. For more details we refer to the review article for surface processes [19].

1.2.1. Adsorption/desorption–spin flip mechanism

A spin flip at the site x is a spontaneous change in the order parameter, 0 is converted to 1 and vice versa. Physically this mechanism describes the desorption of a particle from the surface

to the gas phase and conversely the adsorption of a particle from the gas phase to the surface. Typically the desorption mechanism depends on the interactions with neighbors manifested in the potential J, as well as the external filed h. An obvious requirement on the dynamics is that they should leave the Gibbs states invariant and this condition is called a detailed balance law. Typical choices of such dynamics are the Glauber and Metropolis dynamics.

1.2.2. Surface diffusion–spin exchange dynamics

A spin exchange between the neighboring sites x and y is a spontaneous exchange of the values of the order parameter at x and y. Physically this mechanism describes the diffusion of a particle on a surface, where sites cannot be occupied by more than one particle. The simplest such dynamics are the Kawasaki and Metropolis dynamics.

1.3. Mesoscopic models

At large space/time scales and for long range potentials with interaction range γ^{-1} it turns out that the small scale fluctuations of the Ising systems are suppressed and an almost deterministic pattern emerges described by suitable integrodifferential equations. The passage in the limit $\gamma \to 0$ (the interaction range is γ^{-1}), which is related to coarse graining of quantities like the thermodynamical pressure, coverage, etc., is known as the Lebowitz–Penrose limit [12]. Along these lines we can study the asymptotic limit of the coarse-grained variable corresponding to a local coverage in space,

$$u_\gamma(x,t) = |B_x|^{-1} \sum_{y \in B_x} \sigma_t(y),$$

where B_x is a ball centered at x containing enough points so that, (a) the random fluctuations will be (formally) suppressed due to the law of large numbers, and (b) spatial variations in the coverage are still captured. In the case of adsorption/desorption dynamics in asymptotic limit $\gamma \to 0$, we get a closed equation for the coverage, $u_\gamma(x,t) \approx u(\gamma x, t)$, and u solves the mesoscopic equation [7,16],

$$u_t = \Psi\big(-\beta(J * u + h)\big)\big[1 - u - \exp(-\beta h) u \exp(-\beta J * u)\big], \tag{1.1}$$

where $\Psi = \Psi(r)$ is associated with the microscopic dynamics: typical choices include $\Psi(r) = (1+e^r)^{-1}$ (Glauber dynamics), $\Psi(r) = e^{-r/2}$ or $\Psi(r) = e^{-r^+}$ (Metropolis dynamics).

Equation (1.1) is equipped with a comparison principle, at least when $J \geqslant 0$, and it has one or three steady states. When intermolecular forces between the adsorbates are strong we may have coexistence of dilute and dense phases, each one corresponding to a different steady state of Eq. (1.1). For instance, when $h = -J_0/2$, (1.1) has three steady states when

$$\beta > \beta_c = \frac{4}{J_0},$$

where $J_0 = \int J(r)\,dr$. The stable states correspond to the dense and the dilute phases of the system, i.e. we have bistability. Standing waves, for $h = -J_0/2$, and traveling waves, when $h \neq -J_0/2$, but still in the presence of multiple steady states, for Eq. (1.1) exist, and are crucial for the long space/time cluster evolution analysis, since they connect high and low density phases,

across a cluster boundary. The rigorous existence, uniqueness and stability of such solutions follows from the analysis in [6], which covers a broad class of integrodifferential equations that have a comparison principle. Note that for even potentials which are not necessarily radial we obtain direction-dependent standing and traveling waves [17].

In the case of surface diffusion it can be shown [21] that $u_\gamma(x, t\gamma^{-2}) \approx u(\gamma x, t)$, and u solves (for $h = 0$)

$$u_t - \nabla \cdot \left\{ \mu[u] \nabla \left(\frac{\delta E[u]}{\delta u} \right) \right\} = 0, \tag{1.2}$$

where $\mu[u]$ is the mobility and $E[u]$ is the free energy,

$$E[u] = -\frac{1}{2} \iint J(r - r') u(r) u(r')\, dr\, dr' + \int \frac{1}{\beta} \big[u \ln u + (1-u) \ln(1-u) \big]\, dr.$$

In the case of Metropolis/Kawasaki dynamics (1.2) was derived in [21] where the mobility is $\mu[u] = \Psi(0)\beta u(1-u)$. Typical choices of Ψ's associated with the microscopic diffusion dynamics are $\Psi(r) = 2(1+e^r)^{-1}$ (Kawasaki dynamics) and $\Psi(r) = e^{-r^+}$ (Metropolis dynamics).

Note that in both types of equations the coverage u satisfies $0 \leqslant u \leqslant 1$ due to the presence of the term $u(1-u)$ in the mobilities, which enforces the exclusion principle (i.e. at most one particle per lattice site) at the mesoscopic level. Equation (1.2) includes two competing mechanisms: a diffusion term associated with the entropy in $E[u]$, which competes with the attractive potential $J \geqslant 0$. We expect that when the inverse temperature β is large enough ($\beta \geqslant \beta_c$), the particles will tend to organize in clusters, overcoming the diffusive effects. These heuristics can become more clear using a linearization argument around a constant coverage u_0, yielding a regime of *spinodal decomposition* [19].

1.3.1. Mesoscopic models for multiple micromechanisms

Typically surface processes take place simultaneously and interact. For instance we can consider [14,18] a combination of Arrhenius adsorption/desorption dynamics, Metropolis surface diffusion and simple unimolecular reaction; the corresponding mesoscopic equation is:

$$u_t - D\nabla \cdot \big[\nabla u - \beta u(1-u) \nabla J_m * u \big] - \big[k_a p(1-u) - k_d u \exp(-\beta J_d * u) \big] + k_r u = 0. \tag{1.3}$$

Here D is the diffusion constant, k_r, k_d and k_a denote, respectively the reaction, desorption and adsorption constants and p is the partial pressure of the gaseous species. The partial pressure p is related to the external field h in (1.1) and here is assumed to be a constant, although realistically it is given by the fluids equations in the gas phase. The steady states of (1.3) and (1.1) are identical and when $J_d = J_m$ and $k_r = 0$, they also share the same standing wave. However there are no general rigorous results available on the existence of traveling waves for (1.3); some numerical simulations were carried out in [14] indicating the existence of *nonmonotone* traveling waves. Finally, it is easy to see that, when $k_r = 0$, the free energy $E[u]$ is a Lyapunov functional for (1.3).

1.3.2. Relation to the Cahn–Hilliard and Allen–Cahn models

Next we briefly discuss the connections of the mesoscopic equations with well-known models for phase separation such as the Allen–Cahn and the Cahn–Hilliard models. If we rescale space

as $x \mapsto x/\epsilon$ the potential J gives rise to the approximation of the Dirac distribution $J^\epsilon(x) = \epsilon^{-d} J(\frac{x}{\epsilon})$. Then after a simple change of variables and formally expanding in Taylor series,

$$J^\epsilon * u(x) = \int J(z)u(x+\epsilon z)\,dz = \int J(z)\left[u(x) + \epsilon \nabla u(x)\cdot z + \frac{\epsilon^2}{2} z^T \nabla^2 u(x) z + O\big(\epsilon^3\big)\right] dz.$$

Ignoring the $O(\epsilon^3)$ terms and assuming that J is radially symmetric, i.e. $J(r) = J(|r|)$, we have that

$$J^\epsilon * u(x) \approx J_0 u(x) + \frac{\epsilon^2}{2} J_2 \Delta u(x),$$

where $J_0 = \int J(r)\,dr$ and $J_2 = \int |r|^2 J(r)\,dr$. Then, for instance (1.1), is approximated by a version of the Allen–Cahn equation with nonlinear diffusion,

$$u_t = Du \exp(-\beta J_0 u)\Delta u + c_0\big[1 - u - \exp(-\beta h)u\exp(-\beta J_0 u)\big],$$

where $D = c_0 \frac{\epsilon^2}{2}\beta J_0 \exp(-\beta h)$. Note that the function $f(u) = 1 - u - \exp(-\beta h)u\exp(-\beta J_0 u)$ is bistable or equivalently is the derivative of a double well potential when $\beta > \beta_c = 4/J_0$. We remind the reader that the Allen–Cahn equation has the nondimensional form

$$u_t = \Delta u + W'(u),$$

where W is the double well potential $W(u) = (u^2 - 1)^2$.

In the case of the surface diffusion we can rewrite the free energy as

$$E[u] = \frac{1}{4}\iint J(r - r')\big[u(r) - u(r')\big]^2\,dr\,dr' + \int W_\beta(u)\,dr,$$

$W_\beta(u) = \frac{1}{2} J_0 u(1-u) + \frac{1}{\beta}[u\ln u + (1-u)\ln(1-u)]$. W_β is a double-well potential provided $\beta > \beta_c = 4/J_0$. Then, rescaling and expanding the convolution as before we have that

$$E[u] \approx \tilde{E}[u] := \int \frac{\epsilon^2 J_2}{8}|\nabla u|^2 + W_\beta(u)\,dr, \tag{1.4}$$

after omitting the higher order terms. This is the standard Ginsburg–Landau functional, in which case (1.2) becomes a Cahn–Hilliard-type equation

$$u_t - \nabla\cdot\left\{\mu[u]\nabla\left(\frac{\delta\tilde{E}[u]}{\delta u}\right)\right\} = 0, \tag{1.5}$$

with nontrivial mobility $\mu(u) = Du(1-u)$; recall that in the standard Cahn–Hilliard model $\mu(u) = 1$. Notice that the truncations in the gradient expansions used here disregard higher order effects as well as possible anisotropies in the potential J. However, in the vicinity of the critical temperature the Allen–Cahn and Cahn–Hilliard equations become exact rescaled limits of the mesoscopic models and the underlying particle systems.

1.3.3. A simplified model with multiple microscopic mechanisms

To illustrate the effects of the multiple mechanisms we consider a simplification of (1.3) which retains its fundamental structure and can be exactly obtained from rescalings of (1.2) close to the critical temperature, when $k_r = 0$ and $J_m = J_d = J$:

$$u_t = D\Delta\big(-\Delta u + W'(u)\big) + \Delta u - W'(u), \tag{1.6}$$

W is a double-well potential with wells ± 1, the Cahn–Hilliard term corresponds to surface diffusion, while the Allen–Cahn to adsorption/desorption. We refer to (1.6) as a scalar CH/AC equation.

1.4. Mathematical structure of the scalar CH/AC equation

In the sequel of the paper we study in a rigorous fashion the behavior of the scalar CH/AC equation (1.6), as time is rescaled with ϵ^2 and space is rescaled with ϵ, which describes the long-time behavior of large clusters. Under this diffusive rescaling the equation becomes

$$\begin{cases} \partial_t u = \epsilon^2 D\left(-\Delta\left(\Delta u + \dfrac{f(u)}{\epsilon^2}\right)\right) + \Delta u + \dfrac{f(u)}{\epsilon^2}, \\ u = 1, \quad \text{on } \partial\Omega, \\ u(0,x) = u_0(x), \end{cases} \tag{1.7}$$

where $\Omega \subset \mathbf{R}^N$, $N > 1$, is a smooth, bounded domain.

First we present some remarks on the mathematical structure of (1.6) and (1.7). The free energy

$$F_\epsilon(u) := \frac{1}{2}\int_\Omega \epsilon|\nabla u|^2 + \int_\Omega \frac{1}{\epsilon} W(u) \tag{1.8}$$

equals $\epsilon^{-1}\tilde{E}[u]$, where $\tilde{E}[u]$ is as in (1.4)—up to different coefficients which do not affect qualitative properties. Equation (1.7) is (up to a rescaling in time) a gradient flow for the energy (1.8) with respect to the metric

$$\langle f, g\rangle_{A^\epsilon} := \big\langle f, \big(A^\epsilon\big)^{-1} g\big\rangle, \tag{1.9}$$

where $\langle\cdot,\cdot\rangle$ denotes the L^2-scalar product and

$$A := -D\Delta + I, \quad (Af)(x/\epsilon) = A^\epsilon\big(f(x/\epsilon)\big)$$

are self-adjoint operators w.r.t. to the L^2-scalar product. In particular

$$A^\epsilon = -\epsilon^2 D\Delta + I,$$

i.e. it is a small perturbation of the identity operator, provided the second derivatives are bounded.

Let

$$\mathcal{A}^\epsilon(u) := \Delta u + \epsilon^{-2} f(u), \quad f(u) = -W'(u). \tag{1.10}$$

The Allen–Cahn equation, see [1], becomes under a diffusive rescaling of space and time

$$\partial_t u = \mathcal{A}^\epsilon(u). \tag{1.11}$$

The equation under consideration in this paper, (1.7) has the structure

$$\partial_t u = A^\epsilon\big(\mathcal{A}^\epsilon(u)\big).$$

So (1.7) is *formally* a small (yet singular) perturbation of (1.11), and one could expect that the limit evolution will be described by the same limit evolution as the Allen–Cahn equation, i.e. by motion by mean curvature: $u \to \pm 1$ a.e., and the interface which bounds the region where u is negative moves according to

$$V = \kappa,$$

where V is the velocity of the interface in normal direction, and κ the mean curvature of the interface.

However, the small perturbation by a higher order term becomes relevant close to the interface, where the derivatives of u become large. Therefore, we find qualitatively the same behavior, i.e. motion by mean curvature, but with different coefficients.

We actually obtain

$$V = \mu\sigma\kappa, \tag{1.12}$$

here μ is an effective mobility and σ the surface tension. In order to define μ and σ, we need the standing wave for the one-dimensional Allen–Cahn equation, i.e. a solution (unique up to translations) $q : \mathbf{R} \to (-1, 1)$ of

$$\partial_{zz}^2 u = -f(u), \qquad \lim_{z\to\pm\infty} u(z) = \pm 1.$$

Then μ is given by

$$\mu = 2\bigg(\int_{\mathbf{R}} \chi\,\partial_z q\bigg)^{-1}, \tag{1.13}$$

where χ is defined as

$$A\chi = \partial_z q. \tag{1.14}$$

The mobility is completely different from the Allen–Cahn equation, where the corresponding expression equals [22],

$$2\bigg(\int_{\mathbf{R}} \partial_z^2 q\bigg)^{-1}.$$

Later we will show that the mobility μ is *larger* than the one for the Allen–Cahn equation, i.e. the underlying diffusion mechanism speeds up the cluster evolution. The surface tension σ is defined as [22]

$$\sigma = \int_{-1}^{1} \sqrt{(1/2)W(s)}\, ds = \frac{1}{2}\int_{\mathbf{R}} |\partial_z q|^2$$

which is the same as for the Allen–Cahn equation.

The mobility by using a linear response argument is defined in the following way: look for one-dimensional solutions of

$$\partial_t u = \epsilon^2\left(-D\Delta\left(\Delta u - \frac{f(u)}{\epsilon^2}\right)\right) + \Delta u - \frac{f(u)}{\epsilon^2} + \epsilon^{-1}h, \tag{1.15}$$

i.e. a small forcing is added to f. The solution will be of the form $u(t,x) = q(c(h)t - x) + \mathcal{O}(\epsilon)$, and the function $c(h)$ is (at least at highest order) of the form

$$c(h) = \mu h,$$

which defines the mobility.

In order to find a quantitative expression of the mobility in terms of the one-dimensional profile q, we will need the linearization of (1.7) around a function u:

$$\mathcal{L}_u v := A\big(\Delta v + f'(u)v\big), \qquad \mathcal{L}^\epsilon v := A^\epsilon\big(\Delta v + \epsilon^{-2} f'(u)v\big), \tag{1.16}$$

where $A = -D\Delta + I$ is as above.

For further use we define for $Q(z) \in L^2(\mathbf{R})$ the one-dimensional linear operator

$$\mathcal{L}_1 Q := -D\partial_z^2\big(\partial_z^2 Q + f'\big(q(z)\big)Q\big) + \partial_z^2 Q + f'\big(q(z)\big)Q. \tag{1.17}$$

Note that $\mathcal{L}_1 = A\mathcal{M}$, where

$$\mathcal{M} := \partial_z^2 + f'\big(q(z)\big)$$

is the linearized Allen–Cahn operator.

Now (1.13) can be understood from the following formal asymptotics:

$$c\partial_z q - h = \mathcal{L}_1^\epsilon Q,$$

and the Fredholm solvability condition gives (see for a rigorous derivation Section 2.2)

$$c\int_{\mathbf{R}} \chi\, \partial_z q = \int_{\mathbf{R}} \chi,$$

and as

$$\int_{\mathbf{R}} \chi = \int_{\mathbf{R}} \partial_z q + \underbrace{\int_{\mathbf{R}} \Delta\chi}_{=0} = 1 - (-1) = 2,$$

we obtain

$$c = 2\left(\int_{\mathbf{R}} \chi\, \partial_z q \right)^{-1} h,$$

$$\mu\sigma = \frac{\int_{-\infty}^{\infty} \partial_z^2 q\, d\xi}{\int_{-\infty}^{\infty} \partial_z q\, \chi\, d\xi}. \tag{1.18}$$

Note that by testing

$$-D\partial_{zz}^2 \chi + \chi = \partial_z q$$

with the solution χ we obtain

$$\int \chi^2 \leqslant \int |\partial_z \chi|^2 + \int \chi^2 \leqslant \|\chi\|_2 \|\partial_z q\|_2,$$

and therefore

$$\|\chi\|_2 \leqslant \|\partial_z q\|_2.$$

This implies that

$$\int \chi\, \partial_z q = \int |\partial_z \chi|^2 + \int \chi^2 \leqslant \|\chi\|_2 \|\partial_z q\|_2 \leqslant \|\partial_z q\|_2^2,$$

and therefore

$$\mu\sigma = \frac{\int_{-\infty}^{\infty} \partial_z^2 q\, d\xi}{\int_{-\infty}^{\infty} \partial_z q\, \chi\, d\xi} \geqslant 1,$$

so that the diffusion speeds up the mean curvature flow. Note that for $D = 0$, Eq. (1.14) implies that $\partial_z q = \chi$, that is $\mu\sigma = 1$ which corresponds to the Allen–Cahn equation.

While the limit evolution is—up to coefficients—the same as for the Allen–Cahn equation, the mathematical treatment is necessarily quite different, because the Allen–Cahn equation has a comparison principle, while (1.7) lacks this important property. The limit evolution, on the other hand, has a comparison principle. Hence our Eq. (1.7) is a nonmonotone approximation of a monotone evolution law. Therefore the powerful tools for passing to the limit as $\epsilon \to 0$ beyond singularities of the limit evolution, which are based on the comparison principle (see e.g. [3]) are unavailable in our case. Instead, we show convergence until the first singularity of the limit evolution occurs by making a formal asymptotic expansion rigorous with the help of linear stability, in the spirit of [2].

1.5. Results

In the sequel we study rigorously the scalar CH/AC equation for $D = 1$. Let $\Omega_0 \subset \Omega$ be a compact set with smooth domain, and let $\hat{T}$ be the first time at which the evolution of the boundary $\partial\Omega(t)$, which is determined by (1.12), becomes singular. Let $d(t, x)$ be the signed distance from $\Omega(t)$.

The main theorems are:

Theorem 1.1.

(1) *For any $k > 0$ and any $T < \hat{T}$ there are functions $\bar{u}^{(k)}(t, x)$ such that they solve* (1.7) *up to a right-hand side (residual) $r(\epsilon, k)$ such that*

$$\left\| r(\epsilon, k) \right\|_{C^2} < \epsilon^k$$

for $\epsilon < \epsilon_0(k, T)$ and $t \in [0, T)$.

(2) *Moreover, there exists $C > 0$ and a function $d(t, x, \epsilon)$ such that for $t \in [0, T)$ $\lim_{\epsilon \to 0} |d(t, x, \epsilon) - d(t, x)| = 0$ and*

$$\left| \bar{u}^{(k)}(t, x) - q\left(\epsilon^{-1} d(t, x, \epsilon)\right) \right| \leqslant C\epsilon.$$

Theorem 1.2. *Let $T < \hat{T}$. Then there exists $k, k_0 \in \mathbb{N}$, such that for any $k > k_0$ there exists $\delta = \delta(k)$ with both δ, k depending on the space dimension and ϵ_0 and C depending on T (through the distance from the singular time $\hat{T}$) such that if*

$$\left\| \bar{u}^{(k)}(0, x) - u(0, x) \right\|_{\infty} < \epsilon^k$$

then for any $0 < t \leqslant T$, $\epsilon < \epsilon_0$ and $p = \frac{2(N+4)}{N+2}$, it holds that

$$\left\| \bar{u}^{(k)}(t, x) - u(t, x) \right\|_{L^p} < \epsilon^{\delta}.$$

Following the lines of [2] one can improve this estimate in order to get convergence in C^l, $l \in \mathbb{N}$, if the order of approximation k is taken sufficiently large. Then one gets the following sharp interface limit as a corollary:

Theorem 1.3. *For any $\delta > 0$ and any $T < \hat{T}$ there exist functions $u_0(x)$ such that the solution $u(t, x)$ of* (1.7) *starting from $u_0(x)$ has the property that $u(t, x) > 0$ for $\operatorname{dist}(x, \Omega(t)) > \delta$ and $u(t, x) < 0$ for $\operatorname{dist}(x, \Omega^c(t)) > \delta$ i.e. the zero level set of the solution is close to an interface which evolves by the limit evolution.*

Essentially, Theorem 1.2 is a consequence of Theorem 1.1 and the following spectral estimate:

Theorem 1.4. *There exists $\lambda_0 > 0$ such that for $u = \bar{u}^{(k)}$ as in Theorem* 1.1 *and for all test functions $f \in H_0^{1,2}(\Omega)$*

$$\left\langle f, A^{\epsilon}\left(\Delta + \epsilon^{-2} f'(u)\right) f \right\rangle_{A^{\epsilon}} = \left\langle f, \left(\Delta + \epsilon^{-2} f'(u)\right) f \right\rangle \leqslant \lambda_0 \| f \|_{A^{\epsilon}}. \tag{1.19}$$

1.6. Structure of the paper

The paper is organized as follows. In Section 2 we show that for any required order of the residual in the small parameter ϵ, we can construct asymptotic solutions which have a residual that is of this order. Naturally, we will need many terms in the expansion. Luckily it is not necessary to construct them explicitly, because it can be shown by induction that they have a certain structure, which allows the use of Fredholm's alternative in order to obtain existence and regularity. Following e.g. [4] we treat fast variable (normal to the limit interface) and slow variable (tangential to the interface) as independent variables in $\mathbf{R}^{N+1}$. This allows us to avoid the complications arising from the use of a coordinate system on the limit interface. The approximate solutions converge to ± 1 in the interior and exterior, respectively, of a set whose boundary evolves by the limit evolution law $V = (\mu\sigma)\kappa$.

In Section 3 we show a limit theorem for developed interfaces in the spirit of [2,4,9]: If the approximate solution constructed in Section 2 has a sufficiently small residual, then any solution of Eq. (1.7) with initial condition u_0 sufficiently close to the initial condition will stay close to the approximate solution on the macroscopic timescale, as long as the limit evolution (mean curvature flow) does not encounter a singularity. In order to show this, we make use of the stability of the linearization around the approximate solution. We prove the stability by adapting the result obtained by Chen [5] for the Allen–Cahn equation to our situation where we deal with the scalar CH/AC equation.

2. Asymptotic expansions

In this section Theorem 1.1 is shown with the help of asymptotic expansions, following e.g. [2,9,10,16].

This is done in several steps: First, an approximate solution in a neighborhood of a smooth interface is constructed by expanding around the standing wave profile. Here we use a fast and a slow variable, because the gradients are large. For the same reason the inner expansion will be very different from the one for Allen–Cahn equation: the fourth-order term becomes relevant.

Away from the interface we should in principle expand around ± 1. However, this expansion becomes trivial as we obtain immediately the constant functions ± 1.

The solutions for the inner expansion converge exponentially fast towards their limits as the fast variable tends to $\pm\infty$. This allows to construct the approximate solution by interpolating between inner and outer solution with a cut-off function.

2.1. Inner expansion

We look for approximate solutions of this form:

$$u_i^{M,\epsilon} = q\left(\frac{d^{(0)}(x,t) + \sum_{k=1}^{M} \epsilon^k d^{(k)}(x,t)}{\epsilon}\right) + \sum_{k=1}^{M} \epsilon^k Q^{(k)}\left(\frac{\sum_{k=1}^{M} \epsilon^k d^{(k)}(x,t)}{\epsilon}, x\right), \quad (2.20)$$

where

$$d(x,t,\epsilon) = \sum_{k=0}^{M} \epsilon^k d^{(k)}(x,t)$$

and such that

$$\partial_t u_i^{M,\epsilon} - A^\epsilon\big(\mathcal{A}^\epsilon\big(u_i^{M,\epsilon}\big)\big) = r(\epsilon, M) = O\big(\epsilon^{M-1}\big),$$
$$\big|\nabla d(x,t,\epsilon)\big| - 1 = O\big(\epsilon^M\big). \tag{2.21}$$

We will show existence of $u_i^{M,\epsilon}$ for arbitrary M by induction. In order to do so, it is convenient to follow [4] or [9] and look for $Q^{(k)}(z,x)$, where the fast variable z is in $\mathbf{R}$ and the slow variable x is in a fixed neighborhood of the interface, i.e. in a subset of Ω. This means that we rewrite (1.7) replacing the differential operator ∂_x by

$$\partial_x + \epsilon^{-1}\partial_z$$

and collect terms of same order in ϵ. For each of these terms, we will use the solvability condition obtained from Fredholm's alternative in z and treat x as a parameter.

Of course z and x are not independent variables, but related by

$$\epsilon z - d(x,t,\epsilon) = 0.$$

This will lead to the necessity of adding additional terms of the form

$$g(x,t,\epsilon)\eta(z)\big(z - \epsilon^{-1}d(x,t,\epsilon)\big)$$

to the equation. Here η is a cut-off function which vanishes as $|z| \to \infty$. Note that this does not affect the equation in the "physical" region $\epsilon z - d(x,t,\epsilon) = 0$. Of course

$$g(x,t,\epsilon) = \sum \epsilon^k g^{(k)}(x,t).$$

At order ϵ^{-2} we obtain

$$\partial_z^2 q + f(q) = 0,$$

which justifies (and enforces) the choice of the standing wave q as highest order term in the inner expansion.

2.2. *The first order*

At order ϵ^{-1} we get

$$\partial_z q\big(d_t^{(0)} - \Delta d^{(0)}\big) + \partial_z^3 q\,\Delta d^{(0)} - \eta(z) g^{(0)} d^{(0)} = \mathcal{L}^{(1)} Q^{(1)}, \tag{2.22}$$
$$\big|\nabla d^{(0)}\big|^2 = 1, \tag{2.23}$$

where q and $Q^{(1)}$ are functions of the fast variable $z \in \mathbf{R}$, Δ is the Laplace operator in x. We consider Eq. (2.22) as an equation in z with x and t as parameters. Equation (2.22) is solvable

and has a smooth and exponentially decaying solution (as $|z| \to \infty$) if for all $\chi \in \operatorname{Ker}((\mathcal{L}^{(1)})^*)$ it holds that

$$\chi \perp \left(\partial_z q\left(d_t^{(0)} - \Delta d^{(0)}\right) + \partial_z^3 q \Delta d^{(0)} - \eta(z) g^{(0)} d^{(0)}\right). \tag{2.24}$$

$(\mathcal{L}^{(1)})^* \chi = 0$ if and only if

$$\mathcal{M}\left(-\partial_z^2 \chi + \chi\right) = 0,$$

where $\mathcal{M}$ is the linearized Allen–Cahn operator. Using that $\operatorname{Ker} \mathcal{M} = \partial_z q \mathbf{R}$ we obtain

$$-\partial_z^2 \chi + \chi = a \partial_z q$$

for some $a \in \mathbf{R}$. By linearity it suffices to solve

$$-\partial_z^2 \chi + \chi = \partial_z q. \tag{2.25}$$

(This is uniquely solvable, and by the maximum principle for the operator $-\partial_z^2 + I$ we get $\chi > 0$.)

Thus $\operatorname{Ker} \mathcal{L}^* = \chi \mathbf{R}$ where χ solves (2.25). Now returning back to Eq. (2.22), this equation is solvable for $Q^{(1)}$ if and only if (2.24) holds. That is:

$$\left(\int_{-\infty}^{\infty} \partial_z q \chi \, dz\right) d_t - \left[\int_{-\infty}^{\infty} \partial_z q \chi \, dz - \int_{-\infty}^{\infty} \partial_z^3 q \chi \, dz\right] \Delta d^{(0)} = g^{(0)} d^{(0)} \underbrace{\int_{-\infty}^{\infty} \chi \eta \, dz}_{c}.$$

Using that

$$\int_{-\infty}^{\infty} \partial_z q \left(\chi - \partial_z^2 \chi\right) dz = \int_{-\infty}^{\infty} \partial_z^2 q \, dz$$

and

$$\chi - \partial_z^2 \chi = \partial_z q,$$

we finally obtain

$$\mu^{-1} \partial_t d^{(0)}(x,t) = \sigma \Delta d^{(0)}(x,t) + c g^{(0)}(x,t) d^{(0)}(x,t),$$

where $c = \int_{\mathbf{R}} \chi \eta$.

From (2.23) we derive that for any t, the set $\{x \in \Omega\colon\ d^{(0)}(x,t) = 0\}$ is a hypersurface, where $d^{(0)}$ is the distance from it. On this hypersurface we obtain the limit free boundary problem,

$$V = \mu \sigma \kappa, \quad \mu\sigma \text{ as in (1.18)},$$

because there $d^{(0)}(x,t) = 0$, $\partial_t d^{(0)}(x,t) = V$ and $\Delta d^{(0)}(x,t) = \kappa$. But for x away from the interface, i.e. $d^{(0)} \neq 0$, we could not solve this without g. But as the curvature of parallel surfaces

is a smooth function of the distance and the second fundamental form of the surface, we can solve the equation in a ϵ-independent neighborhood of the interface by choosing

$$g^{(0)}(x,t) := \mu\sigma\big[\Delta d^{(0)}\big(Pr_{\partial\Omega(t)}(x),t\big) - \Delta d^{(0)}(x,t)\big]/\big(cd^{(0)}(x,t)\big).$$

Here $Pr_{\partial\Omega(t)}(x)$ is the projection of the point x on the interface $\partial\Omega(t)$. Hence the solvability condition can be fulfilled for all x, in a neighborhood of the limit interface which does not depend on ϵ.

The cut-off function η has the following purpose: if $|z|\to\infty$, then the equation at each level of ϵ, if considered as equation in x with z as a parameter, should converge to the corresponding equation without the correction term in order to obtain exponential convergence of $Q^{(1)}(z)$ as $|z|\to\infty$.

2.3. The higher orders

Let $k \geqslant 1$. At order ϵ^{k-1} we obtain

$$\mathcal{L}^{(1)}Q^{(k+1)} = \partial_z q\big(\partial_t d^{(k)} - \Delta d^{(k)}\big) - \eta(z)\big(g^{(k)}d^{(0)} + g^{(0)}d^{(k)}\big) + R^{(k)}, \tag{2.26}$$

and from (2.21) at order ϵ^k

$$\nabla d^{(k)}\nabla d^{(0)} = B^{(k)}. \tag{2.27}$$

$R^{(k)}$ depends only on the already known $Q^{(1)}(z,x,t),\dots,Q^{(k)}(z,x,t)$, $d^{(0)}(x,t),\dots,d^{(k-1)}(x,t)$, $g^{(0)}(x,t),\dots,g^{(k-1)}(x,t)$, and $B^{(k)}$ only on $d^{(0)}(x,t),\dots,d^{(k-1)}(x,t)$.

We make the *inductive assumption* that $Q^{(1)}(z,x,t),\dots,Q^{(k)}(z,x,t)$, $d^{(0)}(x,t),\dots,d^{(k-1)}(x,t)$, $g^{(0)}(x,t),\dots,g^{(k-1)}(x,t)$ exist, are *smooth*, and, moreover, the $Q^{(l)}$ decay exponentially as $|z|\to\infty$ uniformly in x,t. Note that it holds for $Q^{(1)}$, because $\partial_z q(z)$ decays exponentially.

The solvability condition

$$\partial_z q\big(\partial_t d^{(k)} - \Delta d^{(k)}\big) - \eta(z)\big(g^{(k)}d^{(0)} + g^{(0)}d^{(k)}\big) + R^{(k)} \perp \operatorname{Ker}\big(\mathcal{L}^{(1)}\big)^*$$

and Eq. (2.27) yield

$$\mu^{-1}\partial_t d^{(k)}(x,t) = \sigma\Delta d^{(k)}(x,t) + cg^{(0)}(x,t)d^{(k)}(x,t) + \hat{R}^{(k)}(x,t), \quad \text{on } \big\{d^{(0)}=0\big\}, \tag{2.28}$$

$$\nabla d^{(k)}\nabla d^{(0)} = B^{(k)} \quad \text{on } U_\delta, \tag{2.29}$$

$$g^{(k)}(x,t) = \big(d^{(0)}(x,t)\big)^{-1}l(x,t) \quad \text{on } U_\delta\setminus\big\{d^{(0)}=0\big\}, \tag{2.30}$$

where U_δ is a δ-neighborhood of the limit interface for some small δ which depends on the interface, but not on ϵ, and

$$l(x,t) = \mu^{-1}\partial_t d^{(k)}(x,t) - \sigma\Delta d^{(k)}(x,t) + cg^{(0)}(x,t)d^{(k)}(x,t) + \hat{R}^{(k)}(x,t).$$

Note that $l(x,t)=0$ on $\{d^{(0)}=0\}$ by (2.28).

This system has a smooth solution $d^{(k)}$, $g^{(k)}$: first note that by using (2.29) Eq. (2.28) can be re-written as a *linear* parabolic PDE for $d^{(k)}$ on the smooth manifold $\{d^{(0)}=0\}$. This PDE on the

manifold has a unique, smooth solution. By the method of characteristics (2.29) can be solved to define $d^{(k)}$ in the entire neighborhood U_δ. It remains to solve for $g^{(k)}$. Obviously $g^{(k)}$ is defined uniquely away from the interface, it remains to show that it is sufficiently smooth everywhere. This follows from the following lemma, which is cited as Corollary 6.5 in [8]:

Lemma 2.1. *If $f \in C^k(\mathbf{R}^n)$, $d(x)$ the distance to a smooth interface, and $f(x) \to 0$ as $d(x) \to 0$, then the equation $hd = f$ has a solution $h \in C^{k-2}$.*

Idea of proof: Use Taylor-expansion of f around a point on the interface, and switch to tangential and normal coordinates at that point. The hypotheses of the lemma implies that one can factor out d in the Taylor series, and h is C^{k-2} up to the boundary.

Thus $d^{(k)}$, $g^{(k)}$, $Q^{(k+1)}$ exist and satisfy the same properties that were assumed of $d^{(k-1)}$, $g^{(k-1)}$, $Q^{(k)}$, and we can conclude by induction.

2.4. Construction of the approximate solution

As $q(z) \to \pm 1$ exponentially fast as $z \to \pm\infty$, and the Q^k and their derivatives converge exponentially fast to zero as $|z| \to \infty$, it is sufficient to choose the constant functions $u_o = +1$ and $u_i = -1$ as outer expansions. Let δ be a small constant such that the distance function from $\partial\Omega(t)$ is smooth for all (x,t) such that $\operatorname{dist}(x, \partial\Omega(t)) < \delta$, $0 \leqslant t \leqslant T$. Moreover let $\zeta : \mathbf{R} \to [0,1]$ be a smooth cut-off function such that $\zeta(r) = 0$ for $r < 1$, $\zeta(r) = 1$ for $r > 2$. The function $d^{(0)}$ is again the signed distance from the limit interface $\partial\Omega(t)$. Let

$$u^{k(M)}(x,t) := \big(1 - \zeta\big(\delta^{-1}d^{(0)}\big) - \zeta\big(-\delta^{-1}d^{(0)}\big)\big)u_i^{M,\epsilon}(x,t) + \zeta\big(\delta^{-1}d^{(0)}\big) - \zeta\big(-\delta^{-1}d^{(0)}\big).$$

This satisfies the boundary conditions. (The assumption that the limit evolution does not encounter a singularity implies that the free boundary $\partial\Omega(t)$ does not touch $\partial\Omega$.) Moreover, because of the exponential convergence of the $Q^{(k)}$ and their derivatives, the residual of $u^{k(M)}$ differs at most by one order from the residual of $u_i^{M,\epsilon}$.

3. Proofs of Theorems 1.2–1.4

Let $R^\epsilon := \bar{u}^{(k)} - u$, where u is a solution of (1.7) and $\bar{u}^{(k)}$ is the approximate solution. The aim is to show that there exists a function $C(T)$ which is independent of ϵ such that

$$\big\|R^\epsilon(T)\big\| \leqslant C(T)\big\|R^\epsilon(0)\big\| + C_\epsilon$$

where $C_\epsilon \to 0$ as $\epsilon \to 0$ for any $T < \hat{T}$ and the norm can be L^p or L^∞, etc. This will prove Theorem 1.2.

Note. $R^\epsilon(0)$ can be assumed small if we restrict to "nice" initial conditions (developed interfaces in the language of [2]). Hence $\|R^\epsilon(T)\| \to 0$ as $\epsilon \to 0$. We will from now on make the simplifying assumption that $R^\epsilon(\cdot,0) = 0$, the extension to the case of $\|R^\epsilon(\cdot,0)\|_p$ sufficiently small is straightforward.

From now on we drop the superscript k and simply write $\bar{u}$ for the approximate solution and u for the actual solution.

Lemma 3.1. *Let $R^\epsilon := \bar{u}^{(k)} - u$ as above, then*

$$\partial_t R^\epsilon = A^\epsilon\big(\mathcal{A}^\epsilon(\bar{u}) - \mathcal{A}^\epsilon(u)\big) + r(k,\epsilon) = \mathcal{L}^\epsilon_{\bar{u}} R^\epsilon + \hat{\mathcal{N}}_\epsilon\big(R^\epsilon\big) + r(k,\epsilon) \tag{3.31}$$

where $\mathcal{L}_{\bar{u}}$ is as in (1.16)*,*

$$\hat{\mathcal{N}}_\epsilon\big(R^\epsilon\big) = \big(-\epsilon^2\Delta + I\big)\mathcal{N}_\epsilon,$$

$$\mathcal{N}_\epsilon = \frac{1}{\epsilon^2}\int_0^1 f\big(\bar{u} + sR^\epsilon\big)\,ds\big(R^\epsilon\big)^2$$

is the linearization error, and $r(k,\epsilon)$ is the residual of the approximate solution given in Theorem 1.1.

Proof. A direct consequence of Theorem 1.1 and the Taylor expansion of the nonlinearity f around $\bar{u}$. □

Remark. We linearize around $\bar{u}$, not about q. The spectral properties should be the same for the linearization around q, as both operators are very close. But the new operator may have small eigenvalues of wrong sign. Chen's theorems in [5] cover the case of linearization around a sufficiently small perturbation of q and apply in our case.

For the sake of simplicity, we drop the ϵ and write R instead of R^ϵ.
From the bounds on the approximate solution we get

Theorem 3.1. *Let $p \in [2,3]$, there exists a positive constant C_p depending only on p, $\|f\|_{C^2([-3C_0,3C_0])}$ and C_0 such that the quantity $\mathcal{N}$ satisfies*

$$R\mathcal{N}(u,R) \leqslant C_p|R|^p, \quad \forall u \in [-C_0, C_0],\ R \in \mathbf{R}.$$

Proof. We refer to [2] for the proof. □

Testing (3.31) with R in appropriate, i.e. $\langle\,,\rangle_{A^\epsilon}$ scalar product (or equivalently testing with $\Psi = A^{-1}R$ in the L^2 scalar product), we obtain

$$\begin{aligned}\frac{1}{2}\partial_t\big\|R(t)\big\|^2_{A^\epsilon} &\leqslant \epsilon^{-1}\big\langle\epsilon\Delta R + \epsilon^{-1}f'(q)R, R\big\rangle_{L^2} + \big\langle\mathcal{N}_\epsilon(R), R\big\rangle_{L^2} + \big\langle r(k,\epsilon), R\big\rangle_{A^\epsilon}\\ &= \text{(I)} + \text{(II)} + \text{(III)}.\end{aligned} \tag{3.32}$$

By Lemma 3.1 we obtain

$$\text{(II)} \leqslant C_p\|R\|_p^p.$$

Moreover by the Hölder inequality and $\|A^{-1}R\|_p \leqslant C\|R\|_p$ we immediately get

Lemma 3.2 *(Estimate on the remainder).*

$$\langle r(k,\epsilon), u^\epsilon \rangle \leqslant \|r(k,\epsilon)\|_{L^{p*}} \|u^\epsilon\|_{L^p},$$

where p^* is the exponent which is dual to p.

Hence,

$$\frac{1}{2}\partial_t \|R(t)\|_{A^\epsilon}^2 \leqslant \int -|\nabla R|^2 + \epsilon^{-2}\int f'(q)(R)^2 + \|R\|_p\big(\epsilon^{-2}\|R\|_p^{p-1} + \|r(k,\epsilon)\|_{L^{p*}}\big). \tag{3.33}$$

Now note that Theorem 1.4 implies

$$-\int |\nabla R|^2 + \epsilon^{-2}\int f'(q)R^2 \leqslant \lambda_0 \|R(t)\|_{A^\epsilon}^2.$$

Therefore we can apply Gronwall's inequality, which yields

$$\sup_{t\leqslant T}\|R(t)\|_{A^\epsilon}^2 \leqslant C(T)\|R\|_{L^p([0,t]\times\Omega)}\big(\epsilon^{-2}\|R\|_{L^p([0,t]\times\Omega)}^{p-1} + \|r(k,\epsilon)\|_{L^{p*}([0,t]\times\Omega)}\big). \tag{3.34}$$

We need an estimate for $\|\nabla R\|_2$. In order to simplify notation, set

$$\|\cdot\|_{L^p(\Omega)} = \|\cdot\|_p, \qquad \|\cdot\|_{L^p([0,t]\times\Omega)} = \|\cdot\|_{p,t}.$$

Since

$$-\epsilon^{-2}\int_0^t\int_\Omega f'(\bar u)R^2 \leqslant \epsilon^{-2}\|R\|_{p,t}^2\big|\{f'(\bar u)<0\}\big|^{1-\frac{2}{p}}\max_{s\leqslant C_0}|f'(s)| \leqslant C\epsilon^{-\frac{2}{p}}\|R\|_{p,t}^2, \tag{3.35}$$

where $|A|$ denotes the Lebesgue measure of the set A. Integrating (3.33) over $(0,t)$, $t\in(0,T]$, yields

$$\|\nabla R\|_{2,t}^2 \leqslant C\epsilon^{-2}\|R\|_{p,t}\big[\epsilon^{-\frac{2}{p}}\|R\|_{p,t} + \epsilon^2\|r(k,\epsilon)\|_{p*,t} + \|R\|_{p,t}^{p-1}\big]. \tag{3.36}$$

Since we use Dirichlet boundary conditions and $p = \frac{2(N+4)}{N+2}$, the Sobolev imbedding theorem implies that:

$$\|R\|_p^p \leqslant C_p\|R\|_2^{\frac{8}{N+2}}\|\nabla R\|_2^{\frac{2N}{N+2}}.$$

Also, note that

$$\begin{aligned}\|R\|_2^2 &= -\int_\Omega R\big(\epsilon^2\Delta - I\big)\big(A^{-1}R\big) = \int_\Omega \epsilon^2\nabla R, \nabla\big(A^{-1}R\big) + \int R\big(A^{-1}R\big)\\ &\leqslant \big(\|(\epsilon\nabla R)\|_2 + \|R\|_{A^\epsilon}\big)\|R\|_{A^\epsilon}.\end{aligned} \tag{3.37}$$

The strategy is to derive from the Sobolev imbedding theorem and by using (3.36) and (3.34) a recursive inequality for $\|R\|_{p,t}$. We estimate

$$\begin{aligned}\|R\|_{p,t}^p &\leqslant C_p \int_0^t \|R\|_2^{\frac{8}{N+2}} \|\nabla R\|_2^{\frac{2N}{N+2}} \\ &\leqslant C \int_0^t \big(\|R\|_{A^\epsilon} + \|\epsilon \nabla R\|_2\big)^{\frac{4}{N+2}} \|R\|_{A^\epsilon}^{\frac{4}{N+2}} \|\nabla R\|_2^{\frac{2N}{N+2}}. \end{aligned} \tag{3.38}$$

Now note that $N \geqslant 2$, i.e. $4/(N+2) \leqslant 1$. Hence we have that for any positive numbers a, b

$$(a+b)^{\frac{4}{N+2}} \leqslant a^{\frac{4}{N+2}} + b^{\frac{4}{N+2}},$$

therefore

$$\int_0^t \|R\|_p^p \leqslant C \int_0^t \|R_\epsilon\|_{A^\epsilon}^{\frac{8}{N+2}} \|\nabla R\|_2^{\frac{2N}{N+2}} + \int_0^t \epsilon^{\frac{4}{N+2}} \|R\|_{A^\epsilon}^{\frac{4}{N+2}} \|\nabla R\|_2^{\frac{2N+4}{N+2}}.$$

By the Hölder inequality in space and by taking the supremum in time over $\|R(\cdot, s)\|_{A^\epsilon}$ we obtain (for a different constant C)

$$\int_0^t \|R\|_{A^\epsilon}^{\frac{8}{N+2}} \|\nabla R\|_2^{\frac{2N}{N+2}} \leqslant C \Big(\sup_{[0,t]} \big\|R(\cdot, s)\big\|_{A^\epsilon}^2 \Big)^{\frac{4}{N+2}} \big(\|\nabla R\|_{2,t}^2\big)^{\frac{N}{N+2}}$$

and

$$\int_0^t \epsilon^{\frac{4}{N+2}} \|R\|_{A^\epsilon}^{\frac{4}{N+2}} \|\nabla R\|_2^{\frac{2N+4}{N+2}} \leqslant C\epsilon^{\frac{4}{N+2}} \Big(\sup_{[0,t]} \big\|R(\cdot, s)\big\|_{A^\epsilon}^2 \Big)^{\frac{2}{N+2}} \|\nabla R\|_{2,t}^2.$$

Note that this term is of the same structure as the corresponding term in [2] and can be estimated in a similar way. We abbreviate

$$a = \|R\|_{p,t} \quad \text{and} \quad r = \big\|r(k, \epsilon)\big\|_{p^*,t}.$$

Then (3.34) and (3.36) yield

$$\begin{aligned} a^p &\leqslant C\big(a\big(\epsilon^{-2} a^{p-1} + r\big)\big)^{\frac{4}{N+2}} \big(\epsilon^{-2} a\big[\epsilon^{-\frac{2}{p}} a + \epsilon^2 r + a^{p-1}\big]\big)^{\frac{N}{N+2}} \\ &\quad + C\epsilon^{\frac{4}{N+2}} \big(a\big(\epsilon^{-2} a^{p-1} + r\big)\big)^{\frac{2}{N+2}} \big(\epsilon^{-2} a\big[\epsilon^{-\frac{2}{p}} a + \epsilon^2 r + a^{p-1}\big]\big). \end{aligned} \tag{3.39}$$

Define

$$T^\epsilon := \sup\big\{t \in (0, T],\ \|R\|_{L^p([0,t]\times\Omega)} \leqslant \epsilon^k\big\},$$

i.e. for $t \leqslant T^\epsilon$ we know that $a \leqslant \epsilon^k$. Now choose ϵ so small that $\epsilon^{k(p-1)} \leqslant \epsilon^k$. (Note $p > 2$.) Moreover we may (by taking sufficiently many terms in the construction of the approximate solution) assume that $r \leqslant \epsilon^k$. (This is not optimal.) Then we obtain from (3.39)

$$a^p \leqslant C\left(\epsilon^{-2}a^p\right)^{\frac{4}{N+2}}\left(\epsilon^{-2-\frac{2}{p}}a^2\right)^{\frac{N}{N+2}} + C\epsilon^{\frac{4}{N+2}}\left(\epsilon^{-2}a^p\right)^{\frac{2}{N+2}}\left(\epsilon^{-2-\frac{2}{p}}a^2\right).$$

As $p = 2(N+4)/(N+2)$, we conclude that there exists a small number $\rho > 0$ and some $l > 0$, both depending only on p and N, such that

$$a^p \leqslant C\epsilon^{-l}a^\rho a^p.$$

If k is chosen sufficiently large, then this implies that at T^ϵ still $a^p < \epsilon^{kp}$, contradicting the definition of T^ϵ. Therefore, T^ϵ must be the maximal time interval on which we can construct the approximate solution with r as required, thus proving the theorem.

We now provide a statement for a better regularity.

Theorem 3.2. *Let the assumptions of Theorem* 1.2 *hold. Let $m > 0$ be any fixed integer and assume that*

$$\left\|\bar{u}(t,x)\right\|_{C^{4m+5,m+\frac{5}{4}}([0,t]\times\Omega)} + \left\|u(t,x)\right\|_{C^{4m+3,m+\frac{3}{4}}([0,t]\times\Omega)} \leqslant \epsilon^{-(4m+6)}$$

for all small positive ϵ. Then for any $0 < t \leqslant T$

$$\left\|\bar{u}(t,x) - u(t,x)\right\|_{C^{4m,m}([0,t]\times\Omega)} \leqslant C\left\|\bar{u}(0,x) - u(0,x)\right\|_{C^{4m-2,m-\frac{1}{2}}([0,t]\times\Omega)}$$

for all sufficiently small positive ϵ.

Proof. We refer to [2] for the proof. □

It remains to show the spectral estimate which was crucial in the preceding computations. Let W be the double well potential such that $W'(u) = -f(u)$, where f as in (1.7).

Theorem 3.3. *There exists a positive constant C_{AC} such that for every $\epsilon \in (0,1]$ and every $\psi \in H^1(\Omega)$*

$$\int_\Omega \epsilon|\nabla\psi|^2 + \frac{1}{\epsilon}W''(q)\psi^2 \geqslant -C_{AC}\epsilon\int_\Omega \psi^2.$$

Proof. We refer to [5, pp. 1382–1383]. □

The linear stability Theorem 1.4 is a direct consequence of the following theorem:

Theorem 3.4. *There exist $\lambda_0 > 0$ and $\epsilon_0 > 0$ such that for every $\epsilon \in (0,\epsilon_0]$ and $\psi \in H_0^1(\Omega)$*

$$\inf_{\substack{\psi\in H^1(\Omega)\\ \epsilon^2\Delta w - w = \psi}} \frac{\int \epsilon|\nabla\psi|^2 + \epsilon^{-1}W''(q)\psi^2\,dx}{\int \epsilon^2|\nabla w|^2 + w^2\,dx} \geqslant -\epsilon\lambda_0. \tag{3.40}$$

Proof. First note that there is nothing to prove if

$$\int \epsilon|\nabla\psi|^2 + \epsilon^{-1}W''(q)\psi^2\,dx > 0,$$

because in such a case the left-hand side of the inequality (3.40) is positive, while the right-hand side is negative. Therefore assume without loss of generality

$$\int \epsilon|\nabla\psi|^2 + \epsilon^{-1}W''(q)\psi^2\,dx \leqslant 0,$$

which implies

$$\int \epsilon^2|\nabla\psi|^2 \leqslant \big\|\big(W''(q)\big)_-\big\|_\infty \int \psi^2. \tag{3.41}$$

Set

$$\epsilon^2\Delta w - w = \psi$$

then

$$\psi^2 = -w\psi + \epsilon^2\Delta w\psi$$

and

$$\int \psi w = -\int \epsilon|\nabla w|^2 - w^2\,dx.$$

Moreover,

$$\int \psi\Delta w = -\int \nabla\psi\nabla w \leqslant \delta\int|\nabla\psi|^2 + \frac{1}{\delta}\int|\nabla w|^2.$$

Then

$$\begin{aligned}\int \psi^2\,dx &\leqslant \int \epsilon^2|\nabla w|^2 + \int w^2 + \delta\int \epsilon^2|\nabla\psi|^2 + \delta^{-1}\int \epsilon^2|\nabla w|^2\\ &\leqslant \int \epsilon^2\big(1+\delta^{-1}\big)|\nabla w|^2 + \int w^2 + \delta\int \epsilon^2|\nabla\psi|^2\\ &\leqslant \big(1+\delta^{-1}\big)\int\big(\epsilon^2|\nabla w|^2 + w^2\big) + \delta\int \epsilon^2|\nabla\psi|^2.\end{aligned}$$

Using the previous estimate together with (3.41) we obtain for $\delta < \|(W''(q))_-\|_\infty^{-1}$

$$\int \psi^2 \leqslant \frac{1+\delta^{-1}}{1-\delta\|(W''(q))_-\|_\infty}\int\big(\epsilon^2|\nabla w|^2 + w^2\big). \tag{3.42}$$

By Theorem 3.3, see [5], and (3.42) we get

$$\iint \epsilon|\nabla\psi|^2 + \frac{1}{\epsilon}W''(q)\psi^2 \geqslant -C_{AC}\frac{1+\delta^{-1}}{1-\delta\|(W''(q))_-\|_\infty}\epsilon\left(\int \epsilon^2|\nabla w|^2 + w^2\right). \quad (3.43)$$

Thus the proof is complete. □

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