

Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint

ISSN 0946 – 8633

On a higher order convective Cahn-Hilliard type equation

Maciek Dominik Korzec¹, Piotr Rybka²

submitted: December 22, 2010

¹ Weierstrass Institute for Applied Analysis and Stochastics (WIAS)
10117 Berlin
Germany
Maciek.Korzec@wias-berlin.de

² Institute of Applied Mathematics and Mechanics
The University of Warsaw
02-097 Warsaw
Poland
rybka@mimuw.edu.pl

No. 1582
Berlin 2010



2000 *Mathematics Subject Classification.* 35A05, 74K35, 35G25, 74H40.

Key words and phrases. Existence theory; global weak solutions; Galerkin approach; uniqueness; small-slope approximation; anisotropic surface energy; coarsening.

Supported by the DFG Research Center MATHEON (Project C10) in Berlin.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: <http://www.wias-berlin.de/>

Abstract

A convective Cahn-Hilliard type equation of sixth order that describes the faceting of a growing surface is considered with periodic boundary conditions. By using a Galerkin approach the existence of weak solutions to this sixth order partial differential equation is established in $L^2(0, T; \dot{H}_{per}^3)$. Furthermore stronger regularity results have been derived and these are used to prove uniqueness of the solutions. Additionally a numerical study shows that solutions behave similarly as for the better known convective Cahn-Hilliard equation. The transition from coarsening to roughening is analyzed, indicating that the characteristic length scale decreases logarithmically with increasing deposition rate.

1 Introduction

A few years ago Savina et al. [18] derived the higher order convective Cahn-Hilliard (HCCH) equation

$$u_t - \delta u u_x - (u_{xx} + u - u^3)_{xxxx} = 0 \quad (1.1)$$

for the description of a growing crystalline surface with small slopes that undergoes faceting. Here, $u = h_x$ is the slope of a 1+1D surface $h(x, t)$ and δ is proportional to the deposition strength of an atomic flux. The main purpose of this work is to prove that unique weak solutions to equation (1.1) exist. The challenge here is not the dimension of the domain, since on simple intervals $[0, L]$ Sobolev's embedding theorems simplify the theory, but the high order of the derivatives, which makes it necessary to derive estimates in appropriate Banach spaces of high order. There is not much literature concerned with partial differential equations that include six lateral derivatives with nonlinearities that contain up to fourth order derivatives. Some work on the equation has been carried out recently [8, 10] and a related problem has been analyzed by Pawłow and Zajączkowski [15]. The authors of the latter reference studied also a sixth order equation, though their problem stems from a different physical phenomenon, namely the phase transition in ternary oil-water-surfactant systems. For the resulting PDE existence and uniqueness results can be established with typical tools of the theory of parabolic equations due to Solonnikov [19]. However, we do not proceed in the same way, since the added convective term destroys a Lyapunov function property. We succeed with a relatively generic Galerkin ansatz that demands clever estimation. Also the here presented approach is completely different than in the work by Korzec et al. [11], where the original 2+1D problem is analyzed. We comment further on this later.

The typical evolution of a solution to (1.1) is depicted in Figure 1. One can observe that at later times, as for $t = 20000$, the coarsening is governed by the interaction of domain walls. These *kinks* and *antikinks* resemble stationary solutions to the HCCH equation. Here, for the surface

h a kink describes the tip of a triangularly shaped surface and an antikink a cusp between two such islands. For the slopes u these kind of surfaces transform to rapid transitions from nearly constant negative states to also approximately flat positive states or the other way round.

A formal similarity to the better known convective Cahn-Hilliard (CCH) equation

$$u_t - \delta u u_x + (u_{xx} + u - u^3)_{xx} = 0 \quad (1.2)$$

is evident. An additional negative Laplacian is applied onto the parabolic terms to obtain the HCCH equation. This apparent resemblance leads to the conjecture that certain features of the solutions may be similar for both PDEs — in fact this is true to a large extent. Here, it will be shown numerically that indeed the solutions are akin. In a prior work it has been found out that branches of stationary solutions in a parameter diagram resemble those of the CCH equation [10]. Again, the high order of the equation makes its treatment nontrivial. For the description of stationary solutions a method of matched asymptotics requires to solve for four successive orders and retain exponentially small terms during the matching procedure. For proving the existence it becomes similarly complex to derive desired bounds. More estimates are needed than for the lower order companion and to get first good estimates a transformed equation is considered.

Because of the formal similarity, the discussion can benefit from recalling existing results for the CCH equation (1.2). Here, δ is some driving force strength and the cubic nonlinearity comes in as $W'(u) = f(u) = u^3 - u$, the derivative of a double well W . It is responsible for a bimodal arrangement of the order parameter u and in general it can have a more complex form. The equation has been derived by Leung [12] for the description of a driven lattice gas and it has been analyzed on coarsening dynamics by Emmott and Bray [4]. The authors found a power law for the increase of the characteristic length scale. Golovin et al. [6] saw that the same equation can be used as continuum model for the formation of facets in crystal growth, i.e. during solidification into a hypercooled melt. Coarsening dynamics have been reconsidered [7, 23] and lead to a more detailed understanding of the ripening process. Golovin et al found out that there is a transition from coarsening to roughening, when the external force parameter δ is increased, and that stable stationary solutions in a certain interval of wave numbers exist. Watson et al. derived a coarsening dynamical system, an ODE that tracks the individual kinks and yields a temporal $t^{1/2}$ scaling law that slows down at later times to a logarithmic law. Podolny et al. analyzed the mechanisms behind the coarsening and found analytical formulas for the motion of kink pairs, explaining the logarithmic regime at later times [16]. However, it seems that periodic stationary solutions exist. These have been found in an ODE system by Zaks et al. [24] and it seems possible that these also appear in late stages of dynamical simulations. Then, of course, the coarsening rates drop to zero. Only recently the existence of absorbing balls and hence a compact attractor has been established by Eden and Kalantarov [3]. It is possible that most of the results have an analogon for the HCCH equation.

Savina et al. found slightly variable power laws close to $t^{1/2}$ for the increase of the characteristic length scale for the higher order equation (1.1). For small values of the deposition numbers coarsening is observed that tends to stop after a sufficiently long period of evolution. This kind of behavior should be accentuated, the ripening not only slows down, it really stops and leaves a stationary domain wall pattern. The characteristic wave numbers in equilibrium do not depend on the length of the underlying periodic domain. Our numerics can be used to recompute the

same coarsening diagram as shown in the originating work (Figure 7 in [18]). For higher values of δ a chaotic regime is reached in which no kinds of equilibrium patterns are available. This has already been mentioned [18] and the transition from coarsening to roughening has been analyzed in more detail for the CCH equation [7]. As also known from the lower order equation [16], the coarsening is driven by ternary events, while pairs of *kinks* only form traveling waves or stationary profiles.

However, in this work more fundamental issues than numerical simulations are in focus. After discussing the transition from coarsening to roughening in Section 2, we show in Section 3 that unique solutions exist. First, some useful lemmata are stated in Section 3.1, then in Section 3.2, we show global existence of weak solutions $u \in L^2(0, T; \dot{H}_{per}^3(\Omega)) \cap L^4(0, T; \dot{L}^4(\Omega))$ with $u_t \in L^2(0, T; H^{-3}(\Omega))$. We extend the result in Section 3.3 by showing $u \in L^2(0, T; \dot{H}_{per}^4(\Omega))$ and $u_x \in L^\infty(0, T; L^\infty(\Omega))$. Finally we prove in Section 3.4 that the solutions are unique. The paper finishes with a summary and a discussion of possible future work.

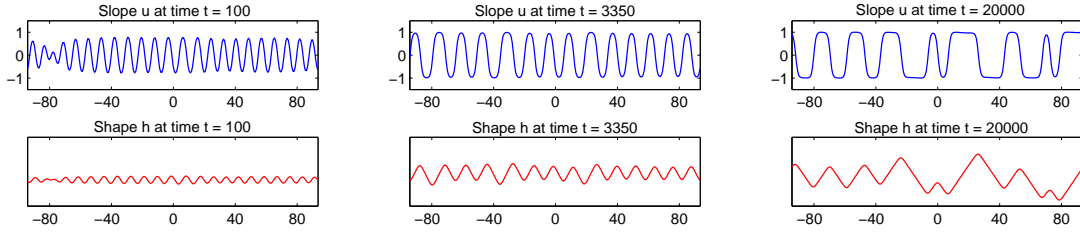


Figure 1: Typical evolution of the solutions to the HCCH equation for small values of δ calculated with a pseudospectral method (here $\delta = 0.01$). Starting with a randomly perturbed zero state small oscillations form that evolve to kink antikink patterns that coarsen. The upper plots show the slopes u , the lower figures depict the actual shape h .

2 From coarsening to roughening

Before proving the theoretical and main results established within this paper in Section 3, we want to discuss general aspects of the solutions to the HCCH equation (1.1) and show results from a numerical study. While the existence and uniqueness results in Section 3 are completely new, Savina and her co-workers made observations that are related to those presented on the following pages in this section. However, we describe the transition from coarsening to roughening in more detail, i.e. we find a logarithmic law for the decrease of the characteristic length of solutions in equilibrium with increasing deposition strength δ . Supported by numerical runs, we think that for small values of the deposition parameter the coarsening tends to stop with an oscillatory surface — though we do not offer a rigorous proof.

First we briefly reproduce the main steps of the derivation of this high order equation. It results from Mullins' surface diffusion formula [14] in presence of an atomic flux F

$$h_t = \sqrt{1 + |\nabla h|^2} (\mathcal{D} \nabla_s^2 \mu + F) \quad . \quad (2.1)$$

Here, the evolving surface is $h = h(x, y, t)$ and \mathcal{D} is a diffusion constant. A formula for the surface Laplacian ∇_s^2 can be found for example in [22]. In the following $|\cdot|$ always denotes the 2-norm for n -dimensional vectors. The chemical potential is written as μ and its definition allows for a huge amount of evolution equations, in particular for the self-assembly of quantum dots, see e.g. [2, 9, 21, 22]. These works extend the model presented here in that an elastic subproblem is considered.

The surface energy for the description of a growing, faceting (strong anisotropic) surface is decomposed into two parts, $\gamma = \gamma_{or} + \gamma_{reg}$. The first component γ_{or} depends on the outward unit normal to constitute preferred orientations. The second, γ_{reg} , is a regularization that is also known as Wilmore term, see e.g. [20]. One obtains the chemical potential for this model by calculating the functional derivative of the surface free energy, which is a surface integral over the surface energy density

$$\mu = \frac{\delta}{\delta h} \int \gamma dS \quad ,$$

where

$$\gamma = \gamma_{or} + \gamma_{reg}, \quad \gamma_{or} = \gamma_{or}(n) = \gamma_{or}(h_x, h_y), \quad \gamma_{reg} = \frac{1}{2}\nu\kappa^2 \quad .$$

The outward unit normal on the surface n can be written as

$$n = (n_1, n_2, n_3)^T = (-h_x, -h_y, 1)^T / \sqrt{1 + |\nabla h|^2}$$

and hence it allows for either using the normal's components or the slopes as arguments of the surface energy term γ_{or} in the regular case. κ is the mean curvature, defined as in the Appendix A, equation (A.1), such that a standard parabola bounded below has positive mean curvature, and ν is a regularization coefficient that determines the length scale over which corners in equilibrium shapes of crystals are smoothed out. The orientation dependent term of the surface energy γ_{or} could be left in a general form, say an arbitrary polynomial in the components of n . However, here it is a sixth order polynomial that suits to describe the surface energy of a crystal with cubic symmetry (derived in [13]),

$$\gamma_{or}(n) = \gamma_0(1 + \gamma_4(n_1^4 + n_2^4 + n_3^4) + \gamma_6(n_1^6 + n_2^6 + n_3^6)) \quad .$$

γ_0 is the surface energy of the (001) orientation and γ_4, γ_6 are dimensionless anisotropy coefficients. If these quantities have a high modulus, without the smoothing term γ_{reg} evolution equation (2.1) can result in backward diffusion, hence here ν is chosen bigger than zero to circumvent this behavior and regularize the problem. Next, the equation is nondimensionalized by using the following characteristic scales,

$$h \rightarrow H_0 H, \quad t \rightarrow \tau T, \quad (x, y) \rightarrow L(X, Y), \quad \mu \rightarrow \frac{\gamma_0}{L} \bar{\mu}, \quad \nabla_s \rightarrow \frac{1}{L} \bar{\nabla}_s$$

that define the characteristic time $\tau = L^4/(\mathcal{D}\gamma_0)$. By application of a long wave approximation — all terms are expanded with respect to the small parameter $\alpha = H_0/L$ and leading order terms are collected — the overall reduced model becomes

$$\begin{aligned} H_T &= \frac{\delta}{2} |\nabla H|^2 + \nabla^4 H + \nabla^6 H \\ &\quad - \nabla^2 [b(H_X^2 H_{YY} + H_Y^2 H_{XX} + 4H_X H_Y H_{XY}) + 3H_X^2 H_{XX} + 3H_Y^2 H_{YY}] . \end{aligned} \quad (2.2)$$

Here, b is an anisotropy coefficient and δ is a quantity proportional to the flux rate. An existence proof for solutions to this equation is under consideration. With help of a fix point argument and by working with Fourier series the existence of unique weak solutions can be established. These results will appear in one of the few related works [11].

The shape described by equation (2.2) is observed in a moving frame with the dimensionless speed δ . By reduction to one lateral dimension and setting $u = H_X$ (and using small letters for time and spatial variables again), one obtains the HCCH equation (1.1). The convective term δuu_x stems from a normal flux, not a heat convection as the name might suggest. The sixth order linearity results from the curvature dependent regularization and all other terms represent the orientation dependent surface energy under surface diffusion.

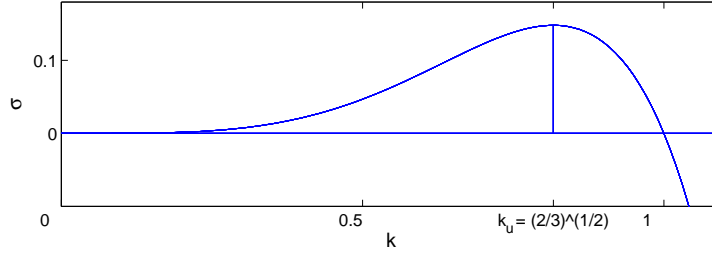


Figure 2: Dispersion relation for the HCCH equation.

Throughout this document, as in the originating work [18], periodicity of the solutions on an interval $\Omega = [0, L]$ is assumed and we should note that for sufficiently smooth solutions mass is conserved, because

$$\frac{d}{dt} \int_{\Omega} u dx = \int_{\Omega} \left(\frac{\delta}{2} u^2 + (u_{xx} + u - u^3)_{xxx} \right) dx = 0 \quad .$$

This property makes use of periodic Sobolev spaces with zero mean

$$\dot{H}_{per}^k(\Omega) = \{f \in H_{per}^k(\Omega) : \int_{\Omega} f dV = 0\} \quad (2.3)$$

reasonable — in particular since here initial conditions $u_0 \in \dot{H}^0(\Omega) = \dot{L}^2(\Omega)$ are used and the zero mean is conserved during evolution. The spaces are typically defined for arbitrary dimensions of the domain Ω , however, for this work it will suffice to consider Ω as one-dimensional interval. A typical simulation run showing the behavior of the surface for smaller values of δ has already been introduced in Figure 1, where $\delta = 0.01$. The simulation results are obtained with help of a pseudospectral method based on the Fourier transform, which premises periodic boundary conditions. The same evolution can be observed when using a finite difference method that uses a sufficiently fine grid. This supports the reliability of our numerical scheme. Starting from a randomly perturbed zero state with equal probability for deviations in positive and negative directions, small oscillations form in the first stage and they evolve to kinks and antikinks that coarsen with time. A linear stability analysis shows that the most unstable wave number is $k_u = \sqrt{2/3}$. This value can be derived by perturbing the zero state by normal modes with the ansatz $u = \epsilon \exp(\sigma t + ikx)$, which gives the characteristic equation $\sigma = -k^6 + k^4$,

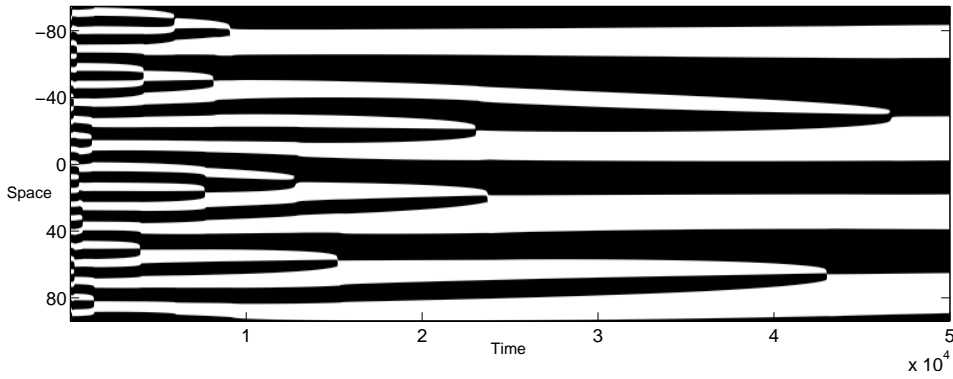


Figure 3: Space time plot for a solution to the HCCH equation for $\delta = 0.01$. White shades correspond to values of u near $+1$ while dark shades indicate $u \approx -1$. Ternary events governing the coarsening are visible throughout the whole evolution, resulting in an Ostwald ripening behavior. The axes are in dimensionless units.

valid to order ϵ and plotted in Figure 2. k_u is a critical point of this polynomial. However, the observed characteristic length in the simulations seems to be above the predicted length of about 1.6π . It shows that the nonlinearities are important already in early stages of the evolution.

An Ostwald-ripening behavior is observed. Kink antikink kink triplets successively merge to simple kinks and the characteristic length of the structures grows. In Figure 3 the behavior is visualized in a spatiotemporal plot for $\delta = 0.01$.

In Figure 4 the evolution on smaller domains $[-10\pi, 10\pi]$ is described to investigate the long-time behavior of the solutions to the HCCH equation dependent on small deposition rates. From earlier studies it seems not clear if coarsening stops or continues logarithmically slow. The presented numerical results indicate that for all values of δ below a certain threshold coarsening indeed does stop.

At earlier times coarsening as in Figure 3 takes place. However, for most values of δ it is not visible on the plots in Figure 4, since it happens at the very early phase of evolution that is not sufficiently resolved to be seen in these plots. For twelve increasing values of δ space time diagrams show how the shapes evolve. To help understanding the grayscale distribution the shape at the latest time point is plotted below. It can be observed that for increasing values of δ the number of stripes in the space time plots grows logarithmically slow in δ . This behavior is supported visually in Figure 5, where maxima for $u > 0$ have been counted and where the x axis representing the deposition parameters is logarithmic to show the moderation of the characteristic frequency growth. For the nonequilibrium solutions the number of maxima has been counted at the latest computed time point $t = 10^5$. However, this figure does not reveal the additional information seen in the previous Figure 4. Apart from stationary solutions (such as for $\delta = 0.05, 0.5$) also traveling waves with various speed rates are observed (e.g. $\delta = 0.07, 3$) and for $\delta = 5$ chaotic behavior is observed that appears for all bigger values of δ . In no reference frame this solutions is in equilibrium. It remains to show that this variety of different solutions indeed can exist, by proving rigorously the existence of solutions.

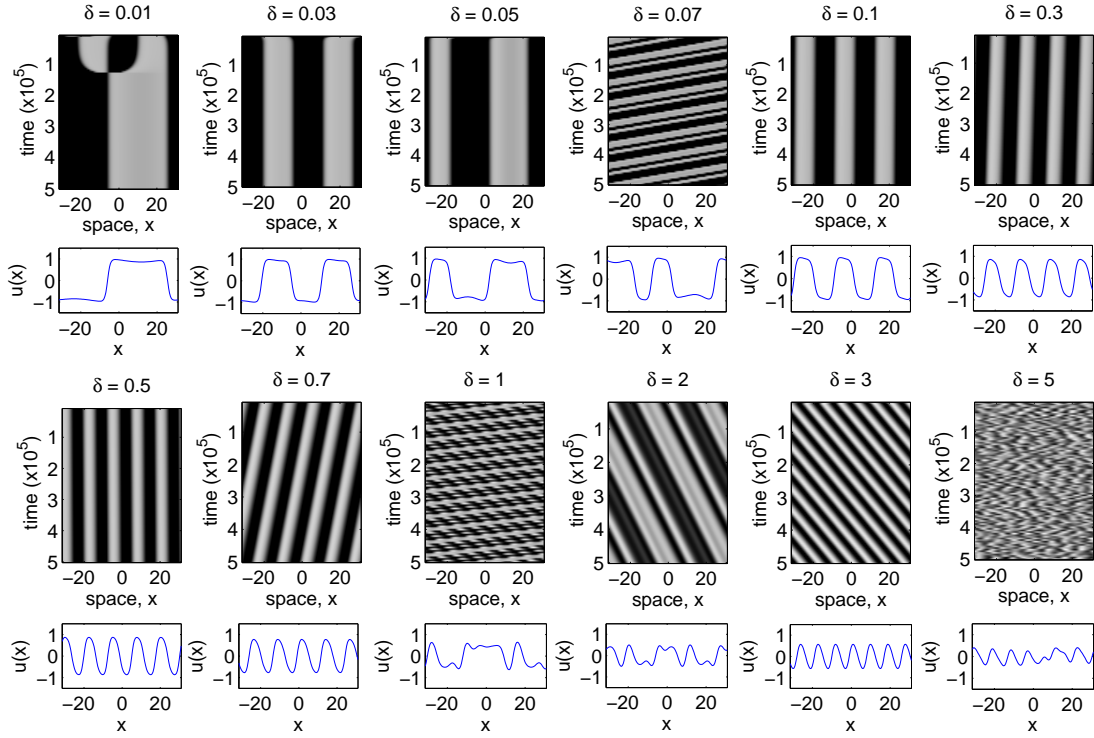


Figure 4: Multi-hump stationary solutions and traveling waves for the HCCH equation for values of δ between 0.01 and 3. The last space time plot visualizes a solution after the transition to chaotic behavior that appears for values of δ above a certain threshold.

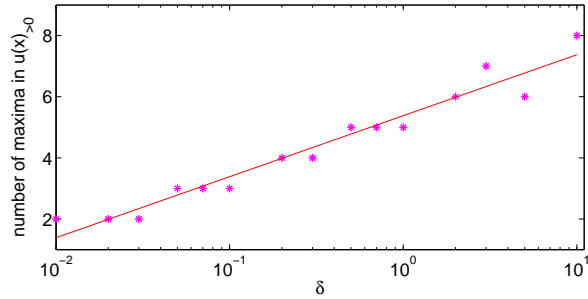


Figure 5: Number of local maxima in the stationary and traveling wave solutions to the HCCH equation for values of δ between 0.01 and 5. The solid curve is a nonlinear least squares data fit.

3 Existence theory

Before we state and prove the existence theorem, we want to introduce a few aspects of certain operators, their eigenvalues and eigenfunctions in one lateral dimension. These are used later during the proofs.

3.1 Preliminaries: Eigenvalues, eigenvectors and powers of Laplacians

The domain under consideration is a simple interval $\Omega = [0, L]$ and we denote the L^2 -norm by $\|\cdot\|$, while other norms obtain a corresponding subscript. We note that with periodic boundary conditions the eigenvalues of the bi-Laplacian $A_2 = \partial_{xxxx}$, the negative tri-Laplacian $A_3 = -\partial_{xxxxx}$ are just powers of the eigenvalues to the negative Laplacian $A_1 = -\partial_{xx}$. For A_k , $k = 1, 2, 3$, we have the eigenvalues $\lambda_{kj} = \lambda_{1j}^k$, and $\lambda_{1j} = (\frac{2\pi j}{L})^2$ for a $[0, L]$ domain. The eigenfunctions are the same for all three operators and they form an orthogonal basis for \dot{H}_{per}^k and an orthonormal basis for \dot{L}^2 . Furthermore, since the A_k are unbounded, symmetric, linear operators with inverse $M_k = A_k^{-1}$ (compact, symmetric, linear operators), the following two theorems, where the pair (A, M) belongs to one of the above operators, can be used (for proofs of all the following lemmata in this section see Robinson's monograph [17]).

Lemma 1 (Hilbert-Schmidt Theorem). *The eigenvalues $\bar{\lambda}_j$ of M defined by the characteristic equation $M\varphi_j = \bar{\lambda}_j\varphi_j$, $j = 1, 2, \dots$ are real and they can be ordered such that $|\bar{\lambda}_{j+1}| \leq |\bar{\lambda}_j|$, $j = 1, 2, \dots$ and $\lim_{j \rightarrow \infty} \bar{\lambda}_j = 0$. The set of eigenfunctions $\{\varphi_j\}_j$ forms an orthonormal basis for \dot{L}^2 and it can be written $Mu = \sum_{j=1}^{\infty} \bar{\lambda}_j(u, \varphi_j)_{L^2} \varphi_j$.*

Lemma 2. *Let A be defined as above as symmetric, linear, unbounded operator with the compact, linear inverse M , than A has an infinite set of eigenvalues $\{\lambda_j\}_j$ that correspond to the set of eigenfunctions $\{\varphi_j\}_j$. They can be ordered such that $|\lambda_{j+1}| \geq |\lambda_j|$, $j = 1, 2, \dots$ and then $\lim_{j \rightarrow \infty} |\lambda_j| = \infty$. Furthermore the eigenfunctions can be chosen as orthonormal basis of \dot{L}^2 and application of A to a function u can be expressed as $Au = \sum_{j=1}^{\infty} \lambda_j(u, \varphi_j)_{L^2} \varphi_j$.*

Now one can easily show estimates of the form

$$\|M_j^{1/2}u\|^2 \leq \bar{\lambda}_1 \|u\|^2 \quad (3.1)$$

or

$$\|u\| \leq C \|A_j u\| \quad , \quad (3.2)$$

for some constant $C > 0$, which will be especially useful in the following. An introduction to fractional operators can also be found in Robinson's book [17].

Another important statement is a compactness result by Aubin and Lions, which will be used to derive strong convergence in L^2 . We use the notation $X \hookrightarrow Y$ for two Banach spaces X and Y , where X is continuously embedded in Y . For a compact embedding we write $X \hookrightarrow\hookrightarrow Y$.

Lemma 3. *Aubin-Lions Lemma Let X_0, X_1, X_2 be three Banach spaces with $X_0 \hookrightarrow\hookrightarrow X_1 \hookrightarrow X_2$. If X_0 and X_1 are reflexive, it holds for all $p \in (1, \infty)$ and conjugate index q that the embedding of*

$$L^p(0, T; X_0) \cap L^q(0, T; X_2)$$

into

$$L^p(0, T; X_1)$$

is compact.

To show continuity in time the following result is useful.

Lemma 4. Let H and \tilde{H} be Hilbert spaces with $H \hookrightarrow \tilde{H} \hookrightarrow H^*$ and let

$$u \in L^2(0, T; H), \quad u_t \in L^2(0, T; H^*),$$

then

$$u \in C^0([0, T], \tilde{H}).$$

Once the L^2 convergence is established the following lemma will be used to handle the nonlinearities.

Lemma 5. For a sequence $(u_n)_n \subset L^2(\Omega)$ that converges in L^2 , $u_n \rightarrow u \in L^2(\Omega)$, there exists a subsequence that converges to u a.e.

In a last step a weak version of the dominated convergence theorem will be used:

Lemma 6. Let $\Omega \subset \mathbb{R}^n$ open, bounded and let $(f_n)_n \subset L^p(\Omega)$, $p > 1$, with $\|f_n\|_{L^p(\Omega)} \leq C$ be a sequence of functions that are pointwise converging a.e. to a function $f \in L^p(\Omega)$. Then $f_n \rightharpoonup f$ in $L^p(\Omega)$.

3.2 Existence of weak solutions

Consider the HCCH equation in the form

$$\begin{aligned} u_t - \delta g(u)_x - (u_{xx} - f(u))_{xxx} &= 0, \quad x \in \mathbb{R}, \delta > 0 \\ u(x, 0) &= u_0(x), \quad x \in \mathbb{R}, \end{aligned} \quad (3.3)$$

with periodic boundary conditions on an interval $\Omega = [0, L]$ for $t \in [0, T]$ and where the nonlinearities are the following polynomials in u ,

$$g(u) = \frac{1}{2}u^2, \quad f(u) = u^3 - u.$$

We use these functions to accentuate the nonlinearities in this PDE. The formulation might be generalized to more general expressions functions, however, we do not follow this possibility in this work.

Theorem 1 (Weak solutions to the HCCH equation). Equation (3.3) on a periodic interval Ω with initial condition $u_0 \in H^1(\Omega)$ has a weak solution: For any $T > 0$ there exists a function

$$u \in L^2(0, T; \dot{H}_{per}^3(\Omega)) \cap L^4(0, T; \dot{L}^4(\Omega)) \cap C^0([0, T], \dot{L}^2(\Omega)) \quad \text{with} \quad u_t \in L^2(0, T; H^{-3}(\Omega))$$

that fulfills

$$\int_{\Omega_T} u_t \varphi \, dx dt + \delta \int_{\Omega_T} g(u) \varphi_x \, dx dt + \int_{\Omega_T} u_{xxx} \varphi_{xxx} \, dx dt - \int_{\Omega_T} f'(u) u_x \varphi_{xxx} \, dx dt = 0, \quad (3.4)$$

$$\text{for all } \varphi \in L^2(0, T, \dot{H}_{per}^3(\Omega))$$

Proof. Consider the Galerkin approximation

$$u^N = \sum_{k=1}^N c_k \varphi_k \quad , \quad (3.5)$$

where u^N is expanded in terms of the eigenfunctions of the negative Laplacian with periodic boundary conditions $\{\varphi_j\}_j$. These functions form an orthonormal basis for \dot{L}^2 and also serve as orthogonal basis of \dot{H}_{per}^k , $k = 1, 2, 3, \dots$. The superscript N in the approximation exclusively stands for the finite-dimensionality of the function and not a power as other superscripts usually stand for. Then the following weak form is defined for u^N

$$\int_{\Omega} u_t^N \varphi dx + \delta \int_{\Omega} \Pi^N[g(u^N)] \varphi_x dx + \int_{\Omega} u_{xxx}^N \varphi_{xxx} dx - \int_{\Omega} \Pi^N[f'(u^N) u_x^N] \varphi_{xxx} dx = 0, \quad (3.6)$$

$$\text{for all } \varphi \in \dot{H}_{per}^3(\Omega) \quad .$$

The orthogonal projection Π^N is defined via

$$\Pi^N\left(\sum_{k=1}^{\infty} b_k \varphi_k\right) = \sum_{k=1}^N b_k \varphi_k \quad , \quad (3.7)$$

mapping \dot{L}^2 functions to a finite dimensional space. It has the property

$$\int_{\Omega} \Pi^N[v] w dx = \int_{\Omega} v \Pi^N[w] dx \quad \forall_{v,w \in \dot{L}^2} \quad . \quad (3.8)$$

Together with the orthogonality of the basis functions this allows to deduce simplified equations from the weak form that have to hold

$$\int_{\Omega} u_t^N \varphi_j dx + \delta \int_{\Omega} g(u^N) (\varphi_j)_x dx + \int_{\Omega} u_{xxx}^N (\varphi_j)_{xxx} dx - \int_{\Omega} f'(u^N) u_x^N (\varphi_j)_{xxx} dx = 0, \quad j = 1, \dots, N \quad .$$

Because of the orthogonality of the chosen basis the first integral just gives the time derivatives of the coefficients. Hence the ODE

$$\dot{c}_j = -\tilde{\lambda}_j c_j + \delta \int_{\Omega} g(u^N)_x \varphi_j dx - \int_{\Omega} f'(u^N) u_x^N (\varphi_j)_{xxx} dx, \quad j = 1, \dots, N \quad (3.9)$$

is derived, where the $\tilde{\lambda}_j$ are the positive eigenvalues of the negative tri-Laplacian. Since the nonlinearities g, f and the basis functions are in C^∞ , the right hand side is a continuous function, dependent on the other coefficients c_k . Hence a solution exists locally in time and it can be extended globally if it does not blow up.

To prove global existence an auxiliary equation will be used. The HCCH equation (3.3) can be written as

$$u_t - \delta g(u)_x + A(f(u) - u_{xx}) = 0 \quad , \quad (3.10)$$

where A is the bi-Laplacian, which is a linear, symmetric, unbounded, positive operator acting on \dot{H}_{per}^4 . Let M be its inverse operator, $M = A^{-1}$, and let the corresponding eigenvalues be denoted by $\lambda_1, \bar{\lambda}_1$ for A and M , respectively, when they are ordered as in the Hilbert-Schmidt Theorem 1.

Applying the compact, linear operator M to (3.10) yields

$$Mu_t - \delta Mg(u)_x + f(u) - u_{xx} = 0 \quad . \quad (3.11)$$

The corresponding weak form for the Galerkin approximation writes

$$\begin{aligned} & \int_{\Omega} M^{1/2}[u_t^N]M^{1/2}[\varphi]dx - \delta \int_{\Omega} M^{1/2}[\Pi^N(g(u^N)_x)]M^{1/2}[\varphi]dx \\ & + \int_{\Omega} u_x^N \varphi_x dx + \int_{\Omega} f(u^N)\Pi^N(\varphi)dx = 0, \quad \varphi \in \dot{H}_{per}^1(\Omega). \end{aligned} \quad (3.12)$$

It was used the property (3.8) and that $M^{1/2}(\Pi^N(v)) = \Pi^N(M^{1/2}v)$, which one can see by recalling the definitions of the fractional operator and of the projection (3.7).

Testing with u^N yields

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|M^{1/2}u^N\|^2 + \|u_x^N\|^2 + \int_{\Omega} (u^N)^4 dx \\ & = \int_{\Omega} (u^N)^2 dx + \delta \int_{\Omega} M^{1/2}[\Pi^N(g(u^N)_x)]M^{1/2}[u^N]dx \quad . \end{aligned} \quad (3.13)$$

As before and as in the following $\|\cdot\|$ denotes the L^2 norm over the space domain Ω . Several estimates will have to be carried out and the appearing positive constants will be denoted by C . Note that these quantities may differ from line to line, even from estimate to estimate. If they are supposed to be fixed numbers, they will be written with some subscript, e.g. C_r for some number r — for small positive constants we also write ϵ . The constants may depend on the size of the domain Ω and the time integral length T .

The terms on the right hand side of (3.13) are estimated as follows

$$\begin{aligned} & \int_{\Omega} (u^N)^2 dx \leq \frac{1}{4} \|(u^N)^2\|_{L^2}^2 + C = \frac{1}{4} \|u\|_{L^4}^4 + C \quad , \\ & \delta \int_{\Omega} M^{1/2}[\Pi^N(g(u^N)_x)]M^{1/2}u^N dx \leq \delta \|M^{1/2}[\Pi^N(g(u^N)_x)]\| \|M^{1/2}u^N\| \\ & \leq \epsilon_1 \frac{\delta \sqrt{\bar{\lambda}_1}}{8} \|u^N\|_{L^4}^4 + \frac{\delta \bar{\lambda}_1}{2\epsilon_1} \|u^N\|^2 \\ & \leq \frac{\delta(\sqrt{\bar{\lambda}_1}\epsilon_1^2 + 2\bar{\lambda}_1\epsilon_2)}{8\epsilon_1} \|u^N\|_{L^4}^4 + C \quad . \end{aligned} \quad (3.14)$$

Here, ϵ_1 and ϵ_2 are arbitrary constants and the quantity C depends on their inverse values.

Furthermore it was used that for any v^N that can be expanded as in (3.5) it is true that

$$\begin{aligned}\|M^{1/2}v_x^N\|^2 &= \int_{\Omega} \sum_{k,l=1}^N \bar{\lambda}_k^{1/2} \bar{\lambda}_l^{1/2} c_k c_l (\varphi_k)_x (\varphi_l)_x dx = \sum_{k,l=1}^N \bar{\lambda}_k^{1/2} \bar{\lambda}_l^{1/2} c_k c_l \int_{\Omega} (-\varphi_k)_{xx} \varphi_l dx \\ &= \sum_{k=1}^N \bar{\lambda}_k^{1/2} c_k^2 \leq \sqrt{\bar{\lambda}_1} \|v^N\|^2 .\end{aligned}$$

This holds, because the eigenvalues of the negative Laplacian are just the roots of the eigenvalues of the bi-Laplacian λ_j on the periodic spaces under consideration. Since $\Pi^N(g(u^N)_x)$ is of the form (3.5) one obtains $\|M^{1/2}[\Pi^N(g(u^N)_x)]\|^2 \leq \sqrt{\bar{\lambda}_1} \|\Pi^N(g(u^N))\|^2 \leq \sqrt{\bar{\lambda}_1} \|g(u^N)\|^2$. Now choosing $\epsilon_1 = 1/(\delta\sqrt{\bar{\lambda}_1})$ (for the case without deposition, $\delta = 0$ we do not need this estimate at all, hence we can assume $\delta > 0$ here) and $\epsilon_2 = 1/(2\delta^2(\bar{\lambda}_1)^{3/2})$ guarantees that the coefficient in front of the L^4 term in (3.14) is equal to 1/4. Then we obtain the overall estimate after integration of (3.13) with respect to time

$$\frac{1}{2} \|M^{1/2}u^N(T)\|^2 + \int_0^T \|u_x^N\|^2 dt + \frac{1}{2} \int_0^T \|u^N\|_{L^4}^4 dt \leq C + \frac{1}{2} \|M^{1/2}u^N(0)\|^2 \leq C ,$$

so that the following bounds can be deduced

$$\begin{aligned}M^{1/2}u^N &\text{ is uniformly bounded in } L^\infty(0, T; \dot{L}^2(\Omega)) , \\ u^N &\text{ is uniformly bounded in } L^2(0, T; \dot{H}_{per}^1(\Omega)) , \\ u^N &\text{ is uniformly bounded in } L^4(0, T; \dot{L}^4(\Omega)) , \\ g(u^N) &\text{ is uniformly bounded in } L^2(0, T; \dot{L}^2(\Omega)) .\end{aligned}$$

The last bound follows directly from the L^4 estimate. The second bound implies by the Sobolev embedding theorem for one-dimensional domains an estimate on u^N in $L^2(0, T; C^0(\Omega))$.

A uniform in time bound is derived by testing (3.11) with u_t^N . It yields with the double well $W(u) = \frac{1}{4}u^4 - \frac{1}{2}u^2$:

$$\begin{aligned}\|M^{1/2}u_t^N\|^2 + \frac{1}{2} \frac{d}{dt} \|u_x^N\|^2 + \frac{1}{2} \frac{d}{dt} \int_{\Omega} W(u^N) dx &= \delta \int_{\Omega} M^{1/2}[\Pi^N g(u^N)_x] M^{1/2}[u_t^N] dx \\ &\leq \frac{\delta^2}{2} \|M^{1/2}[\Pi^N g(u)_x]\|^2 + \frac{1}{2} \|M^{1/2}u_t^N\|^2 \\ &\leq \frac{\delta^2 \sqrt{\bar{\lambda}_1}}{8} \|u\|_{L^4(\Omega)}^4 + \frac{1}{2} \|M^{1/2}u_t^N\|^2 .\end{aligned}$$

Subtracting the last term, multiplication by 2, integration in time, using the L^4 bound and the H^1 bound of the initial condition yield

$$\begin{aligned}\int_0^T \|M^{1/2}u_t^N\|^2 dt + \|u_x^N(T)\|^2 + \int_{\Omega} W(u^N(T)) dx \\ \leq \|u_x^N(0)\|^2 + \frac{\delta^2 \sqrt{\bar{\lambda}_1}}{4} \|u\|_{L^4(\Omega_T)}^4 \leq C .\end{aligned}$$

This gives the following estimate

$$u^N \text{ is uniformly bounded in } L^\infty(0, T; \dot{H}_{per}^1(\Omega)) \text{ ,}$$

which in particular implies by the Sobolev embedding theorem that u^N is continuous in space for almost all times.

Due to the smoothness of f one can further deduce

$$\|f'(u^N)\|_\infty \leq C, \quad \|f''(u^N)\|_\infty \leq C, \dots \text{ .}$$

The original weak equation (3.6) gives with the test function u^N

$$\frac{1}{2} \frac{d}{dt} \|u^N\|^2 + \|u_{xxx}^N\|^2 - \int_{\Omega} f'(u^N) u_x^N u_{xxx}^N dx = 0 \text{ .} \quad (3.15)$$

Periodicity was used with

$$\int_{\Omega} u^N u_x^N u^N dx = \frac{1}{3} \int_{\Omega} ((u^N)^3)_x dx = 0 \text{ ,}$$

which is a property commonly used for the Navier-Stokes or the Korteweg-de-Vries equation.

By using the time uniform bound $|f'(u^N)| \leq C_1$ one can further conclude

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|u^N\|^2 + \|u_{xxx}^N\|^2 &\leq \left| \int_{\Omega} f'(u^N) u_x^N u_{xxx}^N dx \right| \\ &\leq C_1 \int_{\Omega} |u_x^N u_{xxx}^N| dx \\ &\leq C_1 \left(\frac{1}{2\epsilon} \|u_x^N\|^2 + \frac{\epsilon}{2} \|u_{xxx}^N\|^2 \right) \text{ .} \end{aligned}$$

Choosing $\epsilon = 1/C_1$ yields

$$\frac{d}{dt} \|u^N\|^2 + \|u_{xxx}^N\|^2 \leq C \|u_x^N\|^2 \text{ .}$$

Integration in time yields

$$\|u^N(T)\|^2 + \int_0^T \|u_{xxx}^N\|^2 dt \leq C \text{ ,}$$

so that an additional result is established

$$u^N \text{ is uniformly bounded in } L^2(0, T, \dot{H}_{per}^3(\Omega)) \text{ .}$$

From the above results one can further conclude that

$$f'(u^N) u_x^N \text{ is uniformly bounded in } L^2(0, T; \dot{L}^2(\Omega))$$

and the bounds yield also boundedness in the dual space

$$\begin{aligned}
\|u_t^N\|_{H^{-3}} &= \sup_{\varphi \in \dot{H}_{per}^3(\Omega), \|\varphi\|_{H^3}=1} \left| \int u_t^N \varphi dx \right| \\
&\leq \sup_{\varphi \in \dot{H}_{per}^3(\Omega), \|\varphi\|_{H^3}=1} \int |\delta u^N u_x^N \varphi| + |u_{xxx}^N \varphi_{xxx}| + |u_{xx}^N \varphi_{xx}| + |3(u^N)^2 u_x^N \varphi_{xxx}| dx \\
&\leq C \|u_x^N\| (\|\varphi\| + \|\varphi_{xxx}\|) + \|u_{xxx}^N\| \|\varphi_{xxx}\| + \|u_{xx}^N\| \|\varphi_{xx}\| \leq C .
\end{aligned}$$

We have shown that

$$u_t^N \text{ is uniformly bounded in } L^2(0, T; H^{-3}(\Omega)) .$$

This shows the existence of the Galerkin approximation in the weak sense for all times. To show existence of weak solutions, the limit $N \rightarrow \infty$ has to be analyzed. Therefore the reflexive weak compactness theorem gives the following weakly convergent subsequence (as usually not relabeled)

$$\begin{aligned}
u^N &\rightharpoonup u \text{ in } L^2(0, T; \dot{H}_{per}^3(\Omega)) \\
u_t^N &\rightharpoonup u_t \text{ in } L^2(0, T; H^{-3}(\Omega)) \\
f'(u^N) u_x^N &\rightharpoonup \chi_1 \text{ in } L^2(0, T; \dot{L}^2(\Omega)) \\
g(u^N) &\rightharpoonup \chi_2 \text{ in } L^2(0, T; \dot{L}^2(\Omega)).
\end{aligned}$$

The two first weak limits imply by application of the compactness theorem, Lemma 3 with

$$\dot{H}_{per}^3(\Omega) \hookrightarrow \dot{L}^2(\Omega) \hookrightarrow H^{-3}(\Omega)$$

that L^2 convergence of a subsequence is established

$$u^N \rightarrow u \text{ in } L^2(0, T; \dot{L}^2(\Omega)) .$$

Additionally one obtains by application of Lemma 4 that

$$u \in C^0([0, T], \dot{L}^2(\Omega)) .$$

Since Ω is a bounded interval, it further holds $\dot{H}_{per}^3(\Omega) \hookrightarrow \dot{H}_{per}^1(\Omega) \hookrightarrow H^{-3}(\Omega)$ and Lemma 3 yields

$$u_x^N \rightharpoonup u_x \text{ in } L^2(0, T; \dot{L}^2(\Omega)) .$$

The convergence in L^2 is important when dealing with the nonlinearities.

It has to be shown that indeed also with projections the terms $\Pi^N f'(u^N) u_x^N$ and $\Pi^N g(u^N)$ converge weakly. Therefore we consider

$$\Xi^N(\varphi) = \varphi - \Pi^N(\varphi) ,$$

which converges strongly to zero in $L^2(0, T; \dot{L}^2(\Omega))$. Then

$$\int_{\Omega_T} \Pi^N [g(u^N)] \varphi dx dt = \int_{\Omega_T} g(u^N) \varphi dx dt - \int_{\Omega_T} \Xi^N [g(u^N)] \varphi dx dt, \quad \varphi \in L^2(0, T; \dot{L}^2(\Omega)) .$$

The weak convergence for the first integral of the right hand side has been established before. The second integral tends to zero, since

$$\int_{\Omega_T} \Xi^N[g(u^N)]\varphi dxdt = \int_{\Omega_T} g(u^N)\Xi^N[\varphi] dxdt$$

and $\Xi^N[\varphi] \rightarrow 0$ in $L^2(\Omega_T)$. For $\Pi^N[f'(u^N)u_x^N]$ one can proceed analogously, just by replacing g with this nonlinearity. Hence it remains to show that the limits are indeed those anticipated.

The L^2 convergence of u^N , $(u^N)^2$ and u_x^N gives with Lemma 5 a subsequence for that (again without relabeling) $u^N \rightarrow u$, $(u^N)^2 \rightarrow u^2$ and $u_x^N \rightarrow u_x$ a.e. in Ω_T . Then by continuity $g(u^N)$ and $f'(u^N)u_x^N$ converge a.e. to $g(u)$ and $f'(u)u_x$. Lemma 6 with the L^2 bounds yields weak limits $g(u^N) \rightharpoonup g(u)$, $f'(u^N)u_x^N \rightharpoonup f'(u)u_x$ that hold in L^2 , so that by uniqueness of weak limits one has $\chi_1 = f'(u)u_x$ and $\chi_2 = g(u)$, respectively.

As last step it has to be shown that indeed $u(0) = u_0$. Another standard trick can be applied. Therefore we define a test function $\varphi \in C^1([0, T], \dot{H}_{per}^3(\Omega))$ that fulfills $\varphi(T) = 0$. This function is also in $L^2(0, T; \dot{H}_{per}^3(\Omega))$ and partial integration in time of the weak form (3.4) yields

$$\begin{aligned} - \int_{\Omega_T} u \varphi_t dxdt + \left[\int_{\Omega} u \varphi dx \right]_0^T + \delta \int_{\Omega_T} g(u) \varphi_x dxdt \\ + \int_{\Omega_T} u_{xxx} \varphi_{xxx} dxdt - \int_{\Omega_T} f'(u) u_x \varphi_{xxx} dxdt = 0 \quad . \end{aligned} \quad (3.16)$$

Analogously for the Galerkin approximation we have the equation

$$\begin{aligned} - \int_{\Omega_T} u^N \varphi_t dxdt + \left[\int_{\Omega} u^N \varphi dx \right]_0^T + \delta \int_{\Omega_T} \Pi^N(g(u^N)) \varphi_x dxdt \\ + \int_{\Omega_T} u_{xxx}^N \varphi_{xxx} dxdt - \int_{\Omega_T} \Pi^N(f'(u^N)u_x^N) \varphi_{xxx} dxdt = 0 \quad . \end{aligned} \quad (3.17)$$

The weak convergence shows that in the limes the integrals are the same. The bracket terms become $[\int_{\Omega} u^N \varphi dx]_0^T = - \int_{\Omega} u^N(0) \varphi(0) dx$ and $[\int_{\Omega} u \varphi dx]_0^T = \int_{\Omega} u_0 \varphi(0)$. Subtraction of the two weak equations and arbitrariness of $\varphi(0)$ yield $u_0 = u(0)$. \square

3.3 More regularity

We were not able to show uniqueness for the weak solutions established before without further regularity improvement. Here we extend the result from the last section, then we finally prove uniqueness.

Consider the Nierenberg inequality [1] that holds on bounded domains $\Omega \subset \mathbb{R}^n$, $n \leq 3$,

$$\|D^j u\|_{L^p} \leq c_1 \|D^m u\|_{L^r}^a \|u\|_{L^q}^{1-a} + c_2 \|u\|_{L^q}, \quad (3.18)$$

where

$$j/m \leq a \leq 1 \quad \text{and} \quad 1/p = j/n + a(1/r - m/n) + (1-a)/q \quad ,$$

and c_1, c_2 are positive constants. For $p = \infty$ the fraction $1/p$ is interpreted as 0.

This inequality yields for our problem, with $n = 1, j = 1, p = \infty, m = 3, r = 2, q = 2, a = 1/2$, that

$$\|u_x\|_\infty \leq c_1 \|u_{xxx}\|^{1/2} \|u\|^{1/2} + c_2 \|u\|, \quad (3.19)$$

which can be further estimated to

$$\|u_x\|_\infty \leq \frac{c_1}{2} \|u_{xxx}\| + \frac{c_1 + 2c_2}{2} \|u\|, \quad (3.20)$$

and which directly yields with new, but related, constants C_1, C_2 ,

$$\|u_x\|_\infty^2 \leq C_1 \|u_{xxx}\|^2 + C_2 \|u\|^2. \quad (3.21)$$

Integration over time yields $u_x \in L^2(0, T; L^\infty(\Omega))$. However, (3.19) gives also a stronger result by taking the fourth power and using the L^∞ bound on u ,

$$\|u_x\|_\infty^4 \leq C \|u_{xxx}\|^2 + C, \quad (3.22)$$

so that $u_x \in L^4(0, T; L^\infty(\Omega))$. Note that here $C = C(\|u\|_\infty^2)$.

The following calculations are carried out on the level of the Galerkin approximation. Testing the HCCH equation with u_{xx}^N (and ignoring the superscripts again) yields after integration

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|u_x\|^2 + \|u_{xxxx}\|^2 &= \|u_{xxx}\|^2 + \delta \int_\Omega g(u) u_{xxx} dx + \int_\Omega (f''(u) u_x^2 + f'(u) u_{xx}) u_{xxxx} dx \\ &\leq \frac{\delta}{8} \|u\|_{L^4(\Omega)}^4 + (1 + \frac{\delta}{2}) \|u_{xxx}\|^2 + \int_\Omega |(6u u_x^2 + 3u^2 u_{xx}) u_{xxxx}| dx \\ &\leq C + (1 + \frac{\delta}{2}) \|u_{xxx}\|^2 + \int_\Omega 6(\|u\|_\infty u_x^2 + 3\|u\|_\infty^2 |u_{xx}| + |u_{xx}|) |u_{xxxx}| dx \\ &\leq C + (1 + \frac{\delta}{2}) \|u_{xxx}\|^2 + C \|u_{xx}\|^2 + C \int_\Omega u_x^4 dx + \frac{1}{2} \|u_{xxxx}\|^2, \end{aligned}$$

which holds for a. a. times. In the last line we estimate further with help of (3.22)

$$C \int_\Omega u_x^4 dx \leq C \|u_x\|_\infty^4 \leq C \|u_{xxx}\|^2 + C,$$

so that after integration with respect to time we finally obtain by using the established bounds that

$$\frac{1}{2} \|u_x(T)\|^2 + \frac{1}{2} \int_0^T \|u_{xxxx}\|^2 dt \leq C + C \int_0^T \|u_{xxx}\|^2 dt \leq C.$$

Thus we have boundedness of the Galerkin approximation in $L^2(0, T; \dot{H}_{per}^4(\Omega))$. We use this bound to establish that $u_x \in L^\infty(0, T; L^\infty(\Omega))$, which then will be used to show uniqueness of such solutions. First we need to prove an auxiliary lemma.

Lemma 7. Suppose $a, b, c \geq 0$ are functions on $[0, T]$ with $c \in L^2([0, T])$ and let $C > 0$ be a constant. Furthermore assume that the inequality

$$\int_0^T a(s)^2 ds + b(T)^2 \leq \int_0^T a(s)b(s)c(s) ds + C \quad (3.23)$$

holds. Then

$$b(T)^2 \leq 2Ce^{\int_0^T c(s)^2 ds} \quad (3.24)$$

and furthermore

$$\int_0^T a(s)^2 ds \leq 2C \int_0^T c(s)^2 e^{\int_0^T c(p)^2 dp} ds + 2C \quad (3.25)$$

Proof. Inequality (3.23) yields with Young's inequality

$$\int_0^T a(s)^2 ds \leq \int_0^T a(s)b(s)c(s) ds + C \leq \int_0^T \frac{1}{2}a(s)^2 + \frac{1}{2}b(s)^2c(s)^2 ds + C \quad ,$$

hence

$$\frac{1}{2} \int_0^T a(s)^2 ds \leq \frac{1}{2} \int_0^T b(s)^2c(s)^2 ds + C \quad (3.26)$$

Furthermore we get with help of (3.26)

$$\begin{aligned} b(T)^2 &\leq \int_0^T a(s)b(s)c(s) ds + C \\ &\leq \frac{1}{2} \int_0^T c(s)^2 b(s)^2 ds + \frac{1}{2} \int_0^T a(s)^2 ds + C \\ &\leq \int_0^T c(s)^2 b(s)^2 ds + 2C \end{aligned}$$

With $\phi(t) = b(t)^2$ we established

$$\phi(T) \leq \int_0^T c(s)^2 \phi(s) ds + 2C \quad .$$

The standard Gronwall inequality in the integral form yields just (3.24). Using this result in (3.26) gives

$$\begin{aligned} \int_0^T a(s)^2 ds &\leq \int_0^T b(s)^2c(s)^2 ds + 2C \leq \int_0^T c(s)^2 2Ce^{\int_0^s c(p)^2 dp} ds + 2C \\ &\leq 2C \int_0^T c(s)^2 e^{\int_0^T c(p)^2 dp} ds + 2C \quad . \end{aligned}$$

□

For estimating the nonlinearity corresponding to the anisotropy of the model, another estimate will be useful.

Lemma 8. Consider a domain $\Omega \subset \mathbb{R}^n$, let $s > 0, t > s + n/2$ and $u \in H^s(\Omega), \phi \in H^t(\Omega) \cap L^\infty(\Omega)$. Then $\phi u \in H^s(\Omega)$ and it holds for some constant $C > 0$ that

$$\|\phi u\|_{H^s} \leq \|\phi\|_\infty \|u\|_{H^s} + C \|\phi\|_{H^t} \|u\|_{H^{s-1}} \quad . \quad (3.27)$$

Proof. This formula is shown in Proposition 6.16 in Folland [5], if we also take into account the remark preceding this proposition for Sobolev spaces over \mathbb{R}^n . However, the argument requires minor modifications. \square

Let $\Lambda = (-\partial_{xx})^{1/2}$. Then it is in particular $(-\partial_{xx})^{-1} = \Lambda^{-2}$. We can test the HCCH equation, still on a Galerkin level, with $\Lambda^{-2-\alpha}u_t$, where $\alpha > 0$ is a constant to be specified later. We notice that $\Lambda^{-2-\alpha}$ is a self-adjoint operator and that here we use also bracket superscripts^(k) to indicate derivatives of high order.

$$\int_{\Omega} u_t \Lambda^{-2-\alpha} u_t dx - \int_{\Omega} u^{(6)} \Lambda^{-2-\alpha} u_t dx = \delta \int_{\Omega} g(u)_x \Lambda^{-2-\alpha} u_t dx - \int_{\Omega} (u^3 - u)^{(4)} \Lambda^{-2-\alpha} u_t dx \quad (3.28)$$

Let us look separately on each term.

The first term on the left hand side of (3.28) leads to

$$\begin{aligned} \int_{\Omega} u_t \Lambda^{-2-\alpha} u_t dx &= \int_{\Omega} -\partial_{xx} (-\partial_{xx})^{-1} \Lambda^{-\alpha/2} u_t \Lambda^{-2-\alpha/2} u_t dx \\ &= \int_{\Omega} \Lambda^{-2-\alpha/2} u_{xt} \Lambda^{-2-\alpha/2} u_{xt} dx = \|\Lambda^{-2-\alpha/2} u_{xt}\|^2 \quad , \end{aligned}$$

The second term on the left hand side yields

$$- \int_{\Omega} u^{(6)} \Lambda^{-2-\alpha} u_t dx = \int_{\Omega} \Lambda^{2-\alpha/2} u \Lambda^{2-\alpha/2} u_t dx = \frac{1}{2} \frac{d}{dt} \|\Lambda^{2-\alpha/2} u\|^2 \quad .$$

On the right hand side of (3.28) we calculate

$$\begin{aligned} \delta \int_{\Omega} g(u)_x \Lambda^{-2-\alpha} u_t dx &= -\frac{\delta}{2} \int_{\Omega} \Lambda^{-\alpha/2} u^2 \Lambda^{-2-\alpha/2} u_{xt} dx \leq \frac{\delta}{2} \|\Lambda^{-\alpha/2} u^2\| \|\Lambda^{-2-\alpha/2} u_{xt}\| \\ &\leq C \|u^2\|^2 + \frac{1}{4} \|\Lambda^{-2-\alpha/2} u_{xt}\|^2 \quad , \end{aligned}$$

where for the last estimate it was used that for L^2 functions φ it is $\|\Lambda^{-\alpha/2} \varphi\|^2 \leq C \|\varphi\|^2$. Furthermore the two parts of the nonlinearity f give

$$\begin{aligned} \int_{\Omega} u^{(4)} \Lambda^{-2-\alpha} u_t dx &= \int_{\Omega} \Lambda^{2-\alpha/2} u_x \Lambda^{-2-\alpha/2} u_{xt} dx \leq \|\Lambda^{2-\alpha/2} u_x\| \|\Lambda^{-2-\alpha/2} u_{xt}\| \\ &\leq C \|\Lambda^{3-\alpha/2} u\|^2 + \frac{1}{4} \|\Lambda^{-2-\alpha/2} u_{xt}\|^2 \end{aligned}$$

and

$$\begin{aligned} \int_{\Omega} -(u^3)^{(4)} \Lambda^{-2-\alpha} u_t dx &= \int_{\Omega} (3u^2 u_x)_{xx} \Lambda^{-2-\alpha} u_{xt} dx = \int_{\Omega} -\Lambda^{2-\alpha/2} (3u^2 u_x) \Lambda^{-2-\alpha/2} u_{xt} dx \\ &\leq \|\Lambda^{2-\alpha/2} (3u^2 u_x)\| \|\Lambda^{-2-\alpha/2} u_{xt}\|. \end{aligned}$$

Overall we arrived at

$$\begin{aligned} \frac{1}{2} \|\Lambda^{-2-\alpha/2} u_{xt}\|^2 + \frac{1}{2} \frac{d}{dt} \|\Lambda^{2-\alpha/2} u\|^2 & \tag{3.29} \\ \leq C \|u^2\|^2 + C \|\Lambda^{3-\alpha/2} u\|^2 + \|\Lambda^{2-\alpha/2} (3u^2 u_x)\| \|\Lambda^{-2-\alpha/2} u_{xt}\| \end{aligned}$$

and some more work has to be invested.

In order to estimate $\|\Lambda^{2-\alpha/2} (u^2 u_x)\|$ we use Lemma 8. We take $s = 2 - \frac{\alpha}{2}$ and $t = \frac{5}{2} - \frac{\alpha}{2} + \epsilon_1$ for a small positive ϵ_1 to estimate

$$\|\Lambda^{2-\alpha/2} (u^2 u_x)\| \leq \|u^2 u_x\|_{H^{2-\alpha/2}} \leq \|u^2\|_{\infty} \|u_x\|_{H^{2-\alpha/2}} + C \|u_x\|_{H^{1-\alpha/2}} \|u^2\|_{H^{5/2-\alpha/2+\epsilon_1}}.$$

Again we use Lemma 8, here on the last term in the inequality above, with new $s = \frac{5}{2} - \frac{\alpha}{2} + \epsilon_1$, $t = 3 - \frac{\alpha}{2} + \epsilon_1 + \epsilon_2$ and a positive ϵ_2 , to derive

$$\begin{aligned} \|u^2 u_x\|_{H^{2-\alpha/2}} &\leq C \|u\|_{H^{3-\alpha/2}} + C \|u\|_{H^{2-\alpha/2}} \|u\|_{H^{5/2-\alpha/2+\epsilon_1}} \\ &\quad + C \|u\|_{H^{2-\alpha/2}} \|u\|_{H^{3-\alpha/2+\epsilon_1+\epsilon_2}} \|u\|_{H^{3/2-\alpha/2+\epsilon_1}}. \end{aligned}$$

We notice that on the left hand side in (3.29) there is a $\frac{d}{dt} \|\Lambda^{2-\alpha/2} u\|^2$ term, while on the right hand side we have $\|u\|_{H^{2-\alpha/2}}$. In order to get $\frac{d}{dt} \|u\|_{H^{2-\alpha/2}}^2$ we add to equation (3.29) the term $\frac{d}{dt} \|u\|^2$ to both sides. We note that $\frac{d}{dt} \|u\|^2$ is integrable over $[0, T]$ and we arrive at

$$\begin{aligned} \frac{1}{2} \|\Lambda^{-2-\alpha/2} u_{xt}\|^2 + \frac{1}{2} \frac{d}{dt} \|u\|_{H^{2-\alpha/2}}^2 & \\ \leq C \|u^2\|^2 + C \|\Lambda^{3-\alpha/2} u\|^2 + 3 \|\Lambda^{2-\alpha/2} (u^2 u_x)\| \|\Lambda^{-2-\alpha/2} u_{xt}\| + \frac{1}{2} \frac{d}{dt} \|u\|^2 & \\ \leq C + \frac{1}{2} \frac{d}{dt} \|u\|^2 + \|u\|_{H^{3-\alpha/2}}^2 + C \|u\|_{H^{3-\alpha/2}} \|\Lambda^{-2-\alpha/2} u_{xt}\| & \\ + C \|u\|_{H^{2-\alpha/2}} \|\Lambda^{-2-\alpha/2} u_{xt}\| (\|u\|_{H^{5/2-\alpha/2+\epsilon_1}} + \|u\|_{H^{3-\alpha/2+\epsilon_1+\epsilon_2}} \|u\|_{H^{3/2-\alpha/2+\epsilon_1}}). & \end{aligned}$$

Integrating over $[0, T]$, taking into account that $u \in L^2([0, T]; H^3)$, positivity of α and the regularity of the initial condition, $\|u(0)\|_{H^{2-\alpha/2}} < \infty$, we obtain

$$\begin{aligned} \frac{1}{2} \int_0^T \|\Lambda^{-2-\alpha/2} u_{xt}\|^2 dt + \|u(T)\|_{H^{2-\alpha/2}}^2 &\leq \tag{3.30} \\ C + C \int_0^T (\|u\|_{H^{5/2-\alpha/2+\epsilon_1}} + \|u\|_{H^{3-\alpha/2+\epsilon_1+\epsilon_2}} \|u\|_{H^{3/2-\alpha/2+\epsilon_1}}) \|u\|_{H^{2-\alpha/2}} \|\Lambda^{-2-\alpha/2} u_{xt}\| dt. & \end{aligned}$$

At this point we choose α . For an $\epsilon_1 \in (0, \frac{1}{2})$, we set $\alpha = 1 + 2\epsilon_1$ so that $3/2 - \alpha/2 + \epsilon_1 = 1$ and $\|u\|_{H^1}$ may be uniformly estimated due to the L^∞ bound over \dot{H}_{per}^1 established earlier. Moreover, if $\epsilon_2 < \frac{1}{2}$, then

$$3 > 3 - \alpha/2 + \epsilon_1 + \epsilon_2 > 5/2 - \alpha/2 + \epsilon_1 = 2.$$

We may now apply Lemma 7 with

$$a(t) = \|\Lambda^{-2-\alpha/2} u_{xt}\|/\sqrt{2}, \quad b(t) = \|u\|_{H^{2-\alpha/2}}, \quad c(t) = C\|u\|_{H^3}$$

which then yields

$$\|u\|_{H^\sigma} \leq C < \infty. \quad (3.31)$$

Here $\sigma \in (1, \frac{3}{2})$, so that this is an improvement over the uniform estimate on $\|u\|_{H^1}$.

We may use (3.30) again, now with $\alpha < 1$ and ϵ_1 so that $3/2 - \alpha/2 + \epsilon_1 > 1$. We conclude that (3.31) holds with $\sigma \in (\frac{3}{2}, 2)$. As a result we deduce that

$$u_x \in L^\infty(0, T; L^\infty).$$

The uniform bounds on the derivatives will suffice to show uniqueness, i.e. we shall see that sufficiently smooth solutions are unique.

3.4 Uniqueness

To show uniqueness of the solutions, another lemma that results from Young's inequality with ϵ is useful.

Lemma 9. *For any positive ϵ there is a positive constant C such that for all u in \dot{H}_{per}^3 , the following inequality holds.*

$$\|u_{xx}\|^2 \leq \epsilon \|u_{xxx}\|^2 + C\|u\|^2, \quad (3.32)$$

Proof. To show this inequality, use the more obvious interpolation inequality $\|u_x\|^2 \leq \tilde{\epsilon} \|u_{xx}\|^2 + \tilde{C} \|u\|^2$, which is obtained by partial integration and Young's inequality with an arbitrary small $\tilde{\epsilon} > 0$ and a constant $\tilde{C} > 0$ that depends on $\tilde{\epsilon}$. It is used in the following calculation:

$$\begin{aligned} \|u_{xx}\|^2 &\leq \int |u_{xxx} u_x| dx \leq \|u_{xxx}\| \|u_x\| \leq \|u_{xxx}\| (\tilde{\epsilon} \|u_{xx}\|^2 + \tilde{C} \|u\|^2)^{1/2} \\ &\leq \|u_{xxx}\| (\tilde{\epsilon} C_p \|u_{xxx}\| + \tilde{C} \|u\|) \leq (\tilde{\epsilon} \tilde{C} + \bar{\epsilon}) \|u_{xxx}\|^2 + C \|u\|^2 \\ &\leq \epsilon \|u_{xxx}\|^2 + C \|u\|^2. \end{aligned}$$

Here, $C_p > 0$ is a Poincaré constant. In the final steps Young's inequality with $\bar{\epsilon} > 0$ was used, $\bar{\epsilon} = (\tilde{\epsilon} C_p + \bar{\epsilon})$ and the final constant $C > 0$ depends on $\bar{\epsilon}$ and $\tilde{\epsilon}$.

□

Corollary 1. *By application of the Poincaré inequality for the first derivative one can directly derive*

$$\|u_x\|^2 \leq \epsilon \|u_{xxx}\|^2 + C \|u\|^2. \quad (3.33)$$

Again $\epsilon > 0$ can be chosen arbitrarily small and $C > 0$ depends on ϵ .

Theorem 2. *There is at most one weak solution $u \in L^2(0, T; \dot{H}_{per}^4(\Omega)) \cap L^\infty(0, T; W^{1,\infty}(\Omega))$ to the HCCH equation (3.3) with periodic boundary conditions and $u_0 \in H^1(\Omega)$. The solutions depend continuously on the initial conditions.*

Proof. Result (3.21) directly yields that weak solutions to the HCCH equation u fulfill $u_x \in L^2(0, T; L^\infty)$. This will be used in the following. Suppose we have two weak solutions u_1 and u_2 with the same initial condition $u_1(0) = u_2(0) = u_0$. We set $u = u_2 - u_1$ and plug u_i , $i = 1, 2$ into (3.3). The difference of these equations tested with u , which is a legitimate test function, gives the following identity.

$$J := \frac{1}{2} \frac{d}{dt} \int_{\Omega} u^2 + \int_{\Omega} (u_{xxx})^2 dx = \int_{\Omega} (u_{xx})^2 dx + \frac{\delta}{2} \int_{\Omega} (u_2^2 - u_1^2)_x u dx - \int_{\Omega} (u_2^3 - u_1^3)_{xx} u_{xx} dx.$$

The two expressions on the right hand side have to be estimated. Beginning with the convective term we get

$$\begin{aligned} \delta \int_{\Omega} |(u_2^2 - u_1^2)_x u| dx &\leq \delta \int_{\Omega} u^2 |(u_2 + u_1)_x| + |u_x (u_2 + u_1) u| dx \\ &\leq \delta C \|u\|^2 + C \int_{\Omega} |u_x u| dx \\ &\leq C_1 \|u\|^2 + \epsilon_1 \|u_{xxx}\|^2, \end{aligned}$$

where we used the $L^\infty(0, T; L^\infty(\Omega))$ bound for the solutions first derivatives and inequality (3.33) in the last estimate ($\epsilon_1 > 0$ can be chosen arbitrarily small and C_1 depends on δ and ϵ_1). A little bit of care is necessary, since the applied Lemma 9 holds for functions in \dot{H}_{per}^3 . The weak solutions u_1, u_2 are in $L^2(0, T; \dot{H}_{per}^3(\Omega))$, hence the derived estimates hold for a.a. times. This will also be the case for the following estimates.

Now we take care of the cubic term,

$$\begin{aligned} \left| - \int_{\Omega} (u_2^3 - u_1^3)_{xx} u_{xx} dx \right| &= \left| - \int_{\Omega} (u(u_2^2 + u_2 u_1 + u_1^2))_{xx} u_{xx} dx \right| \\ &= \left| \int_{\Omega} u_x (u_2^2 + u_2 u_1 + u_1^2) u_{xxx} dx + \int_{\Omega} u (u_2^2 + u_2 u_1 + u_1^2)_x u_{xxx} dx \right| \\ &\leq C \int_{\Omega} |u_x u_{xxx}| dx + C \int_{\Omega} |u| (|u_1| + |u_2|) (|(u_1)_x| + |(u_2)_x|) u_{xxx} dx \\ &\leq C (\|u_1\|_\infty, \|u_2\|_\infty, \|(u_1)_x\|_\infty, \|(u_2)_x\|_\infty) \|u^2\| + \epsilon_2 \|u_{xxx}\|^2. \end{aligned}$$

In the estimate above we used the uniform bounds on $\|(u_1)_x\|_\infty, \|(u_2)_x\|_\infty$, guaranteed by the assumptions on the solutions. Using Lemma 9 with ϵ_3 for the last remaining term in J gives $\|u_{xx}\|^2 \leq \epsilon_3 \|u_{xxx}\|^2 + C_3 \|u\|^2$. After collecting all inequalities we arrive at the following estimate

$$J \leq \epsilon \|u_{xxx}\|^2 + C_{\delta,\epsilon} \|u\|^2,$$

where $\epsilon = \epsilon_1 + \epsilon_2 + \epsilon_3$ and $C_{\delta,\epsilon} = C_1 + C_2 + C_3$.

Thus, we finally arrive at the estimate,

$$\frac{1}{2} \frac{d}{dt} \|u\|^2 \leq C_{\delta, \epsilon} \|u\|^2 \quad \text{for a. a. } t \in [0, T].$$

An application of Gronwall inequality yields

$$\|u\|^2 \leq \|u(0)\|^2 e^{C_{\delta, \epsilon} t} = 0 \quad \text{for a. a. } t \in [0, T],$$

which shows the continuous dependence on the initial conditions and which gives $u \equiv 0$ a.e. on Ω_T since the initial conditions for both solutions are equal. \square

4 Summary and outlook

In this work we have established fundamental results for a semilinear PDE of sixth order which contains a convective term that stems from an atomic flux impinging normally onto a surface and a second nonlinearity from the anisotropy of the surface energy. It describes the faceting of a growing crystalline surface in 2D. We have shown that unique weak solutions exist in high order periodic Sobolev spaces by using a Galerkin approach. It turned out to be useful to transform the PDE by applying the inverse of the bi-Laplacian. This allowed to show lower order bounds that can be used to proof higher order regularity in $L^2(0, T; \dot{H}_{per}^4(\Omega))$ and we think that establishing even higher regularity is possible, but that it is a wearisome task.

A numerical investigation with help of a pseudospectral method shows that solutions to the HCCH equation behave similarly as to the related CCH equation. While for small values of $\delta \ll 1$ solutions tend to coarsen and stop the ripening process as either stationary or traveling wave solutions, they do not equilibrate for bigger values. Instead they show chaotic behavior and their amplitude shrinks. The characteristic wavelengths of the solutions decreases logarithmically with the deposition parameter δ .

Due to the formal relation to the CCH equation and because of a few calculations we made, it is possible that similar results as in the publications by Zaks et al. [24] can be reproduced analogously for the HCCH equation to describe the periodic stationary patterns observed during simulations of the time dependent problem. However, so far we were not able to prove the existence of an attractor as succeeded by Eden and Kalantarov [3] for the CCH equation. The treatment of the cubic nonlinearity is not as straightforward as in the lower order case, since the additional derivatives make the term less beneficial for certain estimates. For the original 3D model (2.2) we established a different existence proof that does not rely on Galerkin expansions and which will appear soon [11].

It would be interesting to extend the theoretical results for a surface diffusion equation that additionally contains effects from an elastic subproblem. The introduction of such a nonlocal term poses a challenge for a new existence proof. Such a model has been used for example by Korzec et al. [9] for the description of quantum dot self-assembly.

Acknowledgment

MK would like to acknowledge the financial support by the DFG Research Center MATHEON, project C10. Furthermore MK thanks B. Wagner and A. Münch for introducing into this particular topic, L. Recke for further fruitful discussions related to the HCCH equation and R. Huth for pointing out a few mistakes in the manuscript.

A Appendix

The mean curvature of a regular surface $h(x, y, t)$ is

$$\kappa = \frac{h_{xx}(1 + h_y^2) + h_{yy}(1 + h_x^2) - 2h_x h_y h_{xy}}{(1 + |\nabla h|^2)^{\frac{3}{2}}} . \quad (\text{A.1})$$

References

- [1] R. A. Adams. *Sobolev Spaces*. Academic Press, New York, 1975.
- [2] C.-H. Chiu and Z. Huang. Common features of nanostructure formation induced by the surface undulation on the Stranski-Krastanow systems. *Appl. Phys. Lett.*, 89:171904, 2006.
- [3] A. Eden and V. K. Kalantarov. The convective Cahn-Hilliard equation. *App. Math. Lett.*, 20(4):455–461, 2007.
- [4] C. L. Emmott and A. J. Bray. Coarsening Dynamics of a One-Dimensional Driven Cahn-Hilliard System. *Phys. Rev. E*, 54(5):4568–4575, 1996.
- [5] G. B. Folland. *Introduction to Partial Differential Equations*. Princeton University Press, 1995.
- [6] A. A. Golovin, S. H. Davis, and A. A. Nepomnyashchy. A convective Cahn-Hilliard model for the formation of facets and corners in crystal growth. *Phys. D*, 122(1-4):202–230, 1998.
- [7] A. A. Golovin, A. A. Nepomnyashchy, S. H. Davis, and M. A. Zaks. Convective Cahn-Hilliard Models: From Coarsening to Roughening. *Phys. Rev. Lett.*, 86(8):1550, 2001.
- [8] M. D. Korzec. *Continuum modeling, analysis and simulation of the self-assembly of thin crystalline films*. PhD thesis, Technical University in Berlin, 2010.
- [9] M. D. Korzec and P. L. Evans. From bell shapes to pyramids: A reduced continuum model for self-assembled quantum dot growth. *Phys. D*, 239:465–474, 2010.
- [10] M. D. Korzec, P. L. Evans, A. Münch, and B. Wagner. Stationary solutions of driven fourth- and sixth-order Cahn-Hilliard type equations. *SIAM J. Appl. Math.*, 69:348–374, 2008.

- [11] M. D. Korzec, P. Nayar, and P. Rybka. Global weak solutions to a sixth order Cahn-Hilliard type equation. *in preparation*, 2010.
- [12] Kwan-Tai Leung. Theory on morphological instability in driven systems. *Journal of Statistical Physics*, 61(1-2):345–364, October 1990.
- [13] G. B. McFadden, S. R. Coriell, and R. F. Sekerka. Effect of surface tension anisotropy on cellular morphologies. *J. Crystal Growth*, 91(1-2):180–198, 1988.
- [14] W. W. Mullins. Theory of Thermal Grooving. *J. Appl. Phys.*, 28(3):333–339, 1957.
- [15] I. Pawłow and W. M. Zajączkowski. Sixth Order Cahn-Hilliard Type Equation. *to appear*, 2010.
- [16] A. Podolny, M. A. Zaks, B. Y. Rubinstein, A. A. Golovin, and A. A. Nepomnyashchy. Dynamics of domain walls governed by the convective Cahn-Hilliard equation. *Phys. D*, 201:291–305, 2005.
- [17] J. Robinson. *Infinite-Dimensional Dynamical Systems - From Basic Concepts to Actual Calculations*. Cambridge University Press, 2001.
- [18] T. V. Savina, A. A. Golovin, S. H. Davis, A. A. Nepomnyashchy, and P. W. Voorhees. Faceting of a growing crystal surface by surface diffusion. *Phys. Rev. E*, 67:021606, 2003.
- [19] V. A. Solonnikov. Boundary value problems for linear parabolic systems of differential equations of general type. *Trudy Mat. Inst. Steklov*, 83:1–162 (in Russian), 1965.
- [20] B. J. Spencer. Asymptotic solutions for the equilibrium crystal shape with small corner energy regularization. *Phys. Rev. E*, 69:011603, 2004.
- [21] B. J. Spencer, P. W. Voorhees, and S. H. Davis. Morphological instability in epitaxially strained dislocation-free solid films. *Phys. Rev. Lett.*, 67(26):3696–3699, 1991.
- [22] W. T. Tekalign and B. J. Spencer. Evolution equation for a thin epitaxial film on a deformable substrate. *J. Appl. Phys.*, 96(10):5505–5512, 2004.
- [23] S. J. Watson, F. Otto, B. Rubinstein, and S. H. Davis. Coarsening dynamics of the convective Cahn-Hilliard equation. *Phys. D*, 178:127–148, 2003.
- [24] M. A. Zaks, A. Podolny, A. A. Nepomnyashchy, and Alexander A. Golovin. Periodic Stationary Patterns Governed by a Convective Cahn-Hilliard Equation. *SIAM J. Appl. Math.*, 66(2):700–720, 2006.