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Stationary solutions and coarsening of a driven Cahn-Hilliard type equation

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Modeling of self-assembled quantum dots growth

Quantum dots, also so-called artificial atoms, are nano-crystals that are confined in three dimensions and can be used as optoelectronic devices such as blue lasers. Recently a variety of physical continuum models have been proposed to simulate the self-assembled growth process such as molecular beam epitaxy for germanium on silicon. Atoms are deposited layer by layer onto a substrate and an instability occurs at a certain height to form small islands that are pyramidal in shape. These coarsen in time.
Continuum models based on Mullins diffusion formula lead to the evolution equation

$$h_t = \sqrt{1+\|\nabla h\|^2}(F + \mathcal{D}\nabla_s^2 \mu), \quad \mathcal{D} = -\frac{\Omega^2 D_s \sigma}{kT},$$

where ∇_s^2 is the surface Laplacian, F an atomic flux, and $\mathcal{D}$ a quantity containing the atomic volume Ω, a diffusion coefficient D_s, the number of atoms per unit area σ, the absolute temperature T and the Boltzmann constant k.
Depending on the chemical potential μ one can include different physical mechanisms into the model. A simple potential that depends on the anisotropic surface tension is

$$\mu = \frac{\delta}{\delta h}\int \gamma(\nabla h, \nabla^2 h)dS$$

and a particular formula that incorporates cubic symmetry and a Willmore regularization which penalizes the edges can be derived as

$$\gamma(\nabla h, \nabla^2 h) \equiv \gamma(n,\kappa) = \gamma_0 + \gamma_4(n_1^4+n_2^4+n_3^4) + \gamma_6(n_1^6+n_2^6+n_3^6) + \frac{1}{2}\nu\kappa^2 \quad .$$

After a small slope based reduction, one obtains a sixth order evolution equation [1]

$$h_t = \frac{\delta}{2}\|\nabla h\|^2 + \nabla^2\{\nabla^2 h + \nabla^4 h + [(-3h_x^2 - bh_y^2))h_{xx} + (-3h_y^2 - bh_x^2)h_{yy}] - 4bh_x h_y h_{xy}\} \quad ,$$

where δ is proportional to the deposition rate and b is an anisotropy coefficient. Further reduction, i.e. 1D in space and $u = h_x$, yields the higher order convective Cahn-Hilliard (HCCH) equation

$$u_t - \frac{\delta}{2}(u^2)_x = (u_{xx} + u - u^3)_{xxxx} \quad .$$

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[1] Savina et al., *Faceting of a growing crystal surface by surface diffusion*, Physical Review 67, 2003

Stationary solutions of the HCCH equation [2]

- Integrate stationary version of HCCH equation

$\frac{\delta}{2}(A - u^2) = (u_{xx} + u - u^3)_{xxx}$

- 2 equilibrium points dependent on the integration constant

$u^{\pm} = \mp\sqrt{A}$

- look for connections from u^+ to u^-: antikinks
- $dim(W^u(u^{\pm})) = 2 \Rightarrow$ codimension 2
- reversibility $\Rightarrow$ codimension 1
- 2 parameters $\Rightarrow$ can expect solution branches

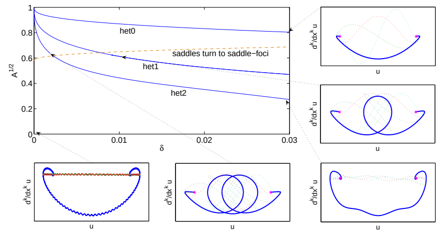

Fig.: Parameter plane with "phase spaces" for certain solutions

Boundary value problem

- 1st order: $U' = LF(U)$ on $[0,1]$
- fix D, add $A' = 0$
- symmetric solution $\longrightarrow$ half domain and...
- ...defines boundary conditions at symmetry point $x = 1$

$$U_1(0) = 1, \quad U_k(0)^2 + U_{k+1}(0)^2 = 0, \quad k = 2,4$$
$$U_1(1) = U_3(1) = U_5(1) = 0$$

- continuation by linear extrapolation in parameter plane
- $het_k, k = 0,1,2,3,\ldots$ as in CCH equation expected
- $A_k \approx 1 - (2k+1)\,2^{1/6}\delta^{1/3}$

Exponential asymptotics

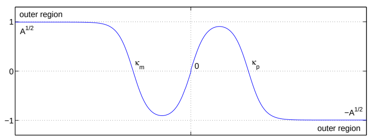

Fig.: Sketch of a het_1 solutions showing the setup for the matching procedure

Results that are in agreement with the numerics; for het_1:

- expand A, κ_m (see figure) and solutions around layers in powers of $\delta^{1/3}$
- solve $\mathcal{O}(\delta^{k/3}), k = 0,1,2,3$ problems
- express one layers solution in terms of the others variable
- retain exponentially small terms
- obtain hump-width Δ in terms of the Lambert W function

$$\Delta = \frac{\sqrt{2}}{6}\ln\left(\frac{\beta}{W(\beta^{1/3})^3}\right), \quad \beta = 2^{11}/(27\delta^2)$$

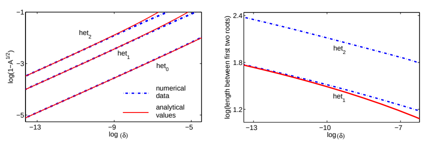

Fig.: Left, log-plot shows expression for A_k; right, distances between the first two roots of the het_1, het_2 solutions, numerically and for het_1 via the analytical expression.

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[2] 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., 2008 (in press)

Coarsening of the HCCH equation

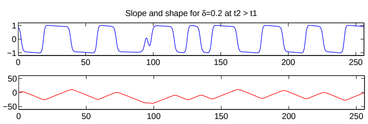

Fig.: slope $u = h_x$ and corresponding shape h

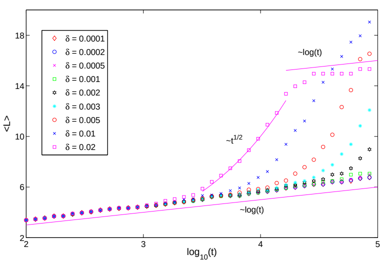

Fig.: Logarithmic timescale versus the characteristic length-scale $<L>$ which is the average distance between two successive kinks

We simulate the HCCH equation in terms of a pseudospectral method for several values of small δ. A term like $(u_{xx} - u^3)_{xxxx}$ is approximated with help of a discrete Fourier transform $\mathcal{F}$ and its inverse $\mathcal{F}^{-1}$

$$\mathcal{F}^{-1}[(ik)^4\mathcal{F}\{(\mathcal{F}^{-1}[(ik)^2\mathcal{F}(u)] - u^3)\}] \quad .$$

Counting zeros of $u = h_x$ lets us study coarsening by computing the average length scale $<L>$, the domain-length divided by the number of zeros.

Coarsening dynamical system ?

Kink-position $k(t) = k_0(t) + \epsilon^{1/3}k_1(t)$ gives speed

$$\dot{k}(t) = \epsilon^{1/3}k_1(t) = -\frac{1}{4}\sum_{k=2}^{4}\lambda_k C_k + \mu_k D_k$$

C_i, D_i depend on distances to neighboring kinks

Discussion

This work describes the stationary solutions of a sixth order driven Cahn-Hilliard type equation which were obtained with a BVP formulation and a matched asymptotics approach which gives analytical expressions for the far-field values and the hump-width. Furthermore a coarsening diagram for small values of δ has been computed and we see

- an initial $\log$ regime which becomes more pronounced the smaller δ is chosen
- a power law regime $\approx t^{1/2}$ and a second $\log$ regime at later stages

Main ongoing work

- coarsening dynamical system for HCCH
- extension to a more realistic model
- simulations and coarsening analysis in 2+1D