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On the Competition of Elastic Energy and Surface Energy in Discrete Numerical Schemes

by

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ON THE COMPETITION OF ELASTIC ENERGY AND SURFACE ENERGY IN DISCRETE NUMERICAL SCHEMES

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Abstract:
The Γ-limit of certain discrete free energy functionals related to the numerical approximation of Ginzburg-Landau models is analysed when the distance h between neighbouring points tends to zero. The main focus lies on cases where there is competition between surface energy and elastic energy. Two discrete approximation schemes are compared, one of them shows a surface energy in the Γ-limit. Finally, numerical solutions for the sharp interface Cahn-Hilliard model with linear elasticity are investigated. It is demonstrated how the viscosity of the numerical scheme introduces an artifical surface energy that leads to unphysical solutions.

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1 Introduction

This article is concerned with the behaviour of certain discrete schemes where there is competition between surface energy and elastic energy. Often, the surface energy will not appear in the limit, but sometimes if the ratio between surface energy and elastic energy is suitable this may be the case. We will compare two discrete approximation schemes that are related to discrete energy functionals $\mathcal{H}_1^h$, $\mathcal{H}_2^h$. These schemes compute the free energy of double well potentials and discretise the deformation gradient ∇u with a step size $h > 0$. In the first example, ∇u is approximated by a two point stencil, and no surface energy appears for $h \searrow 0$. If three or more points are used in the approximation of the deformation gradient, this may be different. The second functional $\mathcal{H}_2^h$ is one simple example which produces a surface energy in the limit.

The choice on $\mathcal{H}_1^h$, $\mathcal{H}_2^h$ is motivated by the approximation of the free energy in physical systems where phase transitions take place and are especially related to phenomena like crystal growth, [2], segregation processes, [7], polymers and particular effects in fluid mechanics as cavitation, [4].

As a practical example, we will consider the Cahn-Hilliard model with linear elasticity where two phases are assumed to occupy a bounded domain $\Omega \subset \mathbb{R}^D$ with Lipschitz boundary. If γ is a given constant where $\sqrt{\gamma}$ is the thickness of the transition layer between two phases, the corresponding free energy has the form

$$\mathcal{F}(\varrho, u) := \int\limits_\Omega \Big(W(\varrho(x)) + \frac{\gamma}{2}|\nabla \varrho(x)|^2 + Q(\varrho(x), u(x)) \Big)\, dx. \qquad (1)$$

Here $\varrho : \Omega \times (0, T_0) \to \mathbb{R}^+$ defines the density of one component of the alloy, $u : \Omega \to \mathbb{R}^D$ the deformation applied to the solid, $T_0 > 0$ is a chosen stop time, $Q(\varrho, u) \geq 0$ the elastic energy density and $W \geq 0$ a double well potential. W has two spatially separated minima ϱ_1, ϱ_2, for instance $W(\varrho) := (\varrho - \varrho_1)^2(\varrho - \varrho_2)^2$. The complete context of the Cahn-Hilliard model with linear elasticity will be outlined in Section 6. The viscosity of the numerical scheme implicitly introduces an artificial surface energy that regularises the solution and leads in computations for the sharp interface model to unphysical solutions.

This work is organised in the following way. In Section 2, a one-dimensional layer of n atoms is considered and a discrete energy functional $\mathcal{G}^h$ is introduced that describes the elastic energy of the chain and accounts for interactions of nearest and second nearest neighbours.

After shortly recapitulating the notion of Γ-convergence in Section 3, the Γ-limit $h \searrow 0$ of $\mathcal{G}^h$ is identified in Section 4. In [5], [6] related results are shown in $L^1(\Omega)$ with different growth conditions on the energy, [1] treats general L^p with $p < \infty$ but assumes periodicity conditions that arise naturally in homogenisation.

The results of Section 4 are the foundations of the analysis in later sections but can be used independently for the understanding of one-dimensional chains. As an application, in Section 5 the two discrete functionals $\mathcal{H}_1^h$, $\mathcal{H}_2^h$ mentioned above are discussed and the behaviour of these two functionals is compared when $h \searrow 0$.

In Section 6, the Cahn-Hilliard model with linear elasticity in case of two phases is reviewed. Mainly, this section is devoted to the interpretation of the numerical solution for the case that γ is set to 0. With the knowledge of Section 4, we can prove that the surface energy inherent in the approximation scheme leads to an unphysical solution. We end up with a discussion of the results.

2 The discrete system

We consider a one-dimensional equally spaced monatomic layer that we identify with a domain $\Omega := (0, L) \subset \mathbb{R}$ of given length $L > 0$.

We suppose that the undeformed reference configuration is given by a discrete system of $n + 1$ atoms with equal distance located at points R_i^h, where

$$R_i^h := ih, \quad 0 \leq i \leq n.$$

Here, the equality $h := L/n$ defines the number n which is to be understood in the sense $n = n(h)$. The limit $h \searrow 0$ corresponds to $n \to \infty$. We allow only those h such that $n \in \mathbb{N}$. By $\widehat{R}_i$, $0 \leq i \leq n$, we denote the position of the i-th atom after the deformation. Finally, by u_i^h, $0 \leq i \leq n$, we denote the displacement of atom i, i.e.

$$u_i^h = \widehat{R}_i^h - R_i^h, \quad 0 \leq i \leq n.$$

For given deformation u^h, we introduce the notation

$$\partial_h u_i^h := \frac{u_i^h - u_{i-1}^h}{h},$$

which is one common way of writing the forward difference quotient. To simplify the notation, we extend u^h and formally set $u_{-1}^h := u_0^h$ such that $\partial_h u_0^h = 0$.

In a first step, we will consider discrete functionals of the form

$$G^h(\{u_i^h\}_{0\le i\le n}) := \sum_{i=1}^{n} \Big(Q_1(\partial_h u_i^h) + Q_2(\partial_h u_{i-1}^h + \partial_h u_i^h) \Big), \tag{2}$$

for given functionals Q_1, $Q_2 : L^p(0,L) \to \mathbb{R}$ with $1 < p < \infty$. The term Q_1 describes interactions of nearest neighbours of atoms, Q_2 accounts for interactions of second-nearest neighbours, see [10].

We make the following assumptions on the growth of the energy functions Q_1, Q_2:

(A1) There exist positive constants c_1, c_2, C_1, C_2, such that

$$c_1|u|^p - c_2 \le Q_1(u) \le C_1|u|^p + C_2 \quad \forall u \in L^p(0,L).$$

(A2) There exist positive constants c_3, c_4, C_3, C_4, such that

$$c_3|u|^p - c_4 \le Q_2(u) \le C_3|u|^p + C_4 \quad \forall u \in L^p(0,L).$$

Finally, in order to rewrite the discrete sum as an integral, we define the rescaling

$$\widetilde{G}^h(u^h) := hG^h(u^h). \tag{3}$$

3 The concept of Γ-convergence

Let $\Omega \subset \mathbb{R}^D$ be an open set with Lipschitz boundary. A family $(E_h)_{h>0}$ of functionals defined on $L^1(\Omega)$ with values in $\mathbb{R}\cup\{\infty\}$ is said to Γ-converge for $h \searrow 0$ to a functional E for a chosen argument $u \in L^1(\Omega)$, if the following two conditions are satisfied:

(i) For all sequences $(u_h)_{h>0} \subset L^1(\Omega)$ with $\lim_{h\searrow 0} \int_\Omega |u_h - u| = 0$ one has

$$E(u) \le \liminf_{h\searrow 0} E_h(u_h).$$

(ii) There exists a sequence $(u_h)_{h>0} \subset L^1(\Omega)$ such that $\lim_{h\searrow 0} \int_\Omega |u_h - u| = 0$ and

$$E(u) \ge \limsup_{h\searrow 0} E_h(u_h).$$

The following theorem explains why the concept of Γ-convergence is so important for the analysis of variational problems.

Theorem 1 *(***Minimimum property of the Γ-limit***)*
Let u_h be a minimiser of E_h in $L^1(\Omega)$ and $u_h \to u$ in $L^1(\Omega)$ as $h \searrow 0$. If E_h additionally Γ-converges for fixed $u \in L^1(\Omega)$ to E as $h \searrow 0$, then u is a minimum of E in $L^1(\Omega)$ and

$$\lim_{h\searrow 0} E_h(u_h) = E(u).$$

The quite simple proof of Theorem 1 is found in [3]. The concept of Γ-convergence goes back to early works by de Giorgi, see [8], [9]. A comprehensive discussion of Γ-convergence is found in the monograph [3], where Γ-convergence is referred to as epi-convergence. One advantage of the concept of Γ-convergence lies in the fact that it is invariant under continuous perturbations.

4 The Γ-limit of the elastic energy functional

In order to study the Γ-limit of $\widetilde{G}^h$ as $h \searrow 0$, it is suitable to analyse the behaviour of $\widetilde{G}^h$ not only as a mapping depending on a set of discrete points, but as a mapping of functions. To this end we follow the work of Braides, Dal Maso and Garroni, [5], and introduce for $h > 0$ the space $\mathcal{A}^h$ of continuous functions on $(0, L)$ which are affine linear on every interval $[R_i^h, R_{i+1}^h]$, $0 \le i \le n-1$.

There is a one-to-one correspondence between $(u_i^h)_{1\le i\le n}$ and its representation in the space $\mathcal{A}^h$. Due to $u_{-1}^h = u_0^h$, this representation can be extended to a constant function in $(-h, 0]$. By $\nabla u^h \in \mathcal{A}^h$ we denote the derivative of u^h defined by $\nabla u^h|_{(R_i^h, R_{i+1}^h)} = \partial_h u^h$ for $1 \le i \le n-1$ and $\nabla u^h \equiv 0$ on $(-h, 0]$.

After continuation of $\partial_h u^h$ to ∇u^h, we can restate the discrete sum of $\widetilde{G}^h$ as a continuous functional,

$$\widetilde{\mathcal{G}}^h(u^h) := \begin{cases} \int_0^L Q_1(\nabla u^h(x)) + Q_2(\nabla u^h(x-h) + \nabla u^h(x))\,dx & \text{if } u \in H^{1,p}(0,L), \\ +\infty & \text{else.} \end{cases} \tag{4}$$

We can show:

Theorem 2 *(*Γ**-limit of the elastic energy functional***)*
Assume that the Assumptions (A1) and (A2) hold for Q_1, Q_2. Then the functional $\widetilde{\mathcal{G}}^h$ Γ-converges for $h \searrow 0$ to a functional $\widetilde{\mathcal{G}} : L^p(0,L) \to \mathbb{R}$ defined by

$$\widetilde{\mathcal{G}}(u) := \begin{cases} \int_0^L V^{**}(\nabla u(x))\,dx & \text{if } u \in H^{1,p}(0,L), \\ +\infty & \text{else.} \end{cases}$$

Here, $V(u) := \overline{Q}_1(u) + Q_2(u)$, where

$$\overline{Q}_1(u) := \frac{1}{2} \min\Big\{ Q_1(u_1) + Q_1(u_2) \mid u_1 + u_2 = 2u \Big\},$$

and V^{**} denotes the convexification of the function V.

The convexification V^{**} of a function V is defined as the greatest convex function less than V, see [14]. The appearance of V^{**} in the Γ-limit is not surprising, but is in accordance with well-known results by L. Modica, [13].

Proof:

(a) Proof of the lim inf-inequality:

Let a sequence $(u^h)_{h>0} \subset L^p(0,L)$ be given with $u^h \to u$ in $L^p(0,L)$. We have to show that

$$\widetilde{\mathcal{G}}(u) \le \liminf_{h\searrow 0} \widetilde{\mathcal{G}}^h(u^h). \tag{5}$$

Obviously, (5) holds if $\liminf_{h\searrow 0} \widetilde{\mathcal{G}}^h(u^h) = +\infty$. Hence we may assume that

$$\liminf_{h\searrow 0} \widetilde{\mathcal{G}}^h(u^h) < \infty \tag{6}$$

or $u^h \in \mathcal{A}^h$ for $h > 0$.

Then we find

$$\begin{aligned}\widetilde{\mathcal{G}}^h(u^h) &= \int_0^L Q_1(\nabla u^h(x)) + Q_2(\nabla u^h(x-h) + \nabla u^h(x))\,dx \\ &\geq (c_1+c_3)\int_0^L |\nabla u^h(x)|^p - (c_2+c_4)L. \qquad (7)\end{aligned}$$

The last is due to Assumptions (A1) and (A2). From (6) and (7) it follows $\sup_{h>0}\|\nabla u^h\|_{L^p(0,L)} < \infty$ and because of $p<\infty$ we obtain $u^h \rightharpoonup u$ in $H^{1,p}(0,L)$ for $h \searrow 0$ and in particular $u \in H^{1,p}(0,L)$.

Now we want to find a sharper estimate from below on $\widetilde{\mathcal{G}}^h$. From the definitions we find

$$\begin{aligned}\widetilde{\mathcal{G}}^h(u^h) &= \int_0^L Q_1(\nabla u^h(x)) + Q_2(\nabla u^h(x-h) + \nabla u^h(x))\,dx \\ &= \sum_{i=1}^n hQ_1(\partial_h u_i^h) + \sum_{i=2}^n hQ_2(\partial_h u_{i-1}^h + \partial_h u_i^h).\end{aligned}$$

In order to treat the second term, we use the following trick, which is a decomposition in even and odd indices and well known in literature. We see

$$\begin{aligned}\widetilde{\mathcal{G}}^h(u^h) &= \sum_{i=1}^n hQ_1(\partial_h u_i^h) + \sum_{i=2}^n hQ_2(\partial_h u_{i-1}^h + \partial_h u_i^h) \\ &= \sum_{\substack{i=2\\ i \text{ even}}}^n \frac{h}{2}(Q_1(\partial_h u_{i-1}^h) + Q_1(\partial_h u_i^h)) + \sum_{\substack{i=2\\ i \text{ even}}}^n hQ_2(\partial_h u_{i-1}^h + \partial_h u_i^h) \\ &\quad + \sum_{\substack{i=3\\ i \text{ odd}}}^n \frac{h}{2}(Q_1(\partial_h u_{i-1}^h) + Q_1(\partial_h u_i^h)) + \sum_{\substack{i=3\\ i \text{ odd}}}^n hQ_2(\partial_h u_{i-1}^h + \partial_h u_i^h) \\ &\quad + \frac{h}{2}Q_1(\partial_h u_1^h) + \frac{h}{2}Q_1(\partial_h u_n^h).\end{aligned}$$

By Assumption (A1) we have

$$\frac{h}{2}Q_1(\partial_h u_1^h) + \frac{h}{2}Q_1(\partial_h u_n^h) \geq -c_2 h$$

which yields

$$\begin{aligned}\widetilde{\mathcal{G}}^h(u^h) &\geq \sum_{\substack{i=2\\ i \text{ even}}}^n h\Big(\overline{Q}_1\big(\frac{\partial_h u_{i-1}^h + \partial_h u_i^h}{2}\big) + Q_2(\partial_h u_{i-1}^h + \partial_h u_i^h)\Big) \\ &\quad + \sum_{\substack{i=3\\ i \text{ odd}}}^n h\Big(\overline{Q}_1\big(\frac{\partial_h u_{i-1}^h + \partial_h u_i^h}{2}\big) + Q_2(\partial_h u_{i-1}^h + \partial_h u_i^h)\Big) + O(h) \\ &= \sum_{i=2}^n hV\Big(\frac{\partial_h u_{i-1}^h + \partial_h u_i^h}{2}\Big) + O(h) \\ &= \int_h^L V\Big(\frac{\nabla u^h(x-h) + \nabla u^h(x)}{2}\Big)\,dx + O(h)\end{aligned}$$

and consequently

$$\widetilde{\mathcal{G}}^h(u^h) \geq \int_h^L V^{**}\Big(\frac{\nabla u^h(x-h) + \nabla u^h(x)}{2}\Big)\,dx + O(h).$$

Now, let $\{x_0, x_1, \ldots, x_m\}$ be a decomposition of $(0, L)$. Introducing the symbol $l^h := \min_{0\le i\le m}\{x_i \mid x_i \ge h\} + 1$ we see

$$\begin{aligned}\widetilde{\mathcal{G}}^h(u^h) &\ge \sum_{i=l^h}^{m}\int_{x_{i-1}}^{x_i} V^{**}\Big(\frac{\nabla u^h(x-h)+\nabla u^h(x)}{2}\Big)\,dx + O(h)\\ &\ge \sum_{i=l^h}^{m}(x_i - x_{i-1})V^{**}\Big(\frac{1}{2}\fint_{x_{i-1}}^{x_i}\nabla u^h(x-h)\,dx + \frac{1}{2}\fint_{x_{i-1}}^{x_i}\nabla u^h(x)\,dx\Big)\\ &\quad + O(h).\end{aligned} \tag{8}$$

Here we used Jensen's inequality

$$\int_S \varphi(u(x))\,dx \ge \varphi\Big(\int_S u(x)\,dx\Big)$$

which holds for any convex real valued function φ.

From elementary estimates we obtain

$$\begin{aligned}&\left|\fint_{x_{i-1}}^{x_i}\nabla u^h(x-h)\,dx - \fint_{x_{i-1}}^{x_i}\nabla u^h(x)\,dx\right|\\ &\quad\le \frac{1}{|x_i - x_{i-1}|}\left(\left|\fint_{x_{i-1}-h}^{x_{i-1}}\nabla u^h(x)\,dx - \fint_{x_{i-1}}^{x_i}\nabla u^h(x)\,dx\right|\right)\\ &\quad\le \frac{1}{|x_i - x_{i-1}|}\left(\fint_{x_{i-1}-h}^{x_{i-1}}|\nabla u^h(x)|\,dx + \fint_{x_{i-1}}^{x_i}|\nabla u^h(x)|\,dx\right)\\ &\quad\le \frac{1}{|x_i - x_{i-1}|}h^{p'}\|\nabla u^h\|_{L^p(0,L)},\end{aligned} \tag{9}$$

where in the last line Hölder's inequality is used and $p' = \frac{p}{p-1}$ is the dual exponent to p.

As the right hand side of (9) tends to 0 as $h \searrow 0$, we find

$$\fint_{x_{i-1}}^{x_i}\nabla u^h(x-h)\,dx \to \fint_{x_{i-1}}^{x_i}\nabla u^h(x)\,dx \to \fint_{x_{i-1}}^{x_i}\nabla u(x)\,dx.$$

For sufficiently small h we furthermore have $l^h = 2$.

From (8) it follows after applying the limes inferior as h tends to 0 and because of the continuity of V^{**}:

$$\begin{aligned}\liminf_{h\searrow 0}\widetilde{\mathcal{G}}^h(u^h) &\ge \sum_{i=2}^{m}(x_i - x_{i-1})V^{**}\Big(\fint_{x_{i-1}}^{x_i}\nabla u(x)\,dx\Big)\\ &\ge \int_{x_1}^{L} V^{**}\Big(\sum_{i=2}^{m}\fint_{x_{i-1}}^{x_i}\nabla u(x)\,dx\,\mathcal{X}_{(x_{i-1},x_i)}(x)\Big)\,dx.\end{aligned}$$

Now we let $m \to \infty$ and we postulate that $x_1 = x_1(m) \to 0$ as $m \to \infty$. This yields

$$\liminf_{h\searrow 0}\widetilde{\mathcal{G}}^h(u^h) \ge \int_0^L V^{**}(\nabla u(x))\,dx.$$

Here we used the fact that according to Assumptions (A1) and (A2)

$$V^{**} \ge (c_1 + c_3)|x|^p - (c_2 + c_4).$$

(b) It remains to show property (ii) in the definition of Γ-convergence.

Let $u \in L^p(0,L)$ be given. Then we have to show the existence of a sequence $(u^h)_{h>0} \subset L^p(0,L)$ such that $u^h \to u$ in $L^p(0,L)$ as $h \searrow 0$ and $\limsup_{h\searrow 0} \widetilde{\mathcal{G}}^h(u^h) \leq \widetilde{\mathcal{G}}(u)$.

Without loss of generality we may assume $u \in H^{1,p}(0,L)$. Otherwise we choose $u^h := u$ for all $h > 0$ and there is nothing to show.

In the following we treat the three cases:

(b1) u is affine linear, i.e. $u(x) = ax + b$; (b2) u is piecewise affine;

(b3) u is an arbitrary function in $H^{1,p}(0,L)$.

For the proof of (b2) we will exploit (b1) and for the proof of (b3) statement (b2). We start with the first assertion.

(b1) u is affine linear, i.e. $u(x) = ax + b$.

Let $n = km$ for some m, $k \in \mathbb{N}$. By definition we have

$$\widetilde{\mathcal{G}}^h(u^h) = \int_0^L Q_1(\nabla u^h(x)) + Q_2(\nabla u^h(x-h) + \nabla u^h(x))\,dx.$$

For the construction we will choose funtions u^h which are periodic in any subinterval of $(0,L)$ with length mh. With this property we find

$$\begin{aligned}
\widetilde{\mathcal{G}}^h(u^h) &= \sum_{i=0}^{k-1}\left[\int_{R^h_{im}}^{R^h_{(i+1)m}} Q_1(\nabla u^h(x))\,dx \right.\\
&\qquad\left. + \int_{R^h_{im+1}}^{R^h_{(i+1)m}} Q_2(\nabla u^h(x-h) + \nabla u^h(x))\,dx\right]\\
&= k\left[\int_0^{R^h_m} Q_1(\nabla u^h(x))\,dx \right.\\
&\qquad\left. + \int_{R^h_m}^{R^h_{2m}} Q_2(\nabla u^h(x-h) + \nabla u^h(x))\,dx\right].
\end{aligned} \tag{10}$$

By convexity of V^{**} and Carathéodory's theorem, see for instance [14], we know that there exists a real number λ with $0 < \lambda < 1$ such that

$$V^{**}(a) = \lambda V(p^+) + (1-\lambda)V(p^-) \tag{11}$$

and

$$a = \nabla u = \lambda p^+ + (1-\lambda)p^- \tag{12}$$

for suitable p^+, $p^- \in \mathbb{R}$.

For given λ we introduce the sets

$$\begin{aligned}
\Omega^h_+ &:= \Omega \cap \cup_{i=0}^{k-1}\,(R^h_{im}, R^h_{im+\lfloor\lambda m\rfloor}],\\
\Omega^h_- &:= \Omega \cap \cup_{i=0}^{k-1}\,(R^h_{im+\lfloor\lambda m\rfloor}, R^h_{(i+1)m}]
\end{aligned}$$

such that $\Omega = \Omega^h_+ \cup \Omega^h_-$. Here, the Gauß bracket $\lfloor\cdot\rfloor : \mathbb{R} \to \mathbb{N}$ is defined by

$$\lfloor\alpha\rfloor := \max\{k \in \mathbb{N} \mid k \leq \alpha\}.$$

We have by definition of V

$$V(p^\pm) = \overline{Q}_1(p^\pm) + Q_2(2p^\pm) = \frac{1}{2}\Big(Q_1(p_1^\pm) + Q_1(p_2^\pm)\Big) + Q_2(2p^\pm)$$

and

$$p^+ = \frac{p_1^+ + p_2^+}{2}, \qquad p^- = \frac{p_1^- + p_2^-}{2}$$

for certain real numbers p_1^+, p_2^+, p_1^-, p_2^-.

We choose $u^h(x) = a^h(x)x + b$ where

$$a^h(x) = \begin{cases} p_1^+ & \text{if } x \in \Omega_+^h \cap \cup_{i=0}^{k-1} \cup_{j=0}^{m/2-1} \ (R_{im+2j}^h, R_{im+2j+1}^h], \\ p_2^+ & \text{if } x \in \Omega_+^h \cap \cup_{i=0}^{k-1} \cup_{j=0}^{m/2-1} \ (R_{im+2j+1}^h, R_{im+2j+2}^h], \\ p_1^- & \text{if } x \in \Omega_-^h \cap \cup_{i=0}^{k-1} \cup_{j=0}^{m/2-1} \ (R_{im+2j}^h, R_{im+2j+1}^h], \\ p_2^- & \text{if } x \in \Omega_-^h \cap \cup_{i=0}^{k-1} \cup_{j=0}^{m/2-1} \ (R_{im+2j+1}^h, R_{im+2j+2}^h]. \end{cases}$$

With this setting, Eq. (10) reads

$$\begin{aligned} \widetilde{\mathcal{G}}^h(u^h) &= kh\Bigg\{ \lfloor \lambda m \rfloor \Big[\frac{1}{2}\Big(Q_1(p_1^+) + Q_1(p_2^+)\Big) + Q_2(2p^+)\Big] \\ &\qquad + (m - \lfloor \lambda m \rfloor)\Big[\frac{1}{2}\Big(Q_1(p_1^-) + Q_1(p_2^-)\Big) + Q_2(2p^-)\Big]\Bigg\} \qquad (13) \\ &= \frac{L}{m}\Big[\lfloor \lambda m \rfloor V(p^+) + (m - \lfloor \lambda m \rfloor) V(p^-)\Big]. \end{aligned}$$

For $m \to \infty$ we have $\lfloor \lambda m \rfloor / m \to \lambda$. Consequently

$$\widetilde{\mathcal{G}}^h(u^h) \to \int_0^L V^{**}(\nabla u(x))\, dx = \widetilde{\mathcal{G}}(u), \quad \text{as } n \to \infty.$$

We still have to show that $u^h \to u$ in $L^p(0, L)$. If we formally set $Q_1(v) := v$ and $Q_2(v) :\equiv 0$ in the derivation of Eq. (13), we obtain the equality

$$\int_0^L \nabla u^h(x)\, dx = L\Big[\frac{\lfloor \lambda m \rfloor}{m} p^+ + \Big(1 - \frac{\lfloor \lambda m \rfloor}{m}\Big) p^-\Big]$$

and in the limit $m \to \infty$ as above

$$\begin{aligned} \lim_{h \searrow 0} \int_0^L \nabla u^h(x)\, dx &= L(\lambda p^+ + (1-\lambda)p^-) = La \\ &= \int_0^L \nabla u(x)\, dx, \qquad (14) \end{aligned}$$

where Eq. (12) was used. Eq. (14) infers $u^h \to u$ in $L^q(0, L)$ for any $1 \le q \le \infty$.

(b2) u is piecewise affine and continuous.

The proof follows easily by a decomposition of $(0, L)$ in those subintervals in which u is continuous and applying Case (b1).

(b3) u is an arbitrary function in $H^{1,p}(0, L)$.

Let $(z^h)_{h>0}$ be a sequence in $\mathcal{A}^h$ with $z^h \to u$ in $H^{1,p}(0,L)$ as $h \searrow 0$. According to (b2) we can find for every $h > 0$ a sequence $(\tilde{z}_j^h)_{j\in\mathbb{N}}$ of functions in $\mathcal{A}^h$ such that $\tilde{z}_j^h \to z^h$ in $L^p(0,L)$ as $j \to \infty$ and

$$\limsup_{j\to\infty} \widetilde{\mathcal{G}}^j(\tilde{z}_j^h) \le \widetilde{\mathcal{G}}(z^h).$$

Consequently

$$\limsup_{h\searrow 0}\ \limsup_{j\to\infty} \widetilde{\mathcal{G}}^j(\tilde{z}_j^h) \le \limsup_{h\searrow 0} \widetilde{\mathcal{G}}(z^h) = \widetilde{\mathcal{G}}(u).$$

Now choose $u^h := \tilde{z}^h_{1/h}$. The functions u^h fulfil $u^h \to u$ in $L^p(0,L)$ and

$$\limsup_{h\searrow 0} \widetilde{\mathcal{G}}^h(u^h) \le \widetilde{\mathcal{G}}(u). \quad \Box$$

5 Application to two discrete free energy functionals

In this section we will apply the results of Section 4 to two discrete functionals that approximate the free energy of a physical system. Even though both functionals look similar, the second may generate a surface energy as $h \searrow 0$.

Let $l_1 < l_2$ be two given numbers (l_1, l_2 are vectors if $D > 1$). As before, h and n are related by the formula $h = L/n$. Let

$$H_1^h(\{u_i^h\}_{0\le i\le n}) := \sum_{i=1}^{n} h^\alpha \Big(\frac{u_i^h - u_{i-1}^h}{h} - l_1\Big)^2 \Big(\frac{u_i^h - u_{i-1}^h}{h} - l_2\Big)^2 \tag{15}$$

for a parameter $0 \le \alpha \le 1$. As before, H_1^h is extended to a functional $\mathcal{H}_1^h$ on functions in $\mathcal{A}^h$.

Theorem 3 *(*Γ**-limit of** $\mathcal{H}_1^h$*)*
The functional $\mathcal{H}_1^h$ Γ-converges for $h \searrow 0$ to a functional $\mathcal{H}_1 : L^p(0,L) \to \mathbb{R}$. Depending on the value of α the functional $\mathcal{H}_1$ can be characterised as follows.

(a) $\alpha = 1$:

$$\mathcal{H}_1(u) = \begin{cases} \int_0^L V^{**}(\nabla u(x))\,dx & \textit{if } u \in H^{1,p}(0,L), \\ +\infty & \textit{else} \end{cases}$$

and $V(v) := (v - l_1)^2(v - l_2)^2$.

(b) $0 \le \alpha < 1$:

$$\mathcal{H}_1(u) = \begin{cases} 0 & \textit{if } u \in H^{1,p}(0,L) \textit{ and } l_1 \le \nabla u(x) \le l_2 \textit{ for a.e. } x \in \Omega, \\ +\infty & \textit{else.} \end{cases}$$

Proof:

(a) The proof is a direct consequence of Theorem 2. We simply have to set $Q_2 :\equiv 0$ and $Q_1(v) := (v - l_1)^2(v - l_2)^2$.

(b) It is evident that $\mathcal{H}_1^h(u) = \infty$ if $u \notin H^{1,p}(0,L)$ or if $\nabla u \notin [l_1, l_2] \subset \mathbb{R}$. Because of $\liminf_{h\searrow 0} \mathcal{H}_1^h(u^h) \ge 0$, it remains to find a 'recovery sequence' $(u^h)_{h>0} \subset$

$H^{1,p}(0,L)$ such that $\lim_{h\searrow 0}\int_0^L |u^h-u|=0$ and $\limsup_{h\searrow 0}\mathcal{H}_1^h(u^h)=0$. As in the proof of Theorem 2 we may assume w.l.o.g. $u(x)=ax+b$. Due to $l_1\le\nabla u\le l_2$ there exists a $\lambda\in[0,1]$ with $a=\nabla u=\lambda l_1+(1-\lambda)l_2$. With Carathéodory's theorem, exactly as in Eqs. (11) and (12) (since $p^+=l_1$, $p^-=l_2$), we find

$$0=\lambda V(l_1)+(1-\lambda)V(l_2)=V^{**}(\nabla u).$$

Let $L/h=km$ and approximate u by functions $u^h(x)=a^h(x)x+b$ which are periodic in any subinterval of $(0,L)$ with length mh. We choose

$$a^h(x)=\begin{cases} l_1 & \text{if } x\in\Omega_+^h,\\ l_2 & \text{if } x\in\Omega_-^h.\end{cases}$$

This yields

$$\begin{aligned}\mathcal{H}_1^h(u^h) &= \int_0^L h^{\alpha-1}V(\nabla u^h(x))\,dx=\sum_{i=0}^{k-1}\int_0^{R_{im}^h} h^{\alpha-1}V(\nabla u^h(x))\,dx\\ &= k\int_0^{R_m^h} h^{\alpha-1}V(\nabla u^h(x))\,dx\\ &= kh^\alpha\Big\{\lfloor\lambda m\rfloor V(l_1)+(1-\lfloor\lambda m\rfloor)V(l_2)\Big\}=0\end{aligned}$$

since $V(l_1)=V(l_2)=0$. $\square$

Next we consider the functional

$$H_2^h(\{u_i^h\}_{0\le i\le n})=\frac{1}{4}\sum_{i=1}^{n-1}h^\alpha\prod_{j=1}^{2}\left[\left(\frac{u_i^h-u_{i-1}^h}{h}-l_j\right)^2+\left(\frac{u_{i+1}^h-u_i^h}{h}-l_j\right)^2\right] \quad (16)$$

and extend it to $\mathcal{H}_2^h$ acting on $\mathcal{A}^h$.

Theorem 4 *(Γ-limit of $\mathcal{H}_2^h$)*
The functional $\mathcal{H}_2^h$ Γ-converges for $h\searrow 0$ to a functional $\mathcal{H}_2: L^p(0,L)\to\mathbb{R}$. Depending on the value of α the functional $\mathcal{H}_2$ can be characterised as follows.

(a) $\alpha=1$:

$$\mathcal{H}_2(u)=\begin{cases}\int_0^L(\tilde V)^{**}(\nabla u(x))\,dx & \textit{if } u\in H^{1,p}(0,L),\\ +\infty & \textit{else}\end{cases}$$

and $\tilde V(v):=(v-l_1)^2(v-l_2)^2$.

(b) $0<\alpha<1$:

$$\mathcal{H}_2(u)=\begin{cases}0, & \textit{if } u\in H^{1,p}(0,L) \textit{ and } \nabla u(x)=l_1 \textit{ or } \nabla u(x)=l_2 \textit{ a.e. } x\in\Omega,\\ +\infty & \textit{else.}\end{cases}$$

(c) $\alpha=0$:

$$\mathcal{H}_2(u)=\begin{cases}(l_2-l_1)^4 j & \textit{if } u\in H^{1,p}(0,L) \textit{ and } \nabla u(x)\in\{l_1,l_2\} \textit{ a.e. } x\in\Omega,\\ +\infty & \textit{else.}\end{cases}$$

Here, $j\in\mathbb{N}$ denotes the number of jumps of ∇u in $(0,L)$.

Notice that

$$\mathcal{H}_2^h(u^h) = \int_0^L h^{\alpha-1} V(\partial_h u^h(x), \partial_h u^h(x+h)). \tag{17}$$

Hence, V depends on two arguments and the earlier proofs cannot be immediately reused.

Proof:

(a) The proof is very similar to Theorem 2.

(b) We observe that if V is defined by (16), (17), then $V = 0$ iff $\partial_h u^h \in \{l_1, l_2\}$. Due to the factor $h^{\alpha-1}$ this is a necessary condition for the Γ-limit to be finite.

(c) From the result in (b) we know that $\mathcal{H}_2^h(u)$ is infinite whenever $\nabla u(x) \notin \{l_1, l_2\}$ for a.e. $x \in \Omega$. Hence the sum (16) counts with a factor $(l_2 - l_1)^4$ how many times $\nabla u^h(x)$ jumps between l_1 and l_2. □

Eq. (16) with $\alpha = 0$ defines a simple functional where a surface energy occurs in the Γ-limit. As the proofs of Theorem 3 show, a surface energy can only be expected if at least three points in the numerical stencil (u_{i-1}^h, u_i^h and u_{i+1}^h for H_2^h) are evaluated.

6 Results on the Cahn-Hilliard system with elasticity

In continuation of the analysis of the last sections we will now investigate a more practical example and study the behaviour of a numerical algorithm for the Cahn-Hilliard equation that shows an interplay between surface energy and elastic energy. The Cahn-Hilliard model with linear elasticity describes the spinodal decomposition of a binary alloy in a homogeneous medium located in a bounded domain $\Omega \subset \mathbb{R}^D$ with Lipschitz boundary under isothermal conditions. A review of the model can be found in [11], numerical computations in two space dimensions for binary alloys are done in [16].

If $\varrho^h > 0$ denotes the density of a chosen constituant of the two-phase alloy and if $u^h : \mathbb{R}^D \to \mathbb{R}^D$ denotes the deformation, the free energy of the system reads

$$\mathcal{F}^h(\varrho^h, u^h) = \int_\Omega \Big(W(\varrho^h(x)) + \frac{\gamma}{2} |\nabla \varrho^h(x)|^2 + V(\varrho^h(x), u^h(x)) \Big)\, dx. \tag{18}$$

The superscript h indicates that the solution (ϱ^h, u^h) is computed for a given regular triangulation of Ω with maximal distance h of two neighbouring vertices. The functional $W(\varrho) \geq 0$ defines a double-well potential with two minima $\varrho_1 \neq \varrho_2$. Frequently used expressions for W are

$$W(\varrho) := \alpha \Big[\varrho \ln \varrho + (1-\varrho) \ln(1-\varrho) \Big] - \frac{\beta \varrho^2}{2}, \tag{19}$$

$$W(\varrho) := \frac{1}{4} \varrho^2 (1-\varrho)^2. \tag{20}$$

In (19), the constant $\alpha > 0$ depends on temperature T (kept constant in this model) and the Boltzmann constant, $\beta > 0$ on the critical temperature (that is the temperature below which the segregation starts). Ansatz (19) can be explained by statistical mechanics. Formula (20) is a Taylor expansion of (19) for certain values of α and β.

In (18), the elastic energy is defined by

$$V(\varrho^h, u^h) := \frac{1}{2}\Big(\varepsilon(u^h) - \overline{\varepsilon}(\varrho^h)\Big) : C\Big(\varepsilon(u^h) - \overline{\varepsilon}(\varrho^h)\Big)$$

where the local strain is given by

$$\varepsilon(u^h) := \frac{1}{2}\Big(\nabla u^h + (\nabla u^h)^t\Big)$$

and

$$\overline{\varepsilon}(\varrho^h) := \overline{\varrho}\varrho^h \mathrm{Id}$$

denotes the elastic energy of the unstressed solid, $\overline{\varrho}$ the lattice misfit. C is the positive definite fourth order elasticity tensor.

ϱ^h is the solution of the diffusion equation

$$\partial_t \varrho^h = \mathrm{div}(M(\varrho^h)\nabla\mu^h) \quad \text{in } \Omega,$$

where the mobility $M(\varrho^h)$ is frequently set to the constant 1 and μ^h denotes the chemical potential. μ^h is the first variation of $f^h(\varrho^h, u^h)$ with respect to ϱ^h, where $\mathcal{F}^h(\varrho^h, u^h) = \int_\Omega f^h(\varrho^h, u^h)$ and $\mathcal{F}^h$ is given by Eq. (18).

The constant $\gamma \geq 0$ in (18) sets the surface energy and is related to the thickness of the transition layer. To study this analytically one considers the rescaled energy $\int_\Omega \frac{1}{\sqrt{\gamma}} W(\varrho(x)) + \sqrt{\gamma}\,|\nabla\varrho(x)|^2 + Q(\varrho(x), u(x))\,dx$ and for ϱ_1, ϱ_2 the metric

$$d(\varrho_1, \varrho_2) \;:=\; \inf\Big\{2\int_{-1}^{1} \sqrt{W(\sigma(t))}|\sigma'(t)|\,dt \;\Big|\; \sigma(-1) = \varrho_1, \sigma(1) = \varrho_2, \sigma : [-1, +1] \to \mathbb{R} \text{ is Lipschitz continuous}\Big\}.$$

As proved in [15] and [11], a curve σ that realises the infimum in the above expression is a geodesic with respect to this metric and the curve σ then realises an interfacial layer with minimal energy $\int_{-\infty}^{\infty} |\sigma'(t)|^2 + W(\sigma(t))dt$. The surface tension $\hat{\sigma}$ is related to d by $\hat{\sigma} = d(\varrho_1, \varrho_2)$ if $\varrho_1 \neq \varrho_2$ are the two minima of W.

The relationship between Formula (18) and the Γ-limit of $\mathcal{F}$ is now the following. Let (ϱ^h, u^h) be the numerical solution for some $h > 0$, that is (ϱ^h, u^h) minimises $\mathcal{F}^h$ and $\varrho = \varrho_1$ or $\varrho = \varrho_2$ in Ω except for a set with a measure proportional to h. For $D = 1$ we have $\varepsilon(u) = \nabla u = u'$ and the elastic energy between two phases converges to

$$\int_\Omega V_\varrho(u) = \int_\Omega \frac{1}{2}(\nabla u - l_1)C(\nabla u - l_2) \tag{21}$$

for some constant $C > 0$ and $l_1 = \varrho_1\overline{\varrho}$, $l_2 = \varrho_2\overline{\varrho}$. This expression is related to Formulation (15) and we see that the limit is an elastic energy. Yet, in the numerical scheme, for $h > 0$, another effect is significant. To see this let us have a look at a transition layer of two neighbouring phases. In a small region, ϱ^h jumps between ϱ_1 and ϱ_2 and ∇u^h between l_1 and l_2. The elastic energy for the discrete scheme with $h > 0$ is hence approximately

$$\int_\Omega \frac{C}{2}\Big(\frac{u_i^h - u_{i-1}^h}{h} - l_1\Big)\Big(\frac{u_i^h - u_{i-1}^h}{h} - l_2\Big) = L\frac{C}{2}(l_1 - l_2)^2 = \frac{LC}{2}\overline{\varrho}^2(\varrho_1 - \varrho_2)^2. \tag{22}$$

The surface energy for a given constant γ along the interface is

$$\int_\Omega \frac{\gamma}{2}|\nabla \varrho^h|^2 = \frac{\gamma}{2}\int_\Omega \frac{(\varrho_1-\varrho_2)^2}{h^2} = \frac{L\gamma}{2h^2}(\varrho_1-\varrho_2)^2. \tag{23}$$

The comparison of (22) and (23) yields the relationship

$$\gamma = C\overline{\varrho}h^2. \tag{24}$$

This means that due to the viscosity of the computational scheme, the numerical solution for $\gamma = 0$ behaves like the solution of the Cahn-Hilliard equation with γ given by (24). As long as $\gamma > 0$, it is well known that the term $\frac{\gamma}{2}|\nabla\varrho|^2$ in the free energy guarantees the coercivity of the functional in $H^{1,2}$ and ensures the existence of a solution to the discrete scheme, see [11]. Therefore, for any $h > 0$, a discrete numerical solution (ϱ^h, u^h) exists. Yet, the limiting equation for $h \searrow 0$ has no solution (ϱ, u) for instance with $\varrho \in C^{0,\frac{1}{4}}([0,T]; L^2(0,L))$, $u \in L^\infty(0,T; H^{1,2}(0,L))$ which is known to be true for $\gamma > 0$, see again [11].

The results of some numerical computations are presented as an illustration in Figure 2 which compares the numerical results of two computations. The pictures on the left hand side show the case $\gamma = 10^{-5}$, the pictures on the right the results after setting $\gamma = 0$ in the algorithm. All computations were done for the two-dimensional domain $\Omega := (0,1)^2 \subset \mathbb{R}^2$. The first line shows the graph of ϱ plotted over Ω. For $\gamma = 0$ one can observe small kinks close to the phase boundary. The second line shows the distribution of the two phases. As can be seen, the transition layer for $\gamma = 0$ is not smooth and follows strongly the underlying triangulation. This can be observed even better in Fig. 1. The third line shows an enlarged section of the graph close to the phase transition which illustrates that for $\gamma = 0$ the transition follows the triangulation.

Competition between elastic energy and surface energy is also of importance for the numerical solution of other two-phase problems of Ginzburg-Landau type. Characteristic for the Ginzburg-Landau approach is an expansion of the energy and a term $\frac{\gamma}{2}|\nabla\varrho^h|^2$ appears in $\mathcal{F}^h$. Consequently, transition layers of width $\sqrt{\gamma}$ are formed and in case of a linear stress strain law (22), (23) continue to hold. Thus, the results carry over to related models like the phase field equations or the Allen-Cahn equation.

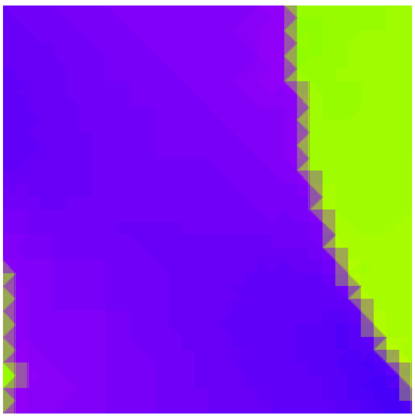
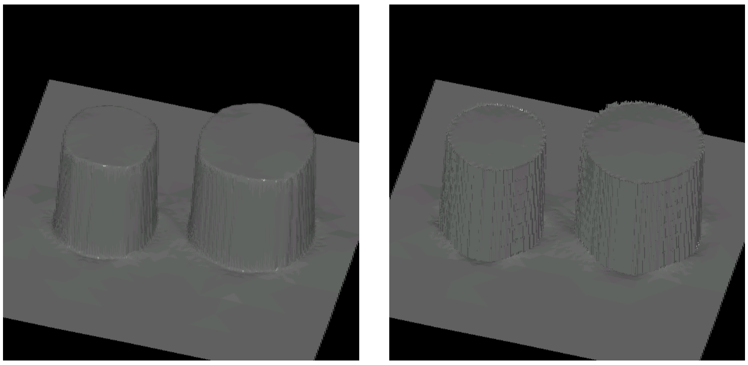


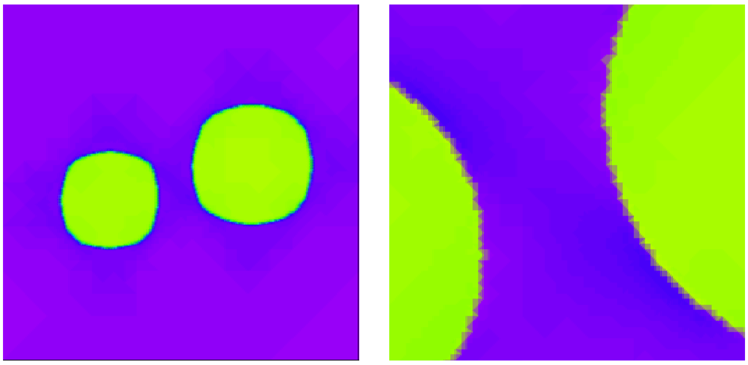
Figure 1: Enlarged picture of the phase distribution for $\gamma = 0$.

7 Discussion and Outlook

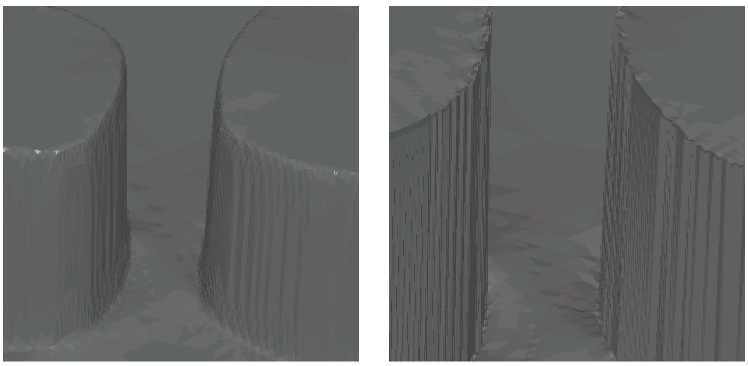
The present article analysed certain discrete approximation schemes related to the computation of free energies in two-phase systems. At one simple example in one space dimension it was demonstrated that if the ratio of elastic and surface energy is suitable this surface energy may still be present in the Γ-limit. This effect may appear in numerical computation schemes and may influence the computations but is frequently not noticed except in border line cases. Therefore, the matter deserves a deeper and more systematic treatment. A further problem is that even small surface tension leads to a multitude of local minima. So, numerical algorithms may get stuck there. This makes it worthwile to implement global minimisation procedures.



Plot of the graph



Distribution of the phases



Enlarged section of the graph

Figure 2: Comparison of numerical results for different values of γ. Left: $\gamma = 10^{-5}$. Right: $\gamma = 0$

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