TWO-PHASE STRUCTURES AS SINGULAR LIMIT OF A ONE-DIMENSIONAL DISCRETE MODEL

T. Blesgen

Max-Planck-Institute for Mathematics in the Sciences, Inselstraße 22-26, D-04103 Leipzig, Germany

Phone: +49-341-9959-804, Fax: +49-341-9959-859

Abstract:
A one-dimensional energy functional that models the elastic free energy of a monatomic chain of atoms occupying a bounded real domain is discussed and the Γ-limit of this functional when the number of particles becomes infinite is derived. The particular ansatz allows for the first time the presence of two coexisting phases in the singular limit and thus can be used as a prototype towards modeling three dimensional cases of physical relevance.

Key Words: Singular Limits, Phase Transitions, Elasticity

1 Introduction

In this article we study the behaviour of a one-dimensional monatomic lattice comprising of $(n+1)$ particles that interact via three and four body potentials that represent the interatomic forces. We are interested in the description of the Γ-limit when $n \to \infty$. This leads to a continuum theory of regular crystals under the idealising assumption that the interatomic distance vanishes in the limit. The notion of Γ-limit goes back to work by de Giorgi, [5]. Γ-limits can be regarded as a convergence related not only to one lattice, but provide a natural framework to formulate convergence with respect to an entire family of lattices, depending on the parameter n. A comprehensive discussion of this issue can be found in [1].

The derivation of a continuum theory relying on atomistic descriptions has only recently become a focus of research after the article [2] studied softening in fracture mechanics. In a similar direction goes [3]. In [6] a stochastic framework is considered, in [8] the topic of phase transitions is discussed by considering oscillations of lattices. In this article, we can extend the analysis in these articles and will discuss a prototype of a free energy functional whose minimisers give rise to two different lattice structures. This energy functional consists of one part that accounts for the local lattice symmetry, a second part that represents the surface energy and a third contribution that stands for the elastic energy.

This work is organised in the following way. In Section 2, a one-dimensional discrete free energy functional $W^n(u^n)$ for deformations u^n is introduced that describes the elastic energy of the atomic chain. In Section 3, the Γ-limit $n \to \infty$ of $W^n(u^n)$ is identified. The article is ended by a short discussion and outlook.

2 The energy functional

Let $\Omega := (0,1) \subset \mathbb{R}$ be the domain that contains a regular monatomic chain.

We suppose that the undeformed discrete reference configuration of Ω is given by a system of $n+1$ atoms with equal distance located at points $R_i^n \in \mathbb{R}$, where

$$R_i^n := ih_n \quad 0 \leq i \leq n.$$

Here, the setting $h_n := 1/n$ defines for given number $n \in \mathbb{N}$ the interatomic distance. The limit $n \to \infty$ corresponds to $h_n \searrow 0$. The index n is always used to indicate the dependency on the number of subdivisions.

By $\widehat{R}_i^n$, $0 \leq i \leq n$ we denote the position of atom i after the deformation. Finally, by u_i^n, $0 \leq i \leq n$ we denote the two-dimensional displacement vector of atom i, given by the relationship

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

For shortness we introduce the numbers $s_1 := 1$, $s_2 := 2$ and $s_3 := \frac{1}{2}$ and let

$$D^n u_i^n := \frac{u_{i+1}^n - u_i^n}{h_n}.$$

This is a forward difference quotient that approximates $(u_i^n)'$ for small h_n.

We will study the behaviour of the following energy functional.

$$W^n(u^n) := \begin{cases} +\infty & \text{if } u_{i+1}^n = u_i^n \text{ for some } i, \\ \sum_{k=1}^3 W_k^n(u^n) & \text{else} \end{cases}$$

where

$$\begin{aligned} W_1^n(u^n) &:= \sum_{i=0}^{n-2} n^\alpha \prod_{k=1}^{3} \Big| s_k - \frac{u_{i+2}^n - u_{i+1}^n}{u_{i+1}^n - u_i^n} \Big|^2, \\ W_2^n(u^n) &:= \sum_{i=0}^{n-3} \Big| 1 - \frac{u_{i+3}^n - u_{i+2}^n}{u_{i+1}^n - u_i^n} \Big|^2, \\ W_3^n(u^n) &:= h_n \sum_{i=0}^{n-2} \Big[\Big(\frac{u_{i+2}^n - u_i^n}{2h_n} - \alpha_1 \Big)^2 \beta_i^n + \Big(\frac{u_{i+2}^n - u_i^n}{2h_n} - \alpha_2 \Big)^2 \gamma_i^n \Big] \end{aligned}$$

and

$$\begin{aligned} \beta_i^n &:= \Big[1 - n^\alpha \Big| 1 - \frac{u_{i+2}^n - u_{i+1}^n}{u_{i+1}^n - u_i^n} \Big|^2 \Big]_+, \\ \gamma_i^n &:= \Big[1 - n^\alpha \Big| 2 - \frac{u_{i+2}^n - u_{i+1}^n}{u_{i+1}^n - u_i^n} \Big|^2 \Big| \frac{1}{2} - \frac{u_{i+2}^n - u_{i+1}^n}{u_{i+1}^n - u_i^n} \Big|^2 \Big]_+. \end{aligned}$$

Here, $0 < \alpha < 1$ and $[\cdot]_+$ denotes the positive part, this is $[x]_+ = x$ for $x \geq 0$ and $[x]_+ = 0$ for $x < 0$.

The concept behind the ansatz for W^n is the following. A minimiser of W_1^n either fulfils $D^n u_{i+1}^n \simeq D^n u_i^n$ which specifies one lattice order that is in the sequel referred to as Phase 1, or $D^n u_{i+1}^n \simeq 2D^n u_i^n$ resp. $D^n u_{i+1}^n \simeq \frac{1}{2} D^n u_i^n$ which characterises Phase 2.

W_2^n represents a surface energy. It counts(and limits) the number of transitions between the two phases, as within a phase one asymptotically has $D^n u_{i+2}^n = D^n u_i^n$. Finally, W_3^n represents an elastic energy. We will show below that β_i^n converges in $L^1(\Omega)$ to the indicator function of Phase 1 and γ_i^n to the indicator function of Phase 2 as $n \to \infty$. α_k corresponds to the elastic constant to Phase k.

The functional W_1^n represents the electrostatic energy due to interatomic potentials that force the atoms to positions of a certain given lattice order. The given example of a doubling (halfing) of the period of $D^n u^n$ is only a first simple example. Energy functionals motivated by real physical applications are higher dimensional and much more complicated.

For the analysis we extend the discrete deformation values $\{u_i^n\}_i$, to piecewise linear functions u^n in $L^2(\Omega) \cap \mathcal{A}^n$, where $\mathcal{A}^n$ denotes the space of piecewise linear functions, see [2]. In this article, discrete quantities are always specified by subscript i.

3 Identification of the Γ-limit for W^n

Now we can state the main result. It characterises the Γ-limit of W^n as n tends to infinity. We use the notation $\chi_1 := \chi$, $\chi_2 := 1 - \chi$. For $u \in H^{1,2}(\Omega)$, $\chi \in BV(\overline{\Omega}, \{0,1\})$ we define

$$E(u,\chi) := \frac{1}{4} \int_\Omega |\nabla \chi| + \sum_{k=1}^{2} \int_\Omega \chi_k \, (u' - \alpha_k)^2.$$

Additionally we introduce $W : L^2(\Omega) \to \mathbb{R}$ by

$$W(u) := \begin{cases} \inf_{\chi \in BV(\overline{\Omega},\{0,1\})} E(u,\chi) & \text{if } u \in H^{1,2}(\Omega) \text{ is strictly monotone,} \\ +\infty & \text{else.} \end{cases}$$

Theorem 1 (**Characterisation of the Γ-limit of** W^n)
The following statements are valid:

(i) The boundedness of the energy functional $W^n(u^n)$ implies the boundedness of $\left(\int_\Omega |(u^n)'|^2\right)_n$ uniformly in n.

(ii) W is the Γ-limit of W^n as $n \to \infty$ with respect to the convergence in $L^2(\Omega)$.

Proof of (i):

Step 1: Construction of the characteristic function χ:

By C we denote various positive constants that may change from line to line.

Let $(u^n) \subset L^2(\Omega)$ be a sequence with $W^n(u^n) \le C$. We set

$$d_k^i := \left| \frac{u_{i+2}^n - u_{i+1}^n}{u_{i+1}^n - u_i^n} - s_k \right|, \quad k_0^i := \operatorname{argmin}\Big\{ k \mapsto d_k^i \mid 1 \le k \le 3 \Big\}.$$

The boundedness of $W_1^n(u^n)$ implies

$$\sum_{i=0}^{n-1} n^\alpha \prod_{k=1}^{3} \left(s_k - \frac{u_{i+2}^n - u_{i+1}^n}{u_{i+1}^n - u_i^n} \right)^2 \le C.$$

Therefore there exists a constant $C > 0$ such that

$$\sup_i d^i_{k^i_0} \le C h_n^{\alpha/2}. \tag{1}$$

For sufficiently large n we can thus define an indicator function χ^n to Phase 1 by

$$\chi^n(x) := \begin{cases} 0 & \text{if } x \in [ih_n, (i+1)h_n),\ i \le n-2,\ k^i_0 \ne 1, \\ 1 & \text{if } x \in [ih_n, (i+1)h_n),\ i \le n-2,\ k^i_0 = 1, \\ \chi^n(1-2h_n) & \text{if } x \in [1-h_n, 1]. \end{cases}$$

Next we show that $\chi^n \in BV(\overline{\Omega}; \{0,1\})$, i.e.

$$\int_\Omega |\nabla \chi^n| \le C. \tag{2}$$

This follows from the boundedness of $W_2^n(u^n)$. Since for large n

$$\frac{u^n_{i+2} - u^n_{i+1}}{u^n_{i+1} - u^n_i} = s_k + o(1) \quad \text{for some } k \in \{1,2,3\},$$

we see that if $\chi^n(x)$ jumps in $x = (i+1)h_n$ between 0 and 1, then

$$\left(1 - \frac{u^n_{i+3} - u^n_{i+2}}{u^n_{i+1} - u^n_i}\right)^2 \ge \frac{1}{4} + o(1)$$

which shows $W_2^n(u^n) \ge \left(\frac{1}{4} + o(1)\right) \int_\Omega |\nabla \chi^n|$ and proves (2). Here we adapted the Landau notation and denote by $o(1)$ terms that tend to 0 as $n \to \infty$.

With (2), well-known compactness results imply the existence of a subsequence (again denoted by) χ^n and a $\chi \in BV(\overline{\Omega}, \{0,1\})$ such that $\chi^n \to \chi$ in $L^1(\Omega)$.

Step 2: Convergence of β^n, γ^n in $L^1(\Omega)$:

We extend the discrete quantities $\{\beta^n_i\}_i$, $\{\gamma^n_i\}_i$ to piecewise constant functions in $L^1(\Omega)$ by the definition

$$\beta^n(x) := \begin{cases} \beta^n_i & \text{if } x \in [ih_n, (i+1)h_n) \text{ and } i \le n-2, \\ 0 & \text{if } x \in [1-h_n, 1]. \end{cases}$$

In the same manner, the extension γ^n of $\{\gamma^n_i\}_i$ is defined.

Now we show that

$$\beta^n \to \chi, \quad \gamma^n \to (1-\chi) \quad \text{in } L^1(\Omega) \text{ for } n \to \infty, \tag{3}$$

where the function $\chi \in BV(\overline{\Omega}, \{0,1\})$ is the limit of χ^n found in Step 1. Without loss of generality we may restrict to $i \le n-2$.

Case 1: $\chi^n(ih_n) = 1$.

Fix a small $\varepsilon > 0$. From the boundedness of $W^n(u^n)$ together with (1) we see that there exists a $n_0 \in \mathbb{N}$ such that

$$\left|1 - \frac{u^n_{i+2} - u^n_{i+1}}{u^n_{i+1} - u^n_i}\right|^2 n^\alpha \le \varepsilon \quad \text{for all } n \ge n_0.$$

So we find $1 \ge \beta^n_i \ge 1 - \varepsilon$ for large n.

Similarly,

$$\Big|2-\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i}\Big|^2\Big|\frac{1}{2}-\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i}\Big|^2\geq h_n^\alpha\quad\text{for all } n\geq n_0$$

and thus $\gamma_i^n=0$ for sufficiently large n.

Case 2: $\chi^n(ih_n)=0$.
Analogous to Case 1 we see that for large n

$$\Big|2-\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i}\Big|^2\Big|\frac{1}{2}-\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i}\Big|^2 n^\alpha\leq\varepsilon,$$

so $1\geq\gamma_i^n\geq 1-\varepsilon$ for large n.
Similarly,

$$\Big|1-\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i}\Big|^2\geq h_n^\alpha$$

and $\beta_i^n=0$ for sufficiently large n.
The discussion of these two cases yields the pointwise convergence of β^n to χ and of γ^n to $1-\chi$. Together with Lebesgue's dominated convergence theorem the proof of (3) is finished.

Step 3: Boundedness of $\int\limits_\Omega |(u^n)'|^2$ uniformly in n:
We choose constants $a\in\mathbb{R}^+$, $b\in\mathbb{R}$ such that

$$\min\{(x-\alpha_1)^2,\,(x-\alpha_2)^2\}\geq ax^2-b.$$

Due to the boundedness of $W_3^n(u^n)$ we thus find that there exist constants C_1, $C_2>0$ such that

$$C_1\geq h_n^2 C_2\sum_{i=0}^{n-2}\Big(\frac{u^n_{i+2}-u^n_i}{2h_n}\Big)^2(\beta_i^n+\gamma_i^n).$$

Since $D^nu^n_{i+1}=s_kD^nu^n_i+o(1)$ for one $k\in\{1,2,3\}$ and large n we find that

$$\Big(\frac{u^n_{i+2}-u^n_i}{2h_n}\Big)^2\geq\Big(1+\frac{1}{2}+o(1)\Big)\Big(\frac{u^n_{i+1}-u^n_i}{2h_n}\Big)^2.$$

The term $(\beta_i^n+\gamma_i^n)$ can for large n be estimated from below by a constant. So we find the existence of a constant $C>0$ with

$$C\geq h_n^2\sum_{i=0}^{n-2}\Big(\frac{u^n_{i+1}-u^n_i}{2h_n}\Big)^2. \tag{4}$$

Due to the estimate $(D^nu^n_{n-1})^2\leq(2+o(1))D^nu^n_{n-2}$ the sum in (4) can be extended to $i=n-1$ and the estimate still holds.

The sum $\sum_i(D^nu^n_i)^2$ is directly related to $\int_\Omega|(u^n)'|^2$ where u^n is the piecewise affine linear extension of $\{u_i^n\}_i$. With (4) extended to $i=n-1$ this finally yields

$$\sup_n\int\limits_\Omega|(u^n)'|^2=\sup_n\,h_n\sum_{i=0}^{n-1}(D^nu^n_i)^2\leq C. \tag{5}$$

Proof of (ii): We assume that the reader is familiar with the concept of Γ-convergence.

Step 4: Lower semicontinuity inequality along the sequence W^n:

We have to show: for every sequence $(u^n)_{n\in\mathbb{N}}$ with $u^n \to u$ in $L^2(\Omega)$ there exists a subsequence $(u^{n_k})_{k\in\mathbb{N}}$ with

$$W(u) \leq \liminf_{k\to\infty} W^{n_k}(u^{n_k}).$$

If $W^n(u^n)$ is unbounded, there is nothing to show. Hence we may assume w.l.o.g. $W^n(u^n) \leq C$ for all n. From (5) follows u^n, $u \in H^{1,2}(\Omega)$ for all $n \in \mathbb{N}$. Because of the reflexivity of the Hilbert space $H^{1,2}(\Omega)$ we know that there exists a subsequence (again denoted by) u^n such that $u^n \rightharpoonup u$, in $H^{1,2}(\Omega)$ for $n \to \infty$.

From Step 2 we know that $\chi^n \to \chi$, $\beta^n \to \chi$, $\gamma^n \to 1-\chi$ in $L^1(\Omega)$ for $n \to \infty$.

Because of $\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i} \geq \frac{1}{2} + o(1)$, for $n \geq n_0$ we find that u^n is monotone for sufficiently large n.

Now we estimate $W^n(u^n)$ from below. We claim

$$\liminf_{n\to\infty} W^n(u^n) \geq E(u,\chi) \geq W(u). \tag{6}$$

In order to prove (6), let us estimate every component of $W^n(u^n)$ separately.

1. $W^n_1(u^n) \geq 0$.

2. Estimate of the surface energy:

$$\liminf_{n\to\infty} W^n_2(u^n) \geq \liminf_{n\to\infty} \left(\frac{1}{4} + o(1)\right) \int_\Omega |\nabla \chi^n| \geq \frac{1}{4} \int_\Omega |\nabla \chi|.$$

3. Estimate of the elastic energy:

For $x \in \Omega$ let $\tilde{u}^n$ be given by

$$\tilde{u}^n(x) := \begin{cases} \frac{u^n(x+2h_n)-u^n(x)}{2h_n} & \text{if } x \in (0, 1-2h_n), \\ 0 & \text{if } x \in [1-2h_n, 1), \end{cases}$$

Using this notation we may rewrite W^n_3,

$$W^n_3(u^n) = \int_\Omega \Big[(\tilde{u}^n - \alpha_1)^2 \beta^n + (\tilde{u}^n - \alpha_2)^2 \gamma^n\Big].$$

Next we show

$$\tilde{u}^n \to u' \quad \text{in } L^2(\Omega) \text{ for } n \to \infty. \tag{7}$$

We observe

$$\Big|\frac{u^n(x+2h_n)-u^n(x)}{2h_n}\Big| \leq \int_0^1 |(u^n)'(x+sh_n)|\, ds \tag{8}$$

and due to the boundedness of u^n in $H^{1,2}(\Omega)$, an application of Hölder's inequality yields the boundedness of the left hand side of (8) uniformly in n.

With Lebesgue's dominated convergence theorem, $\tilde{u}^n \to u'$ in $L^2(\Omega)$ follows. In the same way, the other convergence results in (7) can be derived.

Exploiting (7), with the help of Theorem 3.4, p.74 in [4] we obtain

$$\liminf_{n\to\infty} W_3^n(u^n) \geq \sum_{k=1}^{2} \int_\Omega (u' - \alpha_k)^2 \chi_k.$$

Combining the estimates for $W_l^n(u^n)$, $1 \leq l \leq 3$, (6) is shown.

Step 5: Existence of a "recovery sequence":

We have to find a sequence $(u^n) \subset L^2(\Omega)$ converging to u in $L^2(\Omega)$ with

$$W(u) \geq \limsup_{n\to\infty} W^n(u^n).$$

If $W(u) = +\infty$, there is nothing to show. Due to the monotonicity properties of u demonstrated above we know that the functional $\chi \mapsto E(u,\chi)$ is bounded from below in the BV-norm. Using the compactness properties of $BV(\Omega)$ and the coercivity of E, it is clear that $E(u,\cdot)$ attains its minimum, i.e. $W(u) = E(u,\chi)$ for some $\chi \in BV(\overline{\Omega}, \{0,1\})$.

Next we show that for piecewise affine, strictly monotone u there exists a sequence u^n with $u^n \to u$ and $W^n(u^n) \to E(u,\chi)$. We start with special cases, then generalise.

Case 1: $u' \equiv a_1 > 0$, $\chi \equiv \text{const}$ in Ω:

(a) $\chi \equiv 1$ in Ω:

We simply set $u^n := u$ for all n.

(b) $\chi \equiv 0$ in Ω:

For $x > 0$ choose u^n such that $D^n u_i^n$ is alternating between $\frac{2}{3}a_1$ and $\frac{4}{3}a_1$. Furthermore u^n satisfies $u^n(x=0) = u(x=0)$.

Case 2: $u' \equiv a_1 > 0$, $\chi \equiv 1$ for $0 \leq x \leq \frac{1}{2}$, $\chi \equiv 0$ for $x > \frac{1}{2}$.

The treatment of this case is more difficult. It is not possible to directly combine the two ansatz functions for u^n of Case 1 because for one index i this would mean $D^n u_i^n = a_1 h_n$ and either $D^n u_{i+1}^n = \frac{2}{3}a_1 h_n$ or $D^n u_{i+1}^n = \frac{4}{3}a_1 h_n$, leading to $\lim_{n\to\infty} W_1^n(u^n) = \infty$.

Therefore we have to introduce a transition layer of width h_n^s between the two phases, where $s > 0$ is a small constant to be chosen later.

For convenience we introduce

$$\varphi^n(x) := \begin{cases} a_1 & \text{for } 0 \leq x \leq \frac{1}{2}, \\ a_1 + \frac{a_1}{3} n^s (x - \frac{1}{2}) & \text{for } \frac{1}{2} < x \leq \frac{1}{2} + h_n^s, \\ \frac{4}{3}a_1 & \text{for } \frac{1}{2} + h_n^s < x \leq 1. \end{cases}$$

We set u^n such that $u^n(x=0) = u(x=0)$ and

$$D^n u_i^n := \begin{cases} \varphi^n(ih_n) & \text{for } ih_n \leq \frac{1}{2}, \\ \frac{1}{2}\varphi^n(ih_n),\ \varphi^n(ih_n) \text{ alternating} & \text{for } ih_n > \frac{1}{2}. \end{cases}$$

Let us now analyse what this means for the limit of $W^n(u^n)$. We notice

$$\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i} = s_k \qquad \text{if } (i+1)h_n \le \frac{1}{2} \text{ or } ih_n > \frac{1}{2}. \tag{9}$$

If $\frac{1}{2} < (i+1)h_n \le \frac{1}{2} + h_n^s$ and $ih_n \le \frac{1}{2}$ we have

$$\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i} = s_k\,\frac{\varphi^n((i+1)h_n)}{\varphi^n(ih_n)} = s_k\,\frac{a_1+\frac{a_1}{3}h_n^{1-s}}{a_1} = s_k\left(1+\frac{1}{3}h_n^{1-s}\right) \tag{10}$$

with $s_k = 1$ or $s_k = \frac{1}{2}$. To guarantee the convergence to 0 of the corresponding expressions in W_1^n which are weighted with a factor n^α we require $0 < s < \frac{1-\alpha}{2}$.
If $\frac{1}{2} < ih_n \le \frac{1}{2} + h_n^s$ and $(i+1)h_n > \frac{1}{2} + h_n^s$ we have

$$\frac{u^n_{i+2}-u^n_{i+1}}{u^n_{i+1}-u^n_i} = s_k\,\frac{\varphi^n((i+1)h_n)}{\varphi^n(ih_n)} = s_k\,\frac{\frac{4}{3}a_1}{a_1+\frac{a_1}{3}h_n{}^{-s}h_n^s} = s_k \tag{11}$$

where $s_k = 2$ or $s_k = \frac{1}{2}$.

(9), (10) and (11) cover all possible cases and demonstrate the convergence to 0 of the $D^n u_i^n$-terms in W_1^n. Hence we find $W_1^n(u^n) \to 0$ as $n \to \infty$.

For the estimation of the functional $W_2^n(u^n)$ we have

$$\begin{aligned}\left|1-\frac{u^n_{i+3}-u^n_{i+2}}{u^n_{i+1}-u^n_i}\right|^2 &= \left|1-\frac{1}{2}\frac{\varphi^n((i+2)h_n)}{\varphi^n(ih_n)}\right|^2\\ &= \left|\frac{1}{2}-\frac{1}{2}\,\frac{\varphi^n(ih_n)-\varphi^n((i+2)h_n)}{\varphi^n(ih_n)}\right|^2.\end{aligned}$$

For $I := \frac{\varphi^n(ih_n)-\varphi^n((i+2)h_n)}{\varphi^n(ih_n)}$ simple computations yield

$$I = \begin{cases} 0 & \text{if } (ih_n > \frac{1}{2}) \text{ or } ((i+1)h_n \le \frac{1}{2}) \\ & \text{or } (\frac{1}{2} < ih_n \le \frac{1}{2}+h_n^s \text{ and } (i+2)h_n > \frac{1}{2}+h_n^s), \\ -s_k h_n^{1-s} & \text{if } (ih_n > \frac{1}{2} \text{ and } (i+2)h_n \le \frac{1}{2}+h_n^s) \\ & \text{or } (ih_n \le \frac{1}{2} \text{ and } \frac{1}{2} < (i+1)h_n \le \frac{1}{2}+h_n^s). \end{cases}$$

and for $0 < s < 1$ the convergence of $W_2^n(u^n)$ to $\frac{1}{4}$ can be assured.

For the estimation of $W_3^n(u^n)$, it is clear that outside the strip of width h_n^s the summands in $W_3^n(u^n)$ are exactly equal to

$$h_n^s\Big[\chi(a_1-\alpha_1)^2+(1-\chi)(a_1-\alpha_2)^2\Big].$$

Inside the strip, we have approximately h_n^{s-1} summands, where each summand is of the form h_nC. Thus, for $s > 0$ the part inside the strip tends to 0 for $n \to \infty$.

Case 3: General $\chi \in BV(\overline{\Omega}; \{0,1\})$, u piecewise affine, monotone, continuous:

The construction of u^n can be done by iteratively applying the construction given in Case 2.

Case 4: General monotone $u \in H^{1,2}(\Omega)$:

Let u be a generic monotone function in $H^{1,2}(\Omega)$ and let $\{u^n\}$ be a sequence in $\mathcal{A}^n$ such that $u^n \to u$ in $H^{1,2}(\Omega)$. For every n we can apply Case 3 to find a sequence

$\{w_l^n\}_l$ such that $w_l^n \to u^n$ in $L^2(\Omega)$ as $n \to \infty$ and $\limsup_l W^l(w_l^n) \leq W(u^n)$. Then we have

$$\limsup_{n\to\infty} \limsup_{l\to\infty} W^l(w_l^n) \leq \limsup_{n\to\infty} W(u^n) = W(u), \tag{12}$$

where (12) holds because of the strong convergence of u^n to u in $H^{1,2}(\Omega)$. By diagonalisation, we find a sequence $\tilde{u}^n := w_{l(n)}^n$ such that $\tilde{u}^n \to u$ in $L^2(\Omega)$ and $\limsup_{n\to\infty} W^n(\tilde{u}^n) \leq W(u,v)$. $\square$

4 Discussion and Outlook

The present article analysed the Γ-limit of a one-dimensional lattice as the number of particles tends to infinity in a particular case. The discussed free energy functional represents a first example that gives rise to two different lattice orders. It seems very likely that this concept can be generalised to more than two phases and higher space dimensions although the energy is even more artificial in this case. Physically relevant formulas for the elastic energy replacing $(u' - \alpha_k)^2$ can for instance be found in [7] and are mostly non-linear.

Finally it is important to realize that the concept of Γ-convergence is only partly suitable for the understanding of the static behaviour of solids. This is because the Γ-limit is bound to *global* minimisers whereas the evolution in nature may get stuck in a *local* minimum as the activation energy needed to pass an energy barrier is not available. Unfortunately, at this point no appropriate mathematical instruments seem to be at hand to deal with formulations that arise from this consideration.

References

[1] A. Braides, *Approximation of Free-Discontinuity Problems*, Lecture Notes in Mathematics **1694**, Springer 1998

[2] A. Braides, G. dal Maso and A. Garroni, Variational formulation of softening phenomena in fracture mechanics: the one-dimensional case, *Arch. Rat. Mech. Anal.***146** (1999), 23–58

[3] A. Braides and M.S. Gelli, Limits of discrete systems with long-range interactions, *Journal of Convex Analysis* **9**(2002), 363–399

[4] B. Dacorogna, *Direct Methods in the Calculus of Variations*, Springer 1989

[5] E. De Giorgi, Sulla convergenza di alcune successioni di integrali del tipo dell'area, *Rendiconti di Matematica* **4**(1955), 95–113

[6] O. Iosefescu, C. Licht and G. Michaille, Variational limit of a one-dimensional discrete and statistically homogeneous system of material points, *Asympt. Anal.* **28**(2001), 309–329

[7] J.F. Nye, *Physical Properties of Crystals*, Clarendon Press, Oxford 1964

[8] S. Pagano, R. Paroni, A simple model for phase transitions: from the discrete to the continuum problem, *Quart.Appl.Math.* **61** (2003), 89–109