Chaotic Modeling and Simulation (CMSIM) 1: 29–38, 2011

Pattern Formation of the Stationary Cahn-Hilliard Model

Hansjörg Kielhöfer

University of Augsburg, Germany
(E-mail: hansjoerg.kielhoefer@math.uni-augsburg.de)

Abstract. We investigate critical points of the free energy of the Cahn-Hilliard model of a binary alloy under the constraint of a constant mass. The domain is the unit square. Minimizers of the energy without interfacial energy term are given by a decomposition of the two components of the alloy, but the interfaces between the components are arbitrary. Specific patterns are only formed if an interfacial energy term is present. We select such patterns of minimizers by an approximation of sequences of conditionally critical points of the free energy when the interfacial energy term tends to zero. This is what we call Pattern Formation of the Stationary Cahn-Hilliard Model. Mathematically it is a singular limit process.

We obtain the conditionally critical points by a global bifurcation analysis of the Euler-Lagrange equation for the free energy where the mass is the bifurcation parameter and where the constant homogeneous mixtures give the trivial solutions. By using characteristic symmetries and monotonicities of the bifurcating solutions we show that singular limits exist for all masses in the so-called spinodal region and that they are minimizers of the free energy without interfacial energy term.

Keywords: Cahn-Hilliard model, Spinodal decomposition, Global bifurcation, Geometry of global branches, Singular limit process, Pattern formation, Weierstraß-Erdmann corner condition.

A binary alloy in a vessel Ω can be described by a function $u\colon \Omega \to \mathbb{R}$ as follows: $u(x) \in [0,1]$ means that the mixture contains $u(x) \cdot 100\,\%$ of one component at $x \in \Omega$. The energy density of the alloy is modelled by $W(u)$, where W is a two-well potential (Figure 1).

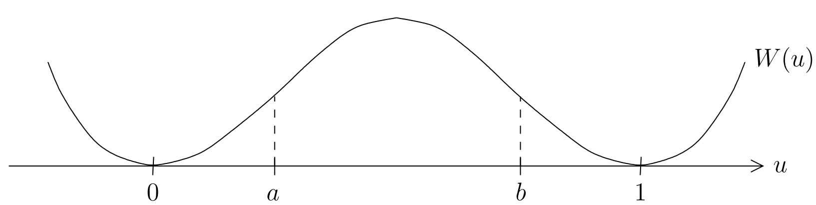


Figure 1

Received: 20 September 2011 / Accepted: 21 October 2011

ISSN 2241-0503

$W(u(x))$ is minimal, if only one component is present at $x \in \Omega$. Any mixture of the two components costs energy. The interval (a,b), where W loses its convexity, is called "spinodal region".

The total energy is given by

$$E_0(u) = \int_\Omega W(u)\,\mathrm{d}x \tag{1}$$

and the mass conservation is formulated as

$$\frac{1}{|\Omega|}\int_\Omega u\,\mathrm{d}x = m \in (0,1). \tag{2}$$

The energy (1) under the constraint (2) is minimal for the following concentrations:

$$u_0(x) = \begin{cases} 0 & \text{for } x \in \Omega_0, \\ 1 & \text{for } x \in \Omega_1, \end{cases} \tag{3}$$

with

$$\begin{aligned} |\Omega_0| &= (1-m)|\Omega|, \\ |\Omega_1| &= m|\Omega|. \end{aligned} \tag{4}$$

The following Figure 2 sketches a possible distribution of the two components in a square Ω. The decomposition of the two components is called "spinodal decomposition".

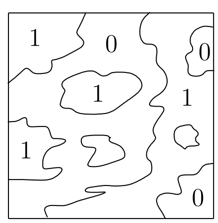


Figure 2

Only the measures of Ω_0 and Ω_1 are determined, their patterns are arbitrary. In experiments, however, certain patterns are preferred, for instance patterns with circular "interfaces".

The model is not yet complete: Taking care of the energy of the interfaces between the two components the total energy is described as

$$E_\varepsilon(u) = \int_\Omega \frac{\varepsilon}{2}\|\nabla u\|^2 + W(u)\,\mathrm{d}x, \quad \varepsilon > 0, \text{ small}, \tag{5}$$

which is called the "Cahn-Hilliard Energy".

Let u_ε be a minimizer of $E_\varepsilon(u)$ under the constraint of mass conservation. One expects for small $\varepsilon > 0$:

$$u_\varepsilon(x) \approx \begin{cases} 0 & \text{for } x \in \Omega_{0,\varepsilon}, \\ 1 & \text{for } x \in \Omega_{1,\varepsilon}, \end{cases}$$

with a profile at the interface of the form (Figure 3)

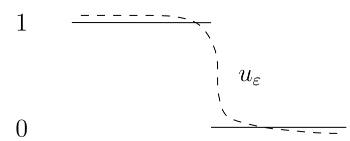


Figure 3

such that for $\varepsilon \searrow 0$

$$u_\varepsilon(x) \longrightarrow u_0(x) = \begin{cases} 0 & \text{for } x \in \Omega_{0,0}, \\ 1 & \text{for } x \in \Omega_{1,0}, \end{cases}$$

and u_0 is a minimizer of $E_0(u)$ under the same constraint.

This "singular limit process" defines the sets $\Omega_{0,0}$ and $\Omega_{1,0}$, in particular their patterns. We call it "Pattern Formation of the Stationary Cahn-Hilliard Model". Due to the "Criterion of Minimal Interface" of Modica from the year 1987, see [5], patterns with circular interfaces are created (Figure 4): If minimizers of (5) under the constraint (2) tend to u_0 in $L^1(\Omega)$ as $\varepsilon \searrow 0$, then the interface between $\Omega_{0,0}$ and $\Omega_{1,0}$ is minimal.

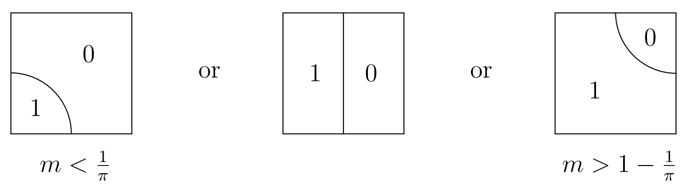


Figure 4. Criterion of Minimal Interface (Modica 1987)

For one-dimensional domains Ω this was already shown by Carr, Gurtin, and Slemrod in 1984, see [1]: The singular limit of conditional minimizers is piecewise constant with one single jump in the interval Ω.

In 1995 Grinfeld and Novick-Cohen [2] classified all conditionally critical points of (5) over an interval. They did not study their singular limits, i. e., their pattern formation.

In the sequel we study the pattern formation of conditionally critical points of (5) over the unit square Ω in $\mathbb{R}^2$. Observe that $|\Omega| = 1$. (Proofs can be found in [3], [4].)

We substitute $m = \lambda$, $u = \lambda + v$ and obtain

$$E_\varepsilon(v, \lambda) = \int_\Omega \frac{\varepsilon}{2} \|\nabla v\|^2 + W(\lambda + v)\,\mathrm{d}x \tag{6}$$

under the constraint

$$\int_\Omega v\,\mathrm{d}x = 0. \tag{7}$$

Conditionally critical points of $E_\varepsilon(v, \lambda)$ satisfy

a) the Euler-Lagrange equation:

$$-\varepsilon \Delta v + W'(\lambda + v) = \text{const.} \quad \text{in } \Omega,$$

b) the natural boundary conditions:

$$\frac{\partial v}{\partial n} = 0 \quad \text{on } \partial\Omega \text{ (Neumann boundary conditions)},$$

c) the constraint of mean value zero:

$$\int_\Omega v \, \mathrm{d}x = 0.$$

Conditions b) and c) are incorporated into a function space X and a) is expressed as

$$\begin{aligned} &G_\varepsilon(v,\lambda) := -\varepsilon\Delta v + W'(\lambda+v) - \textstyle\int_\Omega W'(\lambda+v)\,\mathrm{d}x = 0 \\ &\quad \text{for } (v,\lambda) \in X \times \mathbb{R}. \end{aligned} \tag{8}$$

We have the trivial solution

$$G_\varepsilon(0,\lambda) = 0 \quad \text{for all } \varepsilon > 0,\ \lambda \in \mathbb{R}, \tag{9}$$

which describes by $u \equiv \lambda = m$ a homogeneous mixture.

We look for nontrivial solutions (v, λ) of (8) that bifurcate from the trivial solution line $\{(0,\lambda) \mid \lambda \in \mathbb{R}\}$.

I. In the first part we fix $\varepsilon > 0$ and we consider $\lambda \in \mathbb{R}$ as a variable bifurcation parameter.

I.1 Possible bifurcation points $(0, \lambda)$ have to satisfy

$$\begin{aligned} D_v G_\varepsilon(0,\lambda)v = -\varepsilon\Delta v + W''(\lambda)v &= 0 \quad \text{in } \Omega, \\ \frac{\partial v}{\partial n} &= 0 \quad \text{on } \partial\Omega, \\ \textstyle\int_\Omega v\,\mathrm{d}x &= 0, \end{aligned} \tag{10}$$

for some nontrivial $v \in X$. This linear eigenvalue problem (10) has the solutions $v(x_1, x_2) = \cos n\pi x_1$ and $v(x_1, x_2) = \cos n\pi x_2$ for $n \in \mathbb{N}$ provided $W''(\lambda) = -\varepsilon n^2\pi^2$.

We do not consider these one-dimensional solutions here but we are rather interested in

$$\begin{aligned} v_n(x) &= \cos n\pi x_1 + \cos n\pi x_2 \qquad \text{for } W''(\lambda) = -\varepsilon n^2\pi^2, \\ v_{nn}(x) &= \cos n\pi x_1\, \cos n\pi x_2 \qquad \text{for } W''(\lambda) = -2\varepsilon n^2\pi^2. \end{aligned} \tag{11}$$

The bifurcation points, which are solutions of the "characteristic equation", appear in pairs as depicted in Figure 5:

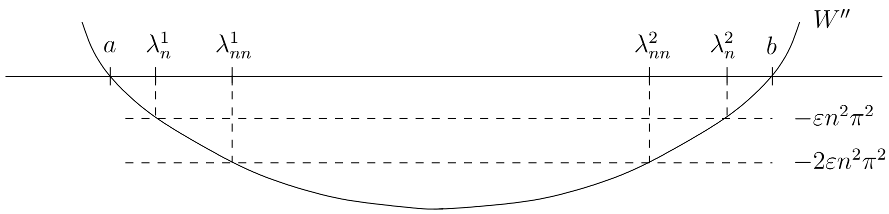
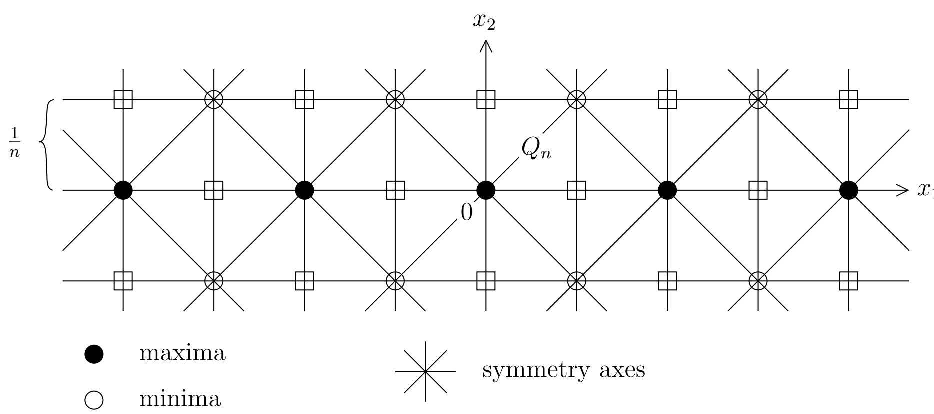


Figure 5

The number of modes $n = 1, \ldots, N(\varepsilon)$, generating bifurcation points in the spinodal region (a, b) as shown in Figure 5, tends to infinity as ε tends to zero.

The symmetries of the eigenfunctions (11) play a crucial role in the subsequent analysis. For v_n they are shown in the following Figure 6:



$Q_n = [0, \frac{1}{n}] \times [0, \frac{1}{n}]$

Figure 6

We define a subspace $X_n \subset X$ by the symmetries (and periodicities) of v_n and we define $X_{nn} \subset X_n \subset X$ by the symmetries (and periodicities) of v_{nn}.

I.2 We solve $G_\varepsilon(v, \lambda) = 0$ for $(v, \lambda) \in X_n \times \mathbb{R}$ as well as for $(v, \lambda) \in X_{nn} \times \mathbb{R}$. The bifurcation points are

$$(0, \lambda_{kn}^1), (0, \lambda_{kn,kn}^1), \text{and } (0, \lambda_{kn}^2), (0, \lambda_{kn,kn}^2), \quad k \in \mathbb{N}, \tag{12}$$

provided

$$W''(\lambda_{kn}^i) = -\varepsilon(kn)^2\pi^2 \quad \text{and} \quad W''(\lambda_{kn,kn}^i) = -2\varepsilon(kn)^2\pi^2 \tag{13}$$

for $i = 1, 2$. A local and global bifurcation analysis then gives the bifurcation diagram sketched in Figure 7:

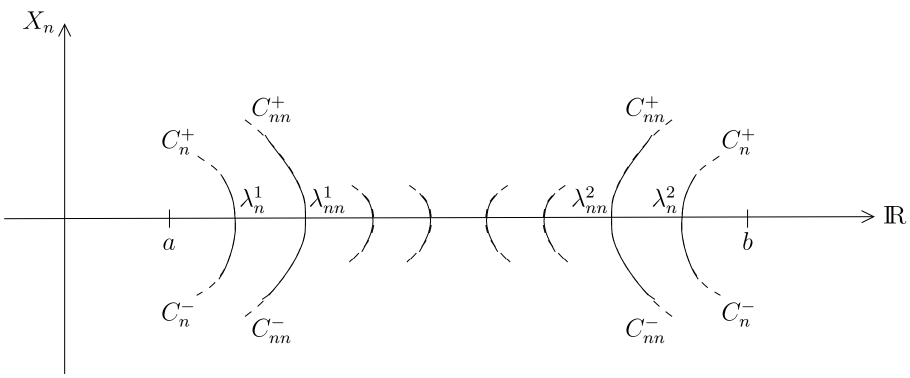


Figure 7

The branches C_n^- and C_{nn}^- are obtained from C_n^+, C_{nn}^+ by "reversion", i. e., by a reflection and a phase shift of half the period in both directions and in one direction, respectively.

By a famous result of Rabinowitz from the year 1971 all bifurcation continua are unbounded or meet the trivial solution line a second time.

I.3 In order to decide which Rabinowitz alternative holds in our case, we determine the geometry of solutions on the global continua C_n^+. (A similar analysis determines the geometry of solutions in C_{nn}^+.) We define an order in $\mathbb{R}^2$ by the positive cone $K = \{x = (x_1, x_2) \mid x_1 \geq 0, x_2 \geq 0\}$ in $\mathbb{R}^2$ (Figure 8):

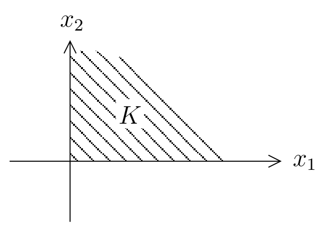


Figure 8

$$x \leq y \quad \Leftrightarrow \quad y - x \in K. \tag{14}$$

The eigenfunction v_n is monotonic in the square $Q_n = [0, \frac{1}{n}] \times [0, \frac{1}{n}]$:

$$x, y \in Q_n,\ x \leq y \quad \Rightarrow \quad v_n(x) \geq v_n(y). \tag{15}$$

By the symmetries (and periodicities) of v_n there is a monotonicity of v_n in all squares of the symmetry lattice.

By using the elliptic maximum principle and the connectivity of C_n^+ it can be shown that the monotonicity (15) is preserved for all solutions of $G_\varepsilon(v, \lambda) = 0$ on C_n^+:

$$x, y \in Q_n,\ x \leq y \quad \Rightarrow \quad v(x) \geq v(y) \tag{16}$$

The consequences of (16) are that the location of the maxima, minima, and saddles is fixed for all solutions on C_n^+. This, in turn, implies that all bifurcating continua C_n^+ and C_{nn}^+ are separated.

I.4 The geometry of solutions on C_n^+ described before helps to derive the following a priori estimates:

$$(v,\lambda) \in C_n^+ \quad \Rightarrow \quad \begin{aligned} &\|v\|_{L^\infty(\Omega)} + |\lambda| \le M_1, \\ &\|v\|_{C^{2+\alpha}(\overline{\Omega})} \le M_2/\varepsilon^2, \end{aligned} \tag{17}$$

where M_1 and M_2 do not depend on $\varepsilon > 0$. The results of I.3 and (17) then yield the global bifurcation diagram sketched in Figure 9:

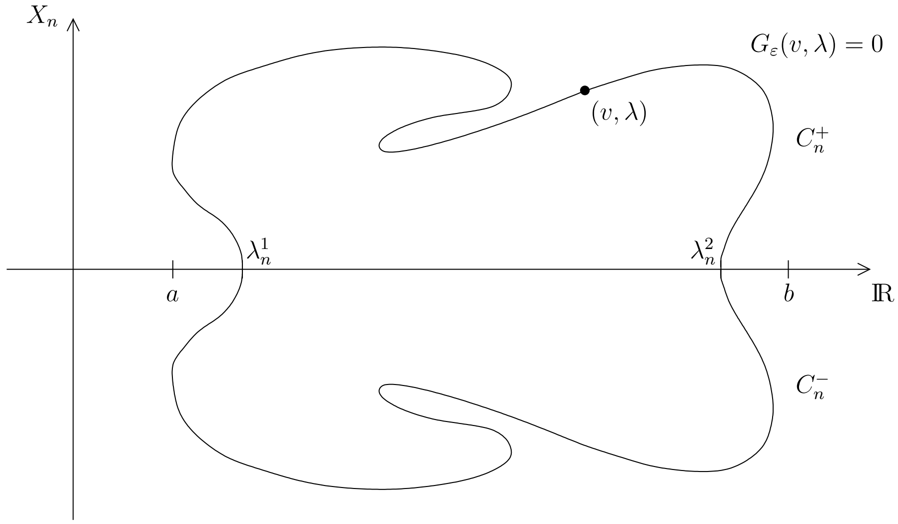


Figure 9

The turning points are explained later.

II. In the second part we fix λ in the spinodal region (a,b) and let ε tend to 0. Since the solution continua C_n^+ depend on ε we change the notation:

$$\begin{aligned} &C_n^+ = C_{n,\varepsilon}^+ \\ &(v,\lambda) \in C_{n,\varepsilon}^+ \quad \Rightarrow \quad v = v_{\lambda,\varepsilon}, \quad \text{where } G_\varepsilon(v_{\lambda,\varepsilon},\lambda) = 0. \end{aligned} \tag{18}$$

II.1 Let $\varepsilon_n \searrow 0$ and consider the sequence $(v_{\lambda,\varepsilon_n})_{n\in\mathbb{N}}$ in $L^p(\Omega)$. The estimates $\|v_{\lambda,\varepsilon_n}\|_{L^\infty(\Omega)} \le M_1$ and $\|v_{\lambda,\varepsilon_n}\|_{C^{2+\alpha}(\overline{\Omega})}\| \le M_2/\varepsilon_n^2$ do not imply that this sequence is relatively compact in $L^p(\Omega)$ for $1 \le p < \infty$. However, by the monotonicity (16) it is relatively compact in $L^p(Q_n)$, and therefore, by the symmetries (and periodicities), it is relatively compact in $L^p(\Omega)$. This follows by an extension of Helly's theorem on one-dimensional monotonic sequences to two dimensions. Thus we can state (w. l. o. g.):

$$\begin{aligned} v_{\lambda,\varepsilon_n} \longrightarrow v_{\lambda,0} \quad &\text{in } L^p(\Omega) \text{ for } 1 \le p < \infty \\ \text{as } \varepsilon_n \searrow 0.& \end{aligned} \tag{19}$$

II.2 The properties of the singular limit $v_{\lambda,0} \in L^p(\Omega)$ are:

a) $\displaystyle\int_\Omega v_{\lambda,0}\,\mathrm{d}x = 0,$

b) $v_{\lambda,0} \in X_n$, $v_{\lambda,0}$ is monotonic in Q_n,

c) $\lambda + v_{\lambda,0} = u_{\lambda,0}$ is a conditionally critical point of $E_0(u) = \int_\Omega W(u)\,\mathrm{d}x$, i. e., $W'(u_{\lambda,0}) = \text{const.}$,

d) $v_{\lambda,0} \neq 0$, i. e., $v_{\lambda,0}$ is nontrivial,

e) $u_{\lambda,0}$ has precisely two values.

Property d) is not obvious. It follows from $W''(u_{\lambda,0}) \geq 0$, which, in turn, is a consequence of the variational characterization of the positive principal eigenvalue of an eigenvalue problem with weight function. Property e) then follows from c) and $W''(u_{\lambda,0}) \geq 0$. Finally,

f) $u_{\lambda,0}$ is a global minimizer of $E_0(u)$ under the constraint $\int_\Omega u\,\mathrm{d}x = \lambda = m \in (a, b)$.

Property f) is not obvious as well. It follows from the second Weierstraß-Erdmann corner condition developed for discontinuous global minimizers of one-dimensional variational problems:

$$\begin{aligned}&W(u_{\lambda,0}) - u_{\lambda,0}W'(u_{\lambda,0}) \text{ is continuous,}\\ &\text{which means constant by e).}\end{aligned} \tag{20}$$

Property (20) admits only the following two values for $u_{\lambda,0}$ which proves f):

$$u_{\lambda,0}(x) = \begin{cases} 0 & \text{for } x \in \Omega_{0,0}, \\ 1 & \text{for } x \in \Omega_{1,0}, \end{cases} \tag{21}$$

where the sets $\Omega_{0,0}$ and $\Omega_{1,0}$ depend on $\lambda = m$. This accomplishes the pattern formation of the stationary Cahn-Hilliard model.

For $n = 4$ we obtain the following pattern in X_n (Figure 10):

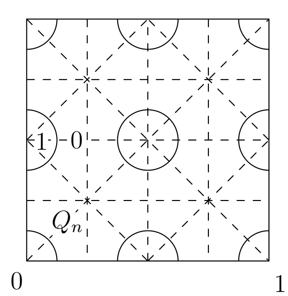


Figure 10

In the symmetry class X_{nn} a pattern for $n = 4$ is the following Figure 11:

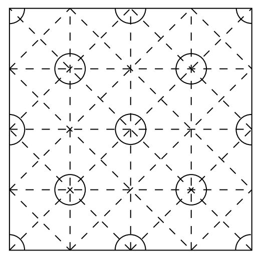


Figure 11

The interfaces are circular, if $u_{\lambda,\varepsilon}$ are conditional mimimizers of $E_\varepsilon(u)$.

However, not all $u_{\lambda,\varepsilon} = \lambda + v_{\lambda,\varepsilon}$, where $(v_{\lambda,\varepsilon}, \lambda) \in C^+_{n,\varepsilon}$, are minimizers with mean value $\lambda = m \in (a, b)$.

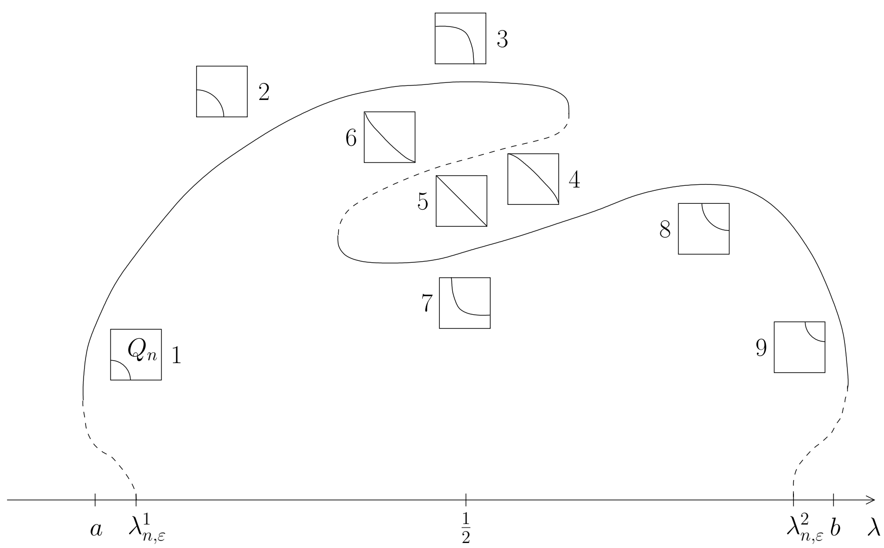


Figure 12

Figure 12 sketches the global continuum $C^+_{n,\varepsilon}$ for small $\varepsilon > 0$. A continuous transition from pattern 1 to pattern 9 in keeping the monotonicity and symmetry of $u_{\lambda,\varepsilon}$ in Q_n is only possible through patterns 4, 5, 6, which are not created by minimizers, since the interface is not minimal. Therefore the continuum has to have two additional turning points, where the stability changes. In particular, the continuum with patterns 4, 5, 6 is unstable, i. e., the critical points $u_{\lambda,\varepsilon}$ are not minimizers. These heuristic arguments for the turning points are verified by a numerical pathfollowing.

References

1.J. Carr, M. E. Gurtin, and M. Slemrod. Structured Phase Transitions on a Finite Interval. Archive for Rational Mechanics and Analysis **86**, 317–351, 1984.

2. M. Grinfeld and A. Novick-Cohen. Counting stationary solutions of the Cahn-Hilliard equation by transversality arguments. Proceedings of the Royal Society of Edinburgh **125A**, 351–370, 1995.
3. H. Kielhöfer. Pattern Formation of the Stationary Cahn-Hilliard Model. Proceedings of the Royal Society of Edinburgh **127A**, 1219–1243, 1997.
4. H. Kielhöfer. Minimizing Sequences Selected via Singular Perturbations, and their Pattern Formation. Archive for Rational Mechanics and Analysis **155**, 261–276, 2000.
5. L. Modica. The Gradient Theory of Phase Transitions and the Minimal Interface Criterion. Archive for Rational Mechanics and Analysis **98**, 123–142, 1987.