

External forces in the continuum limit of discrete systems with non-convex interaction potentials: Compactness for a Γ -development

Marcello Carioni*, Julian Fischer† and Anja Schlömerkemper‡

November 27, 2018

Abstract

This paper is concerned with equilibrium configurations of one-dimensional particle system with non-convex nearest-neighbour and next-to-nearest-neighbour interactions and its passage to the continuum. The goal is to derive compactness results for a Γ -development of the energy with the novelty that external forces are allowed. In particular, the forces may depend on Lagrangian or Eulerian coordinates.

Our result is based on a new technique for deriving compactness results which are required for calculating the first-order Γ -limit: instead of comparing a configuration of n atoms to a global minimizer of the Γ -limit, we compare the configuration to a minimizer in some subclass of functions which in some sense are “close to” the configuration. This new technique is required due to the additional presence of forces with non-convex potentials. The paper is complemented with the study of the minimizers of the Γ -limit.

1 Introduction

The derivation of continuum theories from atomistic models in the context of elasticity theory has been a very active area of research in the previous decades. Prominent mathematical methods, as well as the present paper, are phrased in the context of Γ -convergence; see, e.g., [3] for an introduction. One important problem for which partial results are available is the derivation of continuum models for brittle fracture as a limit of atomistic models. In the limit we expect a variational problem that yields information on the cracks and models the elastic behaviour of the material outside the crack. Such variational models are often referred to as Griffith energies, cf. [16, 26].

Following [4, 22], we focus on one-dimensional systems of particles (e.g. atoms or molecules) which interact with their nearest and next-to-nearest neighbours via some non-convex potential like the classical Lennard-Jones potential. Here, we additionally allow for external forces, including

*Marcello Carioni, Universität Würzburg, Institute of Mathematics, Emil-Fischer-Str. 40, 97074 Würzburg, Germany. Present address: University of Graz, Institute for Mathematics and Scientific Computing, Heinrichstraße 36, 8010 Graz, Austria, Email: marcello.carioni@uni-graz.at

†Julian Fischer, Max Planck Institute for Mathematics in the Sciences, Inselstr. 22, 04103 Leipzig, Germany. Present address: Julian Fischer Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria, Email: julian.fischer@ist.ac.at

‡Anja Schlömerkemper, Universität Würzburg, Institute of Mathematics, Emil-Fischer-Str. 40, 97074 Würzburg, Germany, Email: anja.schloemerkemper@mathematik.uni-wuerzburg.de

dead as well as live loads. That is, the external forces may depend on the position within the reference configuration of the system as well as on the deformation, i.e., on Lagrangian and Eulerian coordinates. We stress that the class of interaction potentials between the particles which we consider in our analysis contains many physically relevant non-convex interaction potentials; the classical Lennard-Jones potential is just one example, cf. Section 3. One-dimensional systems serve as toy-models and may have applications to linear atomic structures like carbon atom wires, cf. e.g. [11] or one-dimensional systems of silicon [21]. However, there are some mathematical results known for higher-dimensional variational problems modeling fracture or image segmentation, cf. [7, 12, 17, 18].

In the setting of one-dimensional chains of atoms as considered here, there are essentially two approaches that lead to a limiting functional that contains information on the elastic behaviour outside cracks as well as information on the cracks. (1) One approach is starting from an energy density of the discrete system which is given by the sum of all interaction potentials between the atoms of the chain. The Γ -limit of this energy yields an integral functional that corresponds to a bulk energy contribution only; information on the size of the fracture is lost since the integrand of that bulk term ($d = 1$ -dimensional) is the convex hull of an effective potential which has its minimum on an unbounded set. One therefore considers the so-called Γ -limit of first order which recovers some information on surface energies ($d - 1 = 0$ -dimensional), i.e. on the energies related to the crack formation. A Γ -development then yields the desired limiting model, cf. [2, 10, 23]. We note that this first approach, which we follow here, allows for large deformations, cf. also [4, 22]. (2) The second approach starts from suitably rescaled energy densities which essentially scale surface and bulk contributions in the same way. The Γ -limit of such rescaled energies leads to a contribution of a linear elastic energy and a part depending on the cracks. The latter approach involves a harmonic approximation around the minimum of the interaction potentials and thus can be considered as an approach in small displacements, cf. [8, 10, 23, 25]. Moreover, there are studies of one-dimensional systems with different scalings for the convex and the concave part of the internal potentials, cf. [9, 5, 6]. For other mathematical approaches to discrete to continuum analysis for fracture mechanics we refer to [13, 14, 19].

Atomic chains with interactions between $K \geq 2$ neighbours were treated in [25]. In computational mechanics one often considers hybrid models; these were mimicked in a discrete-to-continuum limit in [24]. Heterogeneous materials and their continuum limit as well as homogenization in the context of fracture were studied in [20]. With the current paper we set the ground for analysing such systems also in the presence of external forces.

In this paper we first calculate the Γ -limit H of the energy H_n of the discrete system as the number of atoms n tends to infinity (Section 2.1). As one can see from the obtained formula, any information on the number of cracks (i.e., the jump points of macroscopic deformation u) is lost in the Γ -limit: indeed the positive singular part of the derivative of u has no influence on H . Therefore, in order to gain further insight in the limiting behaviour of the considered chain of atoms, we study a higher order description of H_n by employing the development by Γ -convergence. More precisely, one considers the sequence of functionals

$$H_{1,n}^\ell(u_n) := \frac{H_n(u_n) - \inf_u H(u)}{\lambda_n} \quad (1)$$

with the goal of determining a Γ -limit for $H_{1,n}^\ell$, denoted by H^1 and called *first order Γ -limit* or Γ -limit of first order of H_n . Incorporation of forces poses additional challenges, as the value of the minimum of H is not known explicitly and therefore the derivation of properties $H_{1,n}^\ell$ requires a careful analysis.

Here we restrict our attention to the characterization of the minimizers of the zeroth-order Γ -limit and the compactness results relevant for the identification of the first order Γ -limit. The full study of the Γ -development of the discrete energies is postponed to a future work. In order to derive compactness results, one is tempted to employ the method of even-odd interpolation developed in [4] and used in the previous papers. However this fails without proper modifications: the even-odd interpolation strongly modifies the deformation u of the chain of atoms (while preserving the gradient) and therefore it cannot provide enough control of the external force that is depending explicitly on the variable u .

The novel method that we develop for the proof of the compactness results involves the construction of suitable competitors for H that we denote by $v_{1,n}$ and $v_{2,n}$. The goal is to choose $v_{1,n}$ and $v_{2,n}$ such that the difference $\frac{1}{\lambda_n}(H_n(u_n) - \frac{1}{2}(H(v_{1,n}) + H(v_{2,n})))$ provides control of $(u'_n - \gamma)_+$ while at the same time being controlled by $H_{1,n}^\ell(u_n)$. Here, γ is the minimizer of the effective interaction potential and thus the equilibrium condition of u' in the absence of external forces, cf. Assumption \mathcal{A} in Section 3. The definition of $v_{1,n}$ and $v_{2,n}$ is based on a careful step-by-step construction that truncates the slopes of the standard interpolation and introduces jumps in suitably chosen points of the domain (see Section 5).

The outline of the paper is as follows. In Section 2.2 we study properties for minimizers of the zeroth-order Γ -limit in order to gain a preliminary understanding of the first order Γ -limit. More precisely, we characterize the points of the domain (depending of the external force) where a non-elastic behaviour can occur and we relate the size of a crack to the external force. Then we show further regularity results of the minimizers and we prove that there cannot be regions in the domain with a complete compression. This part is inspired by [9], where they consider the special case of a dead load $\Phi(x, u) = -f(x)u(x)$.

In Section 2.3 we state the main results concerning the compactness estimates for the first order Γ -limit: in Theorem 11 (a) we prove that sequences of configurations that keep $H_{1,n}^\ell$ uniformly bounded have only a finite number of bonds such that $(u'_n - \gamma)_+ \geq \varepsilon$. Notice that this result is different to the usual compactness estimates obtained in previous related works as [4, 22]. Indeed, the energy does not provide a control of the distance of u'_n from γ , but only of its positive part. This is an effect due to the presence of the external forces. In Theorem 11 (b) we provide a more precise information on the magnitude of $(u'_n - \gamma)_+$. Finally, in Theorem 11 (c) we prove that the ratio of compression of the material remains uniformly bounded along sequences that keep the rescaled energies $H_{1,n}^\ell$ bounded. This ensures that in the derivation of the first order Γ -limit the singular behaviour of the potentials at zero is immaterial.

The set of assumptions on the interaction potentials that are used throughout the paper (denoted by Assumption \mathcal{A}) will be written explicitly only in Section 3. The reader can go through the statements of the main results assuming that the interaction potentials are two standard Lennard-Jones potentials (see Remark 1).

In Sections 4 and 5 we provide the proofs of the results stated in Section 2.2 (for the properties of minimizers of the limit functional) and Section 2.3 (for the main results about compactness), which concludes the paper.

2 Setting and main results

2.1 Setting

A configuration of the chain of $n + 1$ atoms is described by a map $u_n : \lambda_n \mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$, where we abbreviate $\lambda_n := \frac{1}{n}$, $n \in \mathbb{N}$. As it is customary, we call the set of all possible configurations

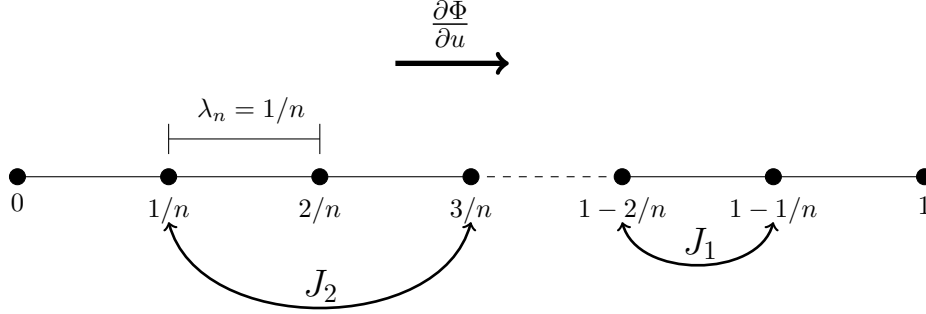


Figure 1: A chain of $n + 1$ atoms with interactions given by the potentials J_1 and J_2 and the external potential Φ .

$\mathcal{A}_n(0, 1)$ and we identify it with the set of all piecewise affine interpolations on $[0, 1]$:

$$\mathcal{A}_n(0, 1) = \{u : [0, 1] \rightarrow \mathbb{R} : u \in C([0, 1]), u(x) \text{ is affine in } (i\lambda_n, (i+1)\lambda_n) \forall i = 0, \dots, n-1\}.$$

We also denote by $u_n^i := u(i\lambda_n)$ the deformed configuration of the i -th atom in the chain. The atoms are assumed to interact with their nearest neighbours and next-to-nearest neighbours; the interactions are described using two non-convex potentials J_1 and J_2 for nearest-neighbour and next-to-nearest neighbour interactions, respectively. We furthermore assume that the external forces are described by a potential $\Phi : [0, 1] \times \mathbb{R} \rightarrow \mathbb{R}$, where the first variable describes the position of the atom in the reference configuration and the second variable describes the position of the atom in the deformed configuration.

Remark 1. *Throughout the paper we assume the potential Φ to be in $C^2([0, 1] \times \mathbb{R})$. Moreover the assumptions on J_j for $j = 1, 2$ are quite classical for the usual convex-concave interaction potentials and they are satisfied by the standard Lennard-Jones potentials. In order to avoid technicalities in this first part of the paper we summarize the set of assumptions satisfied by Φ, J_1 and J_2 in Assumption \mathcal{A} . The precise assumptions will be written explicitly and commented on in Section 3. For the moment the reader can think of them as a standard set of assumptions satisfied by the Lennard-Jones potential. The constant $\gamma > 0$ denotes the minimizer of the effective potential J_0 defined in (5), and $(0, \gamma^c + c)$ for some $c > 0$ is the regime of strict convexity, see [H0] in Assumption \mathcal{A} for details.*

Example 2. *If the external force f depends only on the Lagrangian coordinate, i.e., describes a dead load, the potential simply is*

$$\Phi(x, u(x)) = -f(x)u(x). \tag{2}$$

If the external force also depends on the Eulerian coordinate, which models what is sometimes called live loads, the potential reads

$$\Phi(x, u(x)) = - \int_0^{u(x)} f(x, w) dw.$$

We define the energy associated with a configuration u_n by

$$H_n(u_n) := \sum_{i=0}^{n-1} \lambda_n J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \sum_{i=0}^{n-2} \lambda_n J_2 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) + \sum_{i=0}^n \lambda_n \Phi(i\lambda_n, u_n^i). \quad (3)$$

Moreover, we add Dirichlet boundary conditions in the following way:

$$[B0] \quad u_n^0 = 0 \text{ and } u_n^n = \ell,$$

and we prescribe the slope of the discrete configuration at the boundary, i.e. we require that

$$[B1] \quad u_n^1 = \lambda_n \theta_0 \text{ and } u_n^{n-1} = \ell - \lambda_n \theta_1$$

for some fixed $\theta_0, \theta_1 > 0$. The reader can compare assumptions [B0] and [B1] with [4] where only [B0] is assumed and [22] where additionally [B1] is imposed. The Dirichlet conditions [B0] and [B1] correspond to the situation of a *Hard loading device*. As remarked in [13] and in [14] it is natural to impose four Dirichlet boundary conditions in the case of next-to-nearest neighborhood interactions as they ensure the equilibrium of the discrete system.

We set

$$\mathcal{A}_n^\ell(0, 1) := \{u \in \mathcal{A}_n(0, 1) : [B0] \text{ and } [B1] \text{ hold}\}$$

and

$$H_n^\ell(u_n) = \begin{cases} H_n(u_n) & \text{if } u_n \in \mathcal{A}_n^\ell(0, 1), \\ +\infty & \text{otherwise.} \end{cases} \quad (4)$$

Endowing $\mathcal{A}_n^\ell(0, 1)$ with the L^1 topology we define the (zeroth-order) Γ -limit of H_n^ℓ for $n \rightarrow +\infty$ as

$$H := \Gamma - \lim_{n \rightarrow \infty} H_n^\ell$$

in the L^1 topology (see [3] for an introduction on Γ -convergence).

In order to identify the Γ -limit H we define the effective potential J_0 as the inf-convolution of J_1 and J_2 , i.e.

$$J_0(z) := \inf \left\{ J_2(z) + \frac{1}{2} (J_1(z_1) + J_1(z_2)) : \frac{1}{2}(z_1 + z_2) = z \right\}. \quad (5)$$

Its minimizer is denoted by γ , see Assumption \mathcal{A} . Further, J_0^{**} is the lower convex envelope of J_0 , cf. (15). We also denote by $BV^\ell([a, b])$ the functions $u \in BV((a-1, b+1))$ that are equal to 0 on $(a-1, a)$ and equal to $\ell > 0$ on $(b, b+1)$. Moreover given $u \in BV([a, b])$, the notation $D^s u$ refers to the singular part of the distributional derivative of u , while u' refers to the absolutely continuous part.

Proposition 3. *Suppose that Assumption \mathcal{A} is satisfied. Then the Γ -limit of $(H_n^\ell)_n$ with respect to the $L^1(0, 1)$ topology is given by*

$$H(u) := \begin{cases} \int_0^1 J_0^{**}(u') + \Phi(x, u) \, dx & \text{if } u \in BV^\ell([0, 1]) \text{ and } D^s u \geq 0 \\ +\infty & \text{else.} \end{cases} \quad (6)$$

The derivation of the zeroth-order Γ -limit for functionals of the type of (3) is classical and it has been established in [22] in case $\Phi \equiv 0$ (see also [4, Theorem 4.2] and [6, Theorem 3.2] for earlier related results). We refer to Section 4 for the proof.

As one can see from (6) any information on the number of cracks (i.e., the jump points of u) is lost in the zeroth-order Γ -limit: indeed the positive singular part of the derivative of u has no influence on H . Therefore, in order to gain further insight in the limiting behaviour of the considered chain of atoms, we provide a higher order description of H_n by employing the development by Γ -convergence introduced in [2] (see also [4, 10]). More precisely, one considers the sequence of functionals

$$H_{1,n}^\ell(u_n) := \frac{H_n^\ell(u_n) - \inf_u H(u)}{\lambda_n} \quad (7)$$

with the goal of determining a Γ -limit for $H_{1,n}^\ell$ (denoted by H^1), called *first order Γ -limit* of H_n . The next properties of the minimizers of the limit functional will be useful to study the first order Γ -limit.

2.2 Properties of minimizers of the limit functional

The existence of minimizers of the limit functional is obtained by a classical application of the direct method in the calculus of variations (see, e.g. [15]).

Proposition 4. *Suppose that Assumption \mathcal{A} is satisfied. Then the functional $H : L^1(0, 1) \rightarrow (-\infty, +\infty]$ defined in (6) has a minimizer $u \in BV^\ell([0, 1])$.*

The study of minimizers of the zeroth-order Γ -limit is fundamental for the identification of the first order Γ -limit. Indeed, from (7) it follows that the first-order Γ -limit is infinite for all u in the domain of definition of H with $H(u) - \inf_v H(v) > 0$. For this reason we devote the rest of this section to the study of the properties of minimizers of H .

Note that in the special case $\Phi(x, u) = -f(x)u(x)$ the analysis performed below has already been carried out by Braides, Dal Maso and Garroni in [9].

Depending on the external potential $\Phi(x, u)$ we can identify a region in $[0, 1]$ in which there is elastic behaviour and no cracks. More precisely, we will show that both $(u' - \gamma)_+$ and $D^s u$ necessarily vanishes outside some set determined by the external potential Φ .

Proposition 5. *Suppose that Assumption \mathcal{A} is satisfied. Let $u \in BV^\ell([0, 1])$ be a minimizer of H . Let $F : [0, 1] \rightarrow \mathbb{R}$ be defined by*

$$F(x) := \int_x^1 -\frac{\partial \Phi}{\partial u}(y, u(y)) dy.$$

Let M be the set of (global) maximum points of F . Then the supports of $(u' - \gamma)_+$ and of $D^s u$ are subsets of M .

The following examples show that indeed a minimizer can have jumps both in $(0, 1)$ and at the boundary, as well as a derivative that is strictly bigger than γ .

Example 6. *Let $\Phi(x, w) = 0$ for every x, w . Then $M = [0, 1]$ and it is clear from (15) that any function $u \in BV^\ell([0, 1])$ with slope bigger than γ and non-negative $D^s u$ is a minimizer for H , a case that was already handled in [22].*

Example 7. Let $\Phi(x, u(x)) = -f(x)u(x)$. Thus $-\partial_u \Phi(x, u(x)) = f(x)$. Firstly note that there can only be a crack at $x_0 \in (0, 1)$ if $f(x_0) = 0$. Secondly we consider the case $f(x) < 0$ and $\ell > \gamma$. Then $M = \{1\}$. Assume that $u \in BV^\ell([0, 1])$ is a minimizer of H . If we modify it by defining $\tilde{u} \in BV^\ell([0, 1])$ as

$$\tilde{u}(x) := \int_0^x \min\{u', \gamma\} dx,$$

then $J_0^{**}(\tilde{u}') = J_0^{**}(u')$ and $\Phi(x, \tilde{u}) \leq \Phi(x, u)$. Hence $H(\tilde{u}) = H(u)$ and $1 \in S_{\tilde{u}}$.

The next proposition yields information regarding the behaviour of Φ at the jumps of a minimizer $u \in BV^\ell([0, 1])$ of H .

Proposition 8. Suppose that Assumption \mathcal{A} is satisfied. Let $u \in BV^\ell([0, 1])$ be a minimizer of H . Then given $x_0 \in S_u \cap (0, 1)$ the condition

$$\Phi(x_0, u(x_0-)) = \Phi(x_0, u(x_0+)) = \min_{w \in [u(x_0-), u(x_0+)]} \Phi(x_0, w)$$

is satisfied. If $x_0 \in S_u \cap \{0, 1\}$, then the following holds true:

$$\begin{aligned} \Phi(0, u(0+)) &= \min_{w \in [u(0-), u(0+)]} \Phi(0, w), \\ \Phi(1, u(1-)) &= \min_{w \in [u(1-), u(1+)]} \Phi(1, w). \end{aligned}$$

Next we prove that the derivative of any minimizer of H is bounded away from zero almost everywhere. Physically this means that the ratio of compression of the material is bounded in the continuum limit.

Proposition 9. Suppose that Assumption \mathcal{A} is satisfied. Then any minimizer $u \in BV^\ell([0, 1])$ of H satisfies $\text{ess\,inf}_{x \in [0, 1]} u'(x) > 0$.

We finally compute the Euler-Lagrange equation associated with H . The Euler-Lagrange equation yields continuity of u' on a certain set.

Proposition 10. Suppose that Assumption \mathcal{A} is satisfied. Any minimizer u of H is a solution to the Euler-Lagrange-Equation

$$\int_0^1 J_0^{**'}(u')\phi' + \frac{\partial \Phi}{\partial u}(x, u)\phi dx = 0 \quad \text{for any } \phi \in C_0^\infty([0, 1]). \quad (8)$$

Moreover u' is continuous on the open set

$$M_\gamma := \{x \in [0, 1] : u'(x) < \gamma\}. \quad (9)$$

2.3 Compactness

In this section we state the main results of this paper, the compactness of sequences with bounded rescaled energy $H_{1,n}^\ell$. As mentioned earlier, this is of central importance for the derivation of the first order Γ -limit.

Theorem 11. Suppose that Assumption \mathcal{A} is satisfied. Let $(u_n) \subset \mathcal{A}_n^\ell(0, 1)$ be a sequence of configurations such that $\sup_n H_{1,n}^\ell(u_n) < +\infty$. Then the following statements hold:

(a) For every $\varepsilon > 0$ there exists a constant $C = C(\varepsilon) > 0$ independent of n (but possibly depending on the sequence $(u_n)_n$) such that

$$\#\left\{i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} \geq \gamma + \varepsilon\right\} \leq C(\varepsilon) \quad (10)$$

and

$$\#\left\{i : \left| \frac{u_n^{i+1} - u_n^i}{\lambda_n} - \frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n} \right| \geq \varepsilon\right\} \leq C(\varepsilon). \quad (11)$$

(b) Set $\mathcal{I}_n := \left\{i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} \leq \gamma^c\right\}$. Then there exists $C > 0$ such that

$$\sum_{i \in \mathcal{I}_n} \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma \right)_+^2 \leq C. \quad (12)$$

(c) There holds

$$\liminf_{n \rightarrow \infty} \min_{i \in \{0, \dots, n-1\}} \frac{u_n^{i+1} - u_n^i}{\lambda_n} > 0. \quad (13)$$

Some comments are in order.

Part (a) of Theorem 11 shows that sequences of configurations that keep the rescaled energies $H_{1,n}^\ell$ uniformly bounded have only a finite number of bonds such that $(u_n' - \gamma)_+ \geq \varepsilon$. We remark that in contrast to the previous works [4, 22] we do not expect the L^1 limit of an equibounded sequence to have derivative equal to γ almost everywhere if $\ell \geq \gamma$. This is due to the effect of the external force applied on the system. Part (b) provides a more precise information on the magnitude of $(u_n - \gamma)_+$. In part (c) we prove that the ratio of compression of the material remains uniformly bounded along sequences for which the rescaled energies $H_{1,n}^\ell$ are bounded. This is the asymptotic counterpart of Proposition 9. It ensures that in the derivation of the first order Γ -limit the singular behaviour of the potentials is in fact immaterial. The proofs of parts (a), (b) and (c) of Theorem 11 can be found in Sections 5.1, 5.2 and 5.3, respectively.

As a consequence of Theorem 11 we deduce the following result about the convergence of a sequence of configurations equibounded in energy. The proof is an adaptation of Theorem 3.1 in [5] (see also [4]); it can be found in Section 5.3.

Proposition 12. *Suppose that Assumption \mathcal{A} is satisfied. Let $(u_n)_n \subset \mathcal{A}_n^\ell(0,1)$ be a sequence of configurations such that $\sup_{n \rightarrow +\infty} H_{1,n}^\ell(u_n) < \infty$. Then, up to a subsequence, $u_n \rightarrow u$ strongly in $L^1(0,1)$, where $u \in SBV^\ell([0,1])$ is such that*

(i) $\#S_u < +\infty$,

(ii) $[u] > 0$ in S_u ,

(iii) $u' \leq \gamma$ almost everywhere in $(0,1)$.

Here, $[u]$ denotes the difference of the left and the right limits of u .

As a consequence of Proposition 12, no information is encoded in the first order Γ -limit if all minimizers of H have slope strictly bigger than γ in some set of positive measure or have a non-zero Cantor part of the derivative. Due to the effect of the external force this can happen easily as the following example shows.

Example 13. Consider an arbitrary function $u \in C^2((0, 1))$ such that $u(0) = 0$, $u(1) = \ell$ and $u' > \gamma$. Then choosing $\Phi(x, w) = (u - w)^2$, the function u is the unique minimizer of H . Hence by the previous considerations and Theorem 11 the first order Γ -limit is infinite.

As a positive result we show that under some further assumptions on the external force, there always exists a minimizer of H with derivative bounded by γ . The proof can be found in Section 5.3.

Proposition 14. Suppose that Assumption \mathcal{A} is satisfied. Assume in addition that

$$\text{sign} \frac{\partial \Phi}{\partial u}(x, w) \quad \text{is independent on } w \quad \forall x \in [0, 1] \quad (14)$$

and that $\text{sign} \frac{\partial \Phi}{\partial u}$ only changes its value at finitely many points on $[0, 1]$. Then there exists a minimizer $u \in BV^\ell([0, 1])$ of H with $u'(x) \leq \gamma$ for almost every $x \in (0, 1)$ and $|D^c u|([0, 1]) = 0$.

3 Assumption \mathcal{A} on interaction potentials and external forces

We say that Assumption \mathcal{A} is satisfied if the interaction potentials J_1 and J_2 as well as the effective potential J_0 defined in (5) satisfy conditions [H0]–[H5] and if the external force is described by a potential Φ satisfying condition [\Phi1] stated as follows:

[H0] (strict convexity on a bounded interval) There exists $\gamma^c \in (0, +\infty)$ and $c > 0$ such that J_j is strictly convex in $(0, \gamma^c + c)$ for $j = 0, 1$.

[H1] (regularity) $J_j \in C^2((0, \infty))$ for $j = 0, 1, 2$.

[H2] (uniqueness of minimal energy configurations) For any fixed $z \in (0, \gamma^c)$

$$\min \left\{ J_2(z) + \frac{1}{2} (J_1(z_1) + J_1(z_2)) : \frac{1}{2} (z_1 + z_2) = z \right\}$$

is attained at exactly $z_1 = z_2 = z$.

[H3] (behaviour at infinity) $J_j(z) \rightarrow J_j(\infty) \in \mathbb{R}$ for $z \rightarrow \infty$ for $j = 0, 1, 2$.

[H4] (structure of J_0) J_0 has a unique minimum point $\gamma < \gamma^c$ with $\inf_{z \in [\gamma^c, \infty)} J_0(z) > J_0(\gamma)$.

[H5] $J_j(z) = +\infty$ for $z \leq 0$ and $J_j(z) \rightarrow +\infty$ as $z \rightarrow 0$ for $j = 1, 2$.

We remark that assumption [H0] about the strict convexity of J_1 up to γ^c is needed in part (b) of Theorem 11. The other hypotheses are classical in the context of one dimensional, non-convex discrete to continuum theory (see for example [4, 22]).

Our assumption on the potential Φ is as follows:

[\Phi1] $\Phi \in C^2([0, 1] \times \mathbb{R})$.

Remark 15. Assumptions [H0] and [H4] imply that

$$J_0^{**}(z) := \begin{cases} J_0(z) & z < \gamma, \\ J_0(\gamma) & z \geq \gamma. \end{cases} \quad (15)$$

Remark 16 (Lennard-Jones potentials). The classical Lennard-Jones potentials satisfy the assumptions [H0]–[H5]. Indeed for given $c_1, c_2 > 0$ we define

$$J_1(z) = \frac{c_1}{z^{12}} - \frac{c_2}{z^6} \quad \text{and} \quad J_2(z) = J_1(2z)$$

for $z > 0$ and we extend them to $+\infty$ on $(-\infty, 0]$. One can check that J_1, J_2 and J_0 satisfy [H1]–[H5] (see Remark 4.1 in [22] for the detailed computation).

4 Proofs for Proposition 3 and Section 2.2

Proof of Proposition 3. As the result for $\Phi \equiv 0$ has already been proved in [22] it is enough to show the convergence of the force term for any converging sequence $(u_n)_n \subset \mathcal{A}_n^\ell(0, 1)$.

Consider $(u_n)_n \subset \mathcal{A}_n^\ell(0, 1)$ be a sequence of discrete configurations converging to some limit u in $L^1(0, 1)$. We can suppose without loss of generality that $u'_n > 0$ for every $n \in \mathbb{N}$. Indeed if there exists a sequence n_k such that $u'_{n_k}(x) \leq 0$ in an interval, then $H(u_{n_k}) = +\infty$ for every k and $H(u) = +\infty$ thanks to assumption [H5]. Thus we have

$$\begin{aligned}
& \left| \sum_{i=0}^n \lambda_n \Phi(i\lambda_n, u_n^i) - \int_0^1 \Phi(x, u(x)) dx \right| \\
& \leq \sum_{i=0}^{n-1} \left| \lambda_n \Phi(i\lambda_n, u_n(i\lambda_n)) - \int_{i\lambda_n}^{(i+1)\lambda_n} \Phi(y, u(y)) dy \right| + \lambda_n \sup_{x \in [0, 1], 0 \leq w \leq \ell} |\Phi(x, w)| \\
& \leq \sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} |\Phi(y, u(y)) - \Phi(i\lambda_n, u_n(i\lambda_n))| dy + C\lambda_n \\
& \leq \sum_{i=0}^{n-1} \sup_{x \in [0, 1], 0 \leq w \leq \ell} |\nabla \Phi(x, w)| \left(\lambda_n^2 + \int_{i\lambda_n}^{(i+1)\lambda_n} |u(y) - u_n(i\lambda_n)| dy \right) + C\lambda_n \\
& \leq C \sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} |u(y) - u_n(y)| dy + C \sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} |u_n(y) - u_n(i\lambda_n)| dy + C\lambda_n.
\end{aligned}$$

Thus as $u_n \rightarrow u$ in $L^1(0, 1)$ it is enough to prove that

$$\lim_{n \rightarrow +\infty} \sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} |u_n(y) - u_n(i\lambda_n)| dy = 0. \quad (16)$$

Indeed by the fact that u_n is increasing for every n we have

$$\sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} |u_n(y) - u_n(i\lambda_n)| dy \leq \sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} u_n((i+1)\lambda_n) - u_n(i\lambda_n) dy = \lambda_n \ell$$

that yields (16). □

Proof of Proposition 4. By Proposition 3, H is the Γ -limit of some functional with respect to the $L^1(0, 1)$ -topology. Hence it is lower semicontinuous in $L^1(0, 1)$ (cf., [3, Proposition 1.28]). As the weak-* convergence of $(u_k)_k$ towards u in $BV([0, 1])$ implies that $u_k \rightarrow u$ in $L^1(0, 1)$, H is sequentially lower semicontinuous with respect to weak-* convergence in $BV([0, 1])$.

Moreover, given $(u_k)_k \subset BV^\ell([0, 1])$ of H satisfying $\sup_k H(u_k) < +\infty$ there holds that $u'_k > 0$ because otherwise we had $J_0^{**}(u'_k) = +\infty$ by [H5]. Hence u_k is monotone increasing and bounded by ℓ for every $k \in \mathbb{N}$. Thus $\|u_k\|_{L^1(0, 1)} \leq \int_0^1 \ell dx = \ell$ and $|Du_k|([0, 1]) = \ell - 0$. This implies $\|u_k\|_{BV([0, 1])} \leq C$ uniformly in k .

By the direct method of the calculus of variations we thus get existence of a minimizer (see also [3, Theorem 1.21]). □

Proof of Proposition 5. Assume that the thesis does not hold. We then show that u is not a minimizer of H . Let λ be the measure defined by

$$\lambda(A) := \int_{A \cap [0,1]} (u' - \gamma)_+ dx + D^s u(A \cap [0, 1])$$

for any Borel set $A \subset \mathbb{R}$. If the thesis were wrong, then the support of λ would not be contained in M . Choose a point $m \in M$ and set

$$\tilde{u}(x) := \int_0^x \min\{u', \gamma\} dy + \lambda([0, 1]) \cdot \chi_{\{x:m>m\}}(x).$$

Following our definition of $BV^\ell([0, 1])$ and observing that $Du((-1, x]) = Du([0, x])$ for any $x \in [0, 1]$ we obtain for the right continuous good representative of u , again denoted by u , see [1, Theorem 3.28], that

$$u(x) = \int_0^x u'(y) dy + D^s u([0, x]), \quad x \in [0, 1]. \quad (17)$$

Hence, as $\int_0^x \min\{u', \gamma\} dy - \int_0^x u' dy = -\int_0^x (u' - \gamma)_+ dy$, we infer that

$$\begin{aligned} \tilde{u}(x) - u(x) &= -\lambda([0, x]) + \lambda([0, 1]) \cdot \chi_{\{x:m>m\}}(x) \\ &= -\int_0^x d(\lambda - \lambda([0, 1])\delta_m), \end{aligned}$$

where δ_m denotes the Dirac measure concentrated in the point m . Obviously, $\tilde{u} \in BV^\ell([0, 1])$. We have $u' = \tilde{u}'$ outside the set $\{u' > \gamma\}$, inside of which we have $\tilde{u}' = \gamma$. Since by (15) $J_0^{**}(v) = J_0^{**}(\gamma)$ for $v \geq \gamma$, for $\mu \in [0, 1]$ we calculate

$$H(u) - H((1 - \mu)u + \mu\tilde{u}) = \int_0^1 \Phi(x, u(x)) - \Phi(x, (1 - \mu)u(x) + \mu\tilde{u}(x)) dx.$$

We now show that this contradicts the assumption that u is a minimizer of H . Note that we choose convex combinations of u and \tilde{u} here to ensure that the jumps do not become negative and we are dealing with monotone increasing functions. Dividing by μ and letting $\mu \rightarrow 0$, we obtain

$$\begin{aligned} \frac{d}{d\mu} H((1 - \mu)u + \mu\tilde{u}) \Big|_{\mu=0} &= \int_0^1 \frac{\partial \Phi}{\partial u}(x, u(x)) (\tilde{u}(x) - u(x)) dx \\ &= \int_0^1 \frac{\partial \Phi}{\partial u}(x, u(x)) \left(-\int_0^x d(\lambda - \lambda([0, 1])\delta_m)(y) \right) dx \\ &= \int_0^1 \left(\int_y^1 -\frac{\partial \Phi}{\partial u}(x, u(x)) dx \right) d(\lambda - \lambda([0, 1])\delta_m)(y) \\ &= \int_0^1 F(y) d(\lambda - \lambda([0, 1])\delta_m)(y) = \int_0^1 F(y) d\lambda(y) - \lambda([0, 1])F(m) \\ &= \int_0^1 F(y) - F(m) d\lambda(y) \\ &= \int_{(\text{supp } \lambda) \cap M} F(y) - F(m) d\lambda(y) + \int_{(\text{supp } \lambda) \setminus M} F(y) - F(m) d\lambda(y) \\ &= \int_{(\text{supp } \lambda) \setminus M} F(y) - F(m) d\lambda(y). \end{aligned}$$

Since m is a (global) maximizer of F , we have $F(x) \leq F(m)$ for any $x \in [0, 1]$ and for $x \notin M$ we have $F(x) < F(m)$. Moreover, due to the continuity of F , we have that M is closed. Hence, as we assume by contradiction that the support of λ is not a subset of M , it follows that

$$\left. \frac{d}{d\mu} H((1-\mu)u + \mu\tilde{u}) \right|_{\mu=0} < 0,$$

which yields the desired contradiction as u is supposed to be a minimizer of H . \square

Proof of Proposition 8. We argue by contradiction. To this end, we “split” the jump into two smaller jumps and move one of the jumps a little to the left or right. If $x_0 = 0$ or $x_0 = 1$, we can only move in one direction, thereby explaining the weaker assertions of the proposition at the boundary.

Suppose $\Phi(x_0, u(x_0-)) > \Phi(x_0, w)$ for some $w \in (u(x_0-), u(x_0+)]$. The other case can be handled similarly.

Let $\varepsilon > 0$ be small and define $\tilde{u}_\varepsilon(x) \in BV^\ell([0, 1])$ as

$$\tilde{u}_\varepsilon(x) := \begin{cases} u(x) & \text{for } x \notin [x_0 - \varepsilon, x_0] \\ u(x) + w - u(x_0-) & \text{for } x \in [x_0 - \varepsilon, x_0]. \end{cases}$$

We have

$$\int_0^1 J_0^{**}(u') \, dx = \int_0^1 J_0^{**}(\tilde{u}'_\varepsilon) \, dx \quad (18)$$

and

$$\int_0^1 \Phi(x, \tilde{u}_\varepsilon(x)) - \Phi(x, u(x)) \, dx = \int_{x_0-\varepsilon}^{x_0} \Phi(x, u(x) + w - u(x_0-)) - \Phi(x, u(x)) \, dx. \quad (19)$$

As $x \nearrow x_0$, we have $u(x) \rightarrow u(x_0-)$ and thus $u(x) + w - u(x_0-) \rightarrow w$. Hence by continuity of Φ , (18) and (19), we obtain that

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \frac{H(\tilde{u}_\varepsilon) - H(u)}{\varepsilon} &= \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \int_{x_0-\varepsilon}^{x_0} \Phi(x, u(x) + w - u(x_0-)) - \Phi(x, u(x)) \, dx \\ &= \Phi(x_0, w) - \Phi(x_0, u(x_0-)) < 0. \end{aligned}$$

This is in contradiction to the fact that u is a minimizer of H . \square

Proof of Proposition 9. Let u be a minimizer of H . Suppose by contradiction that u satisfies $\text{essinf}_{x \in [0, 1]} u'(x) = 0$. Fix $m, n \in \mathbb{N}$ such that $m < n$ and set

$$A_n := \left\{ x \in [0, 1] : u'(x) < \frac{1}{n} \right\}$$

and

$$C_m := \left\{ x \in [0, 1] : u'(x) > \frac{1}{m} \right\}.$$

As $\text{essinf}_{x \in [0, 1]} u'(x) = 0$, for every $n \in \mathbb{N}$ one has that $|A_n| > 0$. Moreover

$$\lim_{n \rightarrow +\infty} |A_n| = 0, \quad (20)$$

as otherwise $H(u) = +\infty$. For the same reason there exists $m_0 > 0$ such that for all $m > m_0$ we have $|C_m| > 0$. Next we define a regularization \tilde{u} of u , which increases the derivative of u to $1/m$ where it becomes too small and decreases the derivative on C_m in order to meet the boundary condition at 1. For $x \in [0, 1]$ we set

$$\tilde{u}(x) := \int_{[0,x] \setminus A_n} u'(y) dy + D^s u([0, x]) + \int_{[0,x] \cap A_n} \frac{1}{m} dy + \frac{|C_m \cap [0, x]|}{|C_m|} \int_{A_n} \left(u'(y) - \frac{1}{m} \right) dy.$$

It turns out that $\tilde{u} \in BV^\ell([0, 1])$. Notice in addition that

$$\tilde{u}'(x) = u'(x) \quad \text{for a.e. } x \in [0, 1] \setminus (C_m \cup A_n). \quad (21)$$

By the above definition of \tilde{u} and Equation (17), we obtain for any $x \in [0, 1]$

$$|\tilde{u}(x) - u(x)| \leq \int_{[0,x] \cap A_n} \left| \frac{1}{m} - u'(y) \right| dy + \int_{A_n} \left| \frac{1}{m} - u'(y) \right| dy \frac{|C_m \cap [0, x]|}{|C_m|}.$$

By the definition of A_n and the fact that $u' \geq 0$ the following estimate holds:

$$\sup_{x \in [0,1]} |u(x) - \tilde{u}(x)| \leq \frac{2|A_n|}{m}. \quad (22)$$

Moreover, by [H1] and [H3] we know that J_0^{**} is Lipschitz continuous on $[\frac{1}{2m}, \infty)$ for every $m > 0$. Thus, using (20), for any m large enough there exists $n_0(m)$ such that for all $n \geq n_0$ for a.e. $x \in C_m$ the inequality

$$|J_0^{**}(\tilde{u}'(x)) - J_0^{**}(u'(x))| \leq C(m) \frac{|A_n|}{m}$$

holds.

This yields for any n large enough using [Φ1] as well as Equations (21) and (22)

$$\begin{aligned} & H(\tilde{u}) - H(u) \\ &= \int_{A_n} J_0^{**} \left(\frac{1}{m} \right) - J_0^{**}(u') dx + \int_{C_m} J_0^{**}(\tilde{u}') - J_0^{**}(u') dx + \int_0^1 \Phi(x, \tilde{u}(x)) - \Phi(x, u(x)) dx \\ &\leq \int_{A_n} J_0^{**} \left(\frac{1}{m} \right) - J_0^{**} \left(\frac{1}{n} \right) dx + \int_{C_m} C(m) \frac{|A_n|}{m} dx + \frac{C|A_n|}{m} \\ &\leq |A_n| \left(J_0^{**} \left(\frac{1}{m} \right) - J_0^{**} \left(\frac{1}{n} \right) + \frac{C(m)}{m} + \frac{C}{m} \right). \end{aligned}$$

Selecting n large enough we see that, thanks to hypothesis [H5], the right hand side becomes negative. Hence we have reached a contradiction because u minimizes H . \square

Proof of Proposition 10. Let u be a minimizer of H . For every test function ϕ consider $u + \lambda\phi$ for $\lambda \in \mathbb{R}$. Thanks to the minimality of u we have

$$\frac{H(u + \lambda\phi) - H(u)}{\lambda} \geq 0. \quad (23)$$

By Proposition 9, for λ small enough, $u'(x) + \lambda\phi'(x) > 0$ for almost every $x \in [0, 1]$. Therefore letting $\lambda \rightarrow 0$ in (23) and using assumptions [Φ1], [H1] and [H3] to differentiate under the integral sign we obtain that

$$\int_0^1 J_0^{**'}(u')\phi' + \frac{\partial\Phi}{\partial u}(x, u)\phi dx \geq 0.$$

Then replacing ϕ with $-\phi$ we infer the opposite inequality.

To prove the regularity of u' in M_γ , defined in (9), we notice that the boundedness of u implies that $\frac{\partial \Phi}{\partial u}(x, u)$ is bounded. The Euler-Lagrange equation (8) therefore entails that $J_0^{**'}(u')$ is Lipschitz. Notice that the preimage of $\{0\}$ of the continuous map $J_0^{**'}(u')$ equals $\{x \in [0, 1] : u'(x) \geq \gamma\}$ by the strict monotonicity of $J_0^{**'}(z)$ for $z \leq \gamma$ (assumption [H0]) and the fact that $J_0^{**'}(z)$ is constant for $z \geq \gamma$. Since $\{0\}$ is closed, $\{x \in [0, 1] : u'(x) \geq \gamma\}$ is closed. Hence M_γ is open.

By the continuity of $J_0^{**'}(u')$, the strict monotonicity of $J_0^{**'}$ also implies the continuity of u' on M_γ . \square

5 Proofs for Section 2.3

In what follows we use extensively the following quantity:

$$R(z_1, z_2) := \frac{1}{2} [J_1(z_1) + J_1(z_2)] + J_2\left(\frac{z_1 + z_2}{2}\right) - J_0\left(\frac{z_1 + z_2}{2}\right). \quad (24)$$

First of all we propose a technical lemma that shows that under the assumption of convexity of J_0 and J_1 (see hypothesis [H0]), the functional $R(z_1, z_2)$ is bounded from below quadratically. We will employ this estimate in the proof of part (b) of Theorem 11.

Lemma 17. *Let [H0]–[H5] be satisfied. Then*

$$R(z_1, z_2) \geq c|z_1 - z_2|^2 \text{ for all } 0 < z_1, z_2 < \gamma^c. \quad (25)$$

Proof. By strict convexity of J_1 on $(0, \gamma^c + c)$ (see assumption [H0]), the function $R(a + b, a - b) - C|b|^2$ is still convex in b for $C > 0$ small enough as long as b is such that $a + b, a - b < \gamma^c$. By the definition of J_0 we know that $R(a + b, a - b) \geq 0$. Moreover thanks to hypothesis [H2], $R(a, a) = 0$ whenever $a < \gamma^c$. Hence

$$R(a + b, a - b) = R(a + b, a - b) - R(a, a) \geq C|b|^2$$

for $a + b, a - b < \gamma^c$. Hence (25) follows. \square

We are in position to prove the main theorem. In the next sections we prove separately part (a), (b) and (c) of Theorem 11.

5.1 Proof of part (a) of Theorem 11

Proof. Let $(u_n) \subset \mathcal{A}_n^\ell(0, 1)$ be a sequence of configurations such that $\sup_n H_{1,n}^\ell(u_n) < +\infty$. The first step of the proof of the compactness result for the Γ -limit of first order is the construction of suitable competitors for H that allow to obtain the estimates in (10) and (11). In particular the goal is to define competitors $v_{1,n}$ and $v_{2,n}$ in such a way that the difference $\frac{1}{\lambda_n} (H_n^\ell(u_n) - \frac{1}{2}(H(v_{1,n}) + H(v_{2,n})))$ provides control of the quantities in (10) and (11). Observe in addition that this difference is controlled from above by $H_{1,n}^\ell(u_n)$. We remark that the competitors $v_{1,n}$ and $v_{2,n}$ are not continuous and hence do not belong to $\mathcal{A}_n^\ell(0, 1)$; however, they are admissible functions for H .

We will divide the proof in two steps: the first one is devoted to the construction of the competitors and the second one to the compactness estimates.

Step 1. Construction of the competitors $v_{1,n}$ and $v_{2,n}$

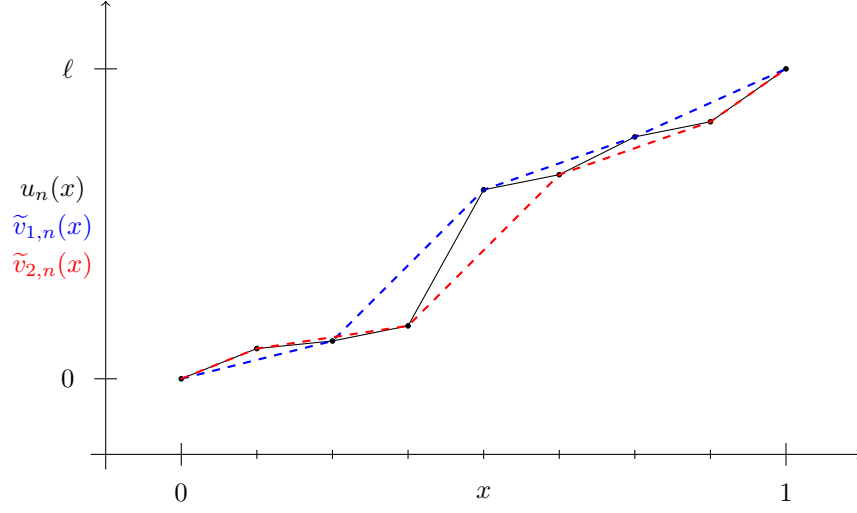


Figure 2: A configuration of the discrete chain (black) and the corresponding naive even-odd interpolators $\tilde{v}_{1,n}$, $\tilde{v}_{2,n}$ (dashed lines, blue, red)

Define first $\tilde{v}_{1,n} : [0, 1] \rightarrow \mathbb{R}$ on the even atoms (and on the n -th one) in the following way:

$$\begin{aligned}\tilde{v}_{1,n}(2k\lambda_n) &:= u_n(2k\lambda_n) \quad \text{for } k \in \mathbb{N}_0, k \leq \frac{n}{2} \\ \tilde{v}_{1,n}(n\lambda_n) &:= u_n(n\lambda_n)\end{aligned}$$

and then by piecewise affine interpolation for all other values of $x \in [0, 1]$. Define $\tilde{v}_{2,n}$ similarly, but prescribing the values of $\tilde{v}_{2,n}$ at 0 , $(2k+1)\lambda_n$ and $n\lambda_n$ instead, for $k \leq \frac{n-1}{2}$.

As usual in this context, the general idea is to use the quantity

$$\begin{aligned}\frac{1}{2}J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) + \frac{1}{2}J_1\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\right) + J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) \\ = J_0\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) + R\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}, \frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\right)\end{aligned}\quad (26)$$

(see (24) for the definition of R) in order to compare $H_n(u_n)$ with $\frac{1}{2}H(\tilde{v}_{1,n}) + \frac{1}{2}H(\tilde{v}_{2,n})$. However, due to the presence of a force term Φ this does not work directly, as the affine interpolation involved in the definition of $\tilde{v}_{i,n}$ may lead to a large difference between u_n and $\tilde{v}_{i,n}$ at some points (see Fig. 2). We thus need to modify the functions $\tilde{v}_{i,n}$ accordingly.

We define $\bar{v}_{1,n}$ to be equal to $\tilde{v}_{1,n}$ everywhere, with the following exception: if the slope of $\tilde{v}_{1,n}$ exceeds γ on an interval $(2k\lambda_n, (2k+2)\lambda_n)$, where γ is as in [H4], we prescribe $\bar{v}_{1,n}$ on the atoms $2k\lambda_n$, $(2k+1)\lambda_n$ and $(2k+2)\lambda_n$ as

$$\begin{aligned}\bar{v}_{1,n}(2k\lambda_n) &:= \tilde{v}_{1,n}(2k\lambda_n), \\ \bar{v}_{1,n}((2k+1)\lambda_n) &:= u_n((2k+1)\lambda_n), \\ \bar{v}_{1,n}((2k+2)\lambda_n) &:= \tilde{v}_{1,n}((2k+2)\lambda_n).\end{aligned}$$

Then, we extend it to $(2k\lambda_n, (2k+2)\lambda_n)$ not by affine interpolation but we instead impose $\bar{v}_{1,n}$ to have slope γ almost everywhere on the interval $(2k\lambda_n, (2k+2)\lambda_n)$. In this way we are forced to

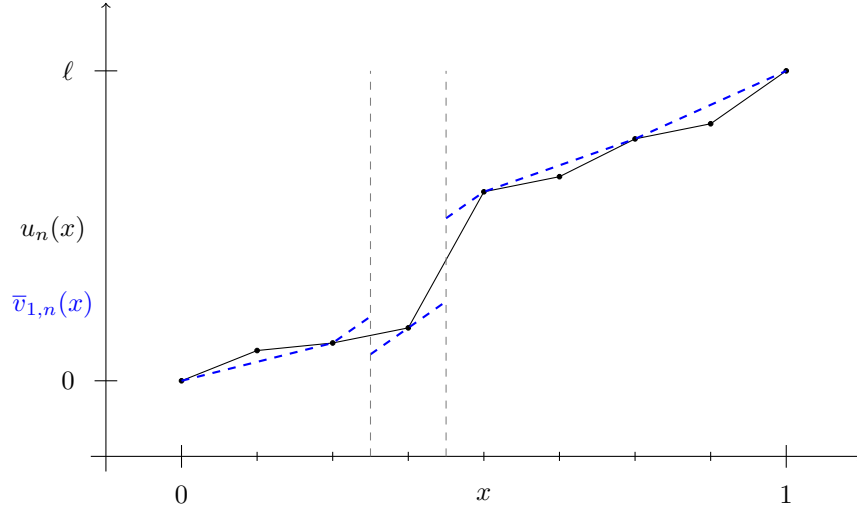


Figure 3: A configuration of the discrete chain (black) and the corresponding adjusted even-odd interpolating function $\bar{v}_{1,n}$ before the final translation step (dashed line, bl)

introduce jumps in some intermediate points of the interval $(2k\lambda_n, (2k+2)\lambda_n)$; in particular we allow for jumps in $(2k + \frac{1}{2})\lambda_n$ and $(2k + \frac{3}{2})\lambda_n$ (cf. Fig. 3).

Finally, we possibly perform a translation to $\bar{v}_{1,n}$ obtaining as a final outcome the function $v_{1,n}$: if the jumps at $(2k + \frac{1}{2})\lambda_n$ or at $(2k + \frac{3}{2})\lambda_n$ are negative, we add a constant to $\bar{v}_{1,n}$ on the interval $((2k + \frac{1}{2})\lambda_n, (2k + \frac{3}{2})\lambda_n)$ in such a way that the negative jump is eliminated and the function becomes continuous at that point again (cf. Fig. 4 and 5). This does not cause another negative jump to appear on the other end of the interval, since we are in the case of the slope of $\bar{v}_{1,n}$ being larger than γ on $(2k\lambda_n, (2k+2)\lambda_n)$.

The definition of $v_{2,n}$ is performed using the obvious modifications: on the intervals $(2k - 1)\lambda_n, (2k + 1)\lambda_n)$ one applies to $\tilde{v}_{2,n}$ the same procedure used to construct $v_{1,n}$ from $\tilde{v}_{1,n}$.

Step 2. Compactness estimates

Now we are in a position to prove the statements of part (a) of Theorem 11. By (26) and the definition of $\tilde{v}_{1,n}$ above, the following equality holds for any even $0 \leq i \leq n - 2$:

$$\begin{aligned} & \frac{1}{2} J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \frac{1}{2} J_1 \left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n} \right) + J_2 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) \\ &= \frac{1}{2\lambda_n} \int_{i\lambda_n}^{(i+2)\lambda_n} J_0(\tilde{v}'_{1,n}) dx + R \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}, \frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n} \right). \end{aligned} \quad (27)$$

An analogous equality holds for i odd and $\tilde{v}_{2,n}$. Taking the sum with respect to i ranging from 0

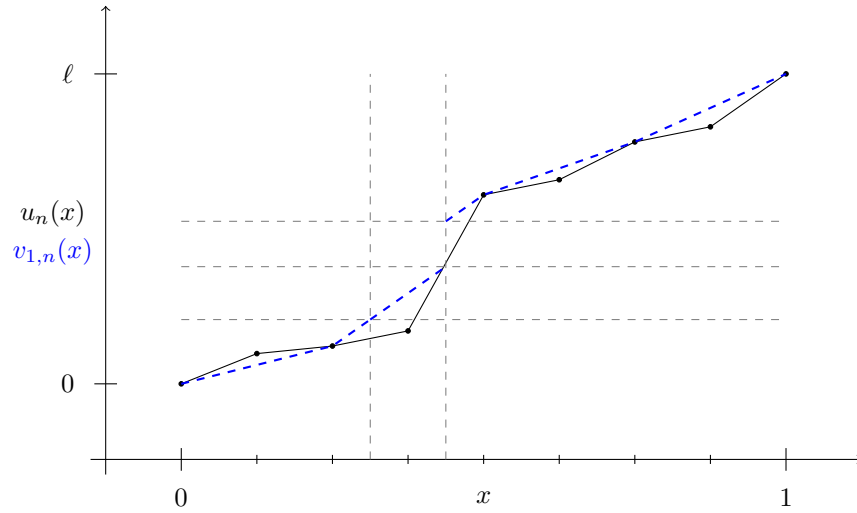


Figure 4: A configuration of the discrete chain (black) and the corresponding adjusted even-odd interpolating function $v_{1,n}$ after the final translation step (dashed line, blue); the left discontinuity has been fixed during the translation step

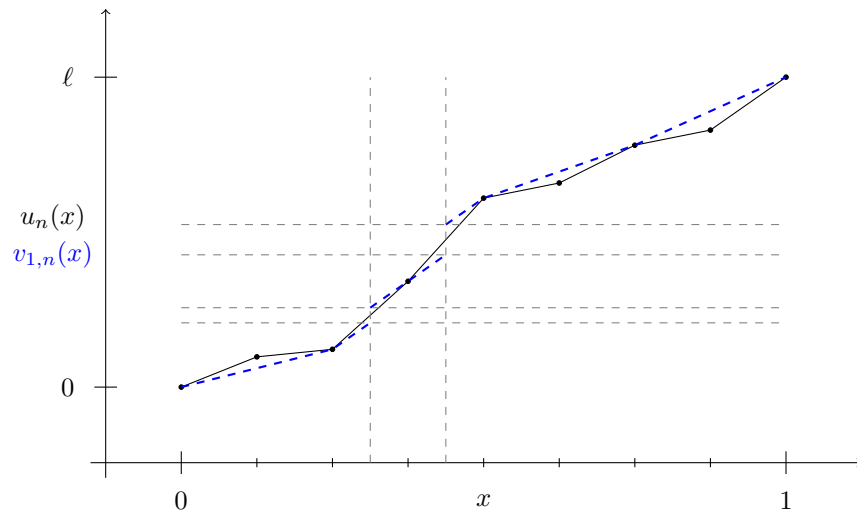


Figure 5: A slightly different configuration of the discrete chain (black) and the corresponding adjusted even-odd interpolating function $v_{1,n}$ (dashed line, blue); here no translation was required as no “backward” jump occurred as a result of the modification of $\tilde{v}_{1,n}$ and consequently $v_{1,n}$ remains discontinuous at two points.

to $n - 2$ and multiplying by λ_n , we therefore obtain

$$\begin{aligned}
& \sum_{i=0}^{n-1} \lambda_n J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \sum_{i=0}^{n-2} \lambda_n J_2 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) \\
&= \frac{1}{2} \int_0^1 J_0(\tilde{v}'_{1,n}) dx + \frac{1}{2} \int_0^1 J_0(\tilde{v}'_{2,n}) dx + \sum_{i=0}^{n-2} \lambda_n R \left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) \\
& \quad + \frac{\lambda_n}{2} \left[J_1 \left(\frac{u_n^1 - u_n^0}{\lambda_n} \right) + J_1 \left(\frac{u_n^n - u_n^{n-1}}{\lambda_n} \right) - J_0 \left(\frac{u_n^1 - u_n^0}{\lambda_n} \right) - J_0 \left(\frac{u_n^n - u_n^{n-1}}{\lambda_n} \right) \right],
\end{aligned} \tag{28}$$

where the last line contains the corrections for the segments at the end of the chain. Moreover as the slope of u_n at the boundary is prescribed (see assumption [B1]), the terms in the last line can be estimated by $C\lambda_n$. This yields

$$\begin{aligned}
& \sum_{i=0}^{n-1} \lambda_n J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \sum_{i=0}^{n-2} \lambda_n J_2 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) \\
& \geq \frac{1}{2} \int_0^1 J_0(\tilde{v}'_{1,n}) dx + \frac{1}{2} \int_0^1 J_0(\tilde{v}'_{2,n}) dx + \sum_{i=0}^{n-2} \lambda_n R \left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - C\lambda_n.
\end{aligned} \tag{29}$$

Notice that for $1 \leq i \leq n - 1$ even we have that $u_n^i = v_{1,n}(i\lambda_n)$ and the function $v_{1,n}$ is Lipschitz with slope less or equal than γ in $((i - \frac{1}{2})\lambda_n, (i + \frac{1}{2})\lambda_n)$. Therefore by Lipschitz continuity of Φ (see assumption [Φ 1]), we infer

$$\begin{aligned}
& \frac{1}{\lambda_n} \int_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} \Phi(x, v_{1,n}(x)) dx - \Phi(i\lambda_n, u_n^i) \leq \frac{1}{\lambda_n} \int_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} |\Phi(x, v_{1,n}(x)) - \Phi(i\lambda_n, u_n^i)| dx \\
& \leq C\lambda_n + \frac{C}{\lambda_n} \int_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} |v_{1,n}(x) - u_n^i| dx \leq C\lambda_n.
\end{aligned} \tag{30}$$

For $1 \leq i \leq n - 1$ odd we can distinguish two cases. If $\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} > \gamma$ we have, by the construction in the previous step that $|u_n^i - v_{1,n}(i\lambda_n)| \leq C\lambda_n$. On the other hand if $\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} \leq \gamma$ we have $v_{1,n}(i\lambda_n) = \tilde{v}_{1,n}(i\lambda_n) = \frac{u_n^{i+1} + u_n^{i-1}}{2}$. In this case as well it is easy to check that $|u_n^i - v_{1,n}(i\lambda_n)| \leq C\lambda_n$. Therefore, thanks to assumption [Φ 1], we infer

$$\begin{aligned}
& \frac{1}{\lambda_n} \int_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} \Phi(x, v_{1,n}(x)) dx - \Phi(i\lambda_n, u_n^i) \\
& \leq \frac{1}{\lambda_n} \int_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} |\Phi(x, v_{1,n}(x)) - \Phi(i\lambda_n, v_{1,n}(i\lambda_n))| dx + |\Phi(i\lambda_n, v_{1,n}(i\lambda_n)) - \Phi(i\lambda_n, u_n^i)| \\
& \leq C\lambda_n.
\end{aligned} \tag{31}$$

Analogous estimates hold for $v_{2,n}$.

Then, multiplying inequalities (30) and (31) by $\lambda_n/2$ and summing from 1 to $n-1$, we obtain

$$\begin{aligned}
& \sum_{i=0}^n \lambda_n \Phi(i\lambda_n, u_n^i) \\
& \geq \frac{1}{2} \int_0^1 \Phi(x, v_{1,n}) dx + \frac{1}{2} \int_0^1 \Phi(x, v_{2,n}) dx + \lambda_n \Phi(0, 0) + \lambda_n \Phi(1, \ell) \\
& \quad - \frac{1}{2} \int_0^{\frac{\lambda_n}{2}} \Phi(x, v_{1,n}) + \Phi(x, v_{2,n}) dx - \frac{1}{2} \int_{1-\frac{\lambda_n}{2}}^1 \Phi(x, v_{1,n}) + \Phi(x, v_{2,n}) dx - C\lambda_n \\
& \geq \frac{1}{2} \int_0^1 \Phi(x, v_{1,n}) dx + \frac{1}{2} \int_0^1 \Phi(x, v_{2,n}) dx - C\lambda_n, \tag{32}
\end{aligned}$$

where in the last inequality we used assumption $[\Phi 1]$. Putting together estimates (32) and (29), we infer

$$\begin{aligned}
& \sum_{i=0}^{n-1} \lambda_n J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) + \sum_{i=0}^{n-2} \lambda_n J_2 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) + \sum_{i=0}^n \lambda_n \Phi(i\lambda_n, u_n^i) \\
& \geq \frac{1}{2} \int_0^1 J_0^{**}(v'_{1,n}) + \Phi(x, v_{1,n}) dx + \frac{1}{2} \int_0^1 J_0^{**}(v'_{2,n}) + \Phi(x, v_{2,n}) dx \\
& \quad + \frac{1}{2} \int_0^1 (J_0 - J_0^{**})(\tilde{v}'_{1,n}) dx + \frac{1}{2} \int_0^1 (J_0 - J_0^{**})(\tilde{v}'_{2,n}) dx \\
& \quad + \sum_{i=0}^{n-2} \lambda_n R \left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - C\lambda_n,
\end{aligned}$$

where we have used $J_0^{**}(v'_{i,n}) = J_0^{**}(\tilde{v}'_{i,n})$, as $\tilde{v}'_{i,n}$ only differs from $v'_{i,n}$ on segments with slope of at least γ and $J_0^{**}(z)$ is constant for all $z \geq \gamma$.

Note that the first two integrals on the right-hand side are precisely $\frac{1}{2}H(v_{1,n}) + \frac{1}{2}H(v_{2,n})$. Subtracting this term from both sides of the equation and dividing by λ_n , we obtain that

$$\begin{aligned}
H_{1,n}^\ell(u_n) &= \frac{H_n^\ell(u_n) - \inf H(u)}{\lambda_n} \\
&\geq \frac{H_n^\ell(u_n) - \frac{1}{2}H(v_{1,n}) - \frac{1}{2}H(v_{2,n})}{\lambda_n} \\
&\geq \frac{1}{2\lambda_n} \int_0^1 (J_0 - J_0^{**})(\tilde{v}'_{1,n}) dx + \frac{1}{2\lambda_n} \int_0^1 (J_0 - J_0^{**})(\tilde{v}'_{2,n}) dx \\
&\quad + \sum_{i=0}^{n-2} R \left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - C. \tag{33}
\end{aligned}$$

Notice that the constant C in (33) does not depend on the sequence $(u_n)_n \subset \mathcal{A}_n^\ell(0, 1)$.

Let us prove (10) by contradiction. Given $0 < \varepsilon < \frac{\gamma^c - \gamma}{2}$ define

$$\begin{aligned}
I_n &:= \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} > \gamma + \varepsilon \right\}, \\
J_n &:= \left\{ i : \frac{u_n^{i+2} - u_n^i}{2\lambda_n} > \gamma + \varepsilon/2 \right\}.
\end{aligned}$$

Suppose by contradiction that there exists $\varepsilon > 0$ such that

$$\limsup_{n \rightarrow +\infty} \#I_n = +\infty. \quad (34)$$

First we prove that (34) implies that

$$\limsup_{n \rightarrow +\infty} \#J_n = +\infty. \quad (35)$$

Indeed, using (33) and the equiboundedness of the rescaled energy, we obtain

$$\sum_{i=0}^{n-2} R\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) \leq C. \quad (36)$$

Introduce the notation

$$\mathfrak{J}_n := \left\{ i : \left| \frac{u_n^{i+1} - u_n^i}{\lambda_n} - \frac{u_n^{i+2} - u_n^{i+1}}{2\lambda_n} \right| \geq \frac{\varepsilon}{2} \right\} \cap J_n^c,$$

where we denote by J_n^c the set of indices that do not belong to J_n . By the definition of J_0 we have that $R(z_1, z_2) \geq 0$ for every z_1, z_2 . In addition to that, whenever $\frac{1}{2}(z_1 + z_2) \in (0, \gamma^c)$, we also have that $R(z_1, z_2) = 0$ if and only if $z_1 = z_2 = \frac{1}{2}(z_1 + z_2)$ by [H2]. Therefore, as ε is chosen such that $\varepsilon < \frac{\gamma^c - \gamma}{2}$ and thanks to hypotheses [H1] and [H5], there exists a constant $C(\varepsilon) > 0$ not depending on n such that for every $i \in \mathfrak{J}_n$

$$R\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) \geq C(\varepsilon).$$

Hence from (36) we infer

$$C \geq \sum_{i=0}^{n-2} R\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) \geq \sum_{i \in \mathfrak{J}_n} R\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) \geq (\#\mathfrak{J}_n)C(\varepsilon).$$

We deduce then that $\#\mathfrak{J}_n < C$, where the constant C is not depending on n . By the definition of I_n and J_n we have also that

$$I_n \cap J_n^c = \left\{ i \in I_n \cap J_n^c : \left| \frac{u_n^{i+1} - u_n^i}{\lambda_n} - \frac{u_n^{i+2} - u_n^{i+1}}{2\lambda_n} \right| \geq \frac{\varepsilon}{2} \right\} = I_n \cap \mathfrak{J}_n.$$

As $\#\mathfrak{J}_n < C$, we conclude that $\#(I_n \cap J_n^c) < C$. Then (35) follows as a consequence of (34). Finally, using the inequality (33) we obtain

$$\sum_{i \in J_n} \left(J_0\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - J_0(\gamma) \right) \leq C.$$

Hence (35) yields a contradiction with assumption [H4].

In an analogous way it is possible to obtain (11). □

5.2 Proof of part (b) of Theorem 11

Proof. In order to obtain (12) we estimate in the following way:

$$\begin{aligned}
& \sum_{i \in \mathcal{I}_n} \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma \right)_+^2 \\
&= \sum_{i \in \mathcal{I}_n} \min \left\{ \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma \right)_+^2, (\gamma^c - \gamma)^2 \right\} \\
&= \sum_{i \in \mathcal{I}_n} \min \left\{ \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} - \gamma + \frac{u_n^{i+1} - u_n^i}{2\lambda_n} - \frac{u_n^i - u_n^{i-1}}{2\lambda_n} \right)_+^2, (\gamma^c - \gamma)^2 \right\} \\
&\leq \sum_{i \in \mathcal{I}_n} \min \left\{ 2 \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} - \gamma \right)_+^2 + 2 \left(\frac{u_n^{i+1} - u_n^i}{2\lambda_n} - \frac{u_n^i - u_n^{i-1}}{2\lambda_n} \right)_+^2, (\gamma^c - \gamma)^2 \right\} \\
&\leq \sum_{i \in \mathcal{I}_n} \min \left\{ 2 \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} - \gamma \right)_+^2, (\gamma^c - \gamma)^2 \right\} \\
&\quad + \sum_{i \in \mathcal{I}_n} \min \left\{ 2 \left(\frac{u_n^{i+1} - u_n^i}{2\lambda_n} - \frac{u_n^i - u_n^{i-1}}{2\lambda_n} \right)_+^2, (\gamma^c - \gamma)^2 \right\} \\
&\leq 2 \sum_{i \in \mathcal{I}_n} \min \left\{ \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} - \gamma \right)_+^2, (\gamma^c - \gamma)^2 \right\} + \sum_{i \in \mathcal{I}_n} \left| \frac{u_n^{i+1} - u_n^i}{\lambda_n} - \frac{u_n^i - u_n^{i-1}}{\lambda_n} \right|^2.
\end{aligned}$$

Using (10) in part (a) of Theorem 11 we deduce that for all $i \in \mathcal{I}_n$ but a finite number of indices (independent on n) one has that

$$\frac{u_n^i - u_n^{i-1}}{\lambda_n} < \gamma^c,$$

where c is the constant defined in assumption [H0]. Therefore combining this fact with Lemma 17 and the inequality (33) we infer that

$$\sum_{i \in \mathcal{I}_n} \left| \frac{u_n^{i+1} - u_n^i}{\lambda_n} - \frac{u_n^i - u_n^{i-1}}{\lambda_n} \right|^2 < C.$$

Notice that

$$\mathcal{J}_n := \left\{ i : \frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} > \gamma^c \right\} \subset \left(\left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} > \gamma^c \right\} \cup \left\{ i : \frac{u_n^i - u_n^{i-1}}{\lambda_n} > \gamma^c \right\} \right);$$

hence, thanks to (10) in Theorem 11, its cardinality is finite and independent of n . Therefore

$$\sum_{i \in \mathcal{I}_n} \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma \right)_+^2 \leq 2 \sum_{i \in \mathcal{J}_n^c} \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} - \gamma \right)_+^2 + C. \quad (37)$$

Finally, using the strict convexity of J_0 in $(0, \gamma^c + c)$ (see hypothesis [H0]), from (37) we obtain that

$$\sum_{i \in \mathcal{I}_n} \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma \right)_+^2 \leq C \sum_{i \in \mathcal{J}_n^c} \left(J_0 \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} \right) - J_0^{**} \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} \right) \right) + C \leq C,$$

where in the last inequality we used (33) and the equiboundedness of the rescaled energy. \square

5.3 Proofs of part (c) of Theorem 11 and of the final remarks

Proof of part (c) of Theorem 11. By contradiction suppose that (13) does not hold true. Notice first that, as $J_j(z) = \infty$ for $z \leq 0$ (see [H5]), we may restrict ourselves to sequences of configurations $(u_n)_n$ of the discrete chains with $u_n \rightarrow u$ with $u'_n > 0$. Set $0 < S < \tilde{S}$ and define

$$h(x) := \int_{\lambda_n}^x \chi_{\{u'_n < S\}} dt \quad \text{and} \quad w(x) := \int_{\lambda_n}^x \chi_{\{u'_n > \tilde{S}\}} dt.$$

for $x \in (\lambda_n, 1 - \lambda_n)$ and extended constantly (and in a continuous way) to $(0, 1)$. Then setting $K > 0$, define

$$\tilde{u}_n(x) := u_n(x) + Kh(x) - \frac{Kh(1)w(x)}{w(1)}.$$

One can easily check that $\tilde{u}_n \in \mathcal{A}_n^\ell(0, 1)$. Moreover

$$\tilde{u}'_n(x) = u'_n(x) + K\chi_{\{u'_n < S\}} - \frac{Kh(1)\chi_{\{u'_n > \tilde{S}\}}}{w(1)}.$$

Notice that $h(1) \rightarrow 0$ as $S \rightarrow 0$ uniformly in n . Indeed if, by contradiction, $h(1)$ is bounded away from zero as $S \rightarrow 0$ and along a subsequence $n_k \rightarrow 0$, then using a diagonal argument it is easy to see that $\sup_n H_n(u_n) = +\infty$ contradicting the hypothesis. Moreover for a similar argument it is possible to choose \tilde{S} small enough such that $w(1) > C > 0$ uniformly in n .

Hence choosing S small enough such that $Kh(1)/w(1) \leq \tilde{S}/2$ we ensured that $\tilde{u}'_n(x) > 0$ and therefore $\tilde{u}_n \in \mathcal{A}_n^\ell(0, 1)$. Moreover

$$|\tilde{u}_n - u_n| = K \left| h(x) - h(1) \frac{w(x)}{w(1)} \right| \leq Kh(1).$$

This implies, thanks to assumption $[\Phi 1]$ that

$$\left| \sum_{i=0}^n \lambda_n \Phi(i\lambda_n, u_n^i) - \sum_{i=0}^n \lambda_n \Phi(i\lambda_n, \tilde{u}_n^i) \right| \leq Ch(1).$$

Therefore

$$\begin{aligned} H_n(u_n) - H_n(\tilde{u}_n) &\geq \sum_{i=0}^{n-1} \left[J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - J_1 \left(\frac{\tilde{u}_n^{i+1} - \tilde{u}_n^i}{\lambda_n} \right) \right] \\ &\quad + \sum_{i=0}^{n-2} \left[J_2 \left(\frac{u_n^{i+2} - u_n^i}{\lambda_n} \right) - J_2 \left(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{\lambda_n} \right) \right] - Ch(1). \end{aligned} \quad (38)$$

Among the contribution of the first neighborhood interaction in the previous estimate, we treat the intervals with $u'_n \geq \tilde{S}$ and the intervals with $u'_n < S$ differently (if $S < u'_n \leq \tilde{S}$, then $\tilde{u}'_n = u'_n$). First consider the intervals $(i\lambda, (i+1)\lambda)$ where $u'_n \geq \tilde{S}$. In these intervals we have $|\tilde{u}'_n - u'_n| \leq Kh(1)/w(1) \leq \tilde{S}/2$ for n big enough. Hence thanks to hypothesis [H1] we have

$$J_1 \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} \right) - J_1 \left(\frac{\tilde{u}_n^{i+1} - \tilde{u}_n^i}{\lambda_n} \right) \geq -Ch(1).$$

On the other if $u'_n < S$ on $(i\lambda, (i+1)\lambda)$, then $K < \tilde{u}'_n < S + K$ on these segments. Therefore, thanks to the convexity of J_1 in assumption [H0] (we choose $K + S$ small enough to make J_1 monotone in $(0, K + S)$), we obtain

$$J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) - J_1\left(\frac{\tilde{u}_n^{i+1} - \tilde{u}_n^i}{\lambda_n}\right) \geq J_1(S) - J_1(K)$$

on these segments.

Regarding the next-to-nearest neighbour potentials, we split the sum (38) into the sum of the intervals $(i\lambda_n, (i+1)\lambda_n)$ such that $u'_n \geq \tilde{S}$ either on $(i\lambda_n, (i+1)\lambda_n)$ or $((i+1)\lambda_n, (i+2)\lambda_n)$ where we have (using again hypothesis [H1])

$$J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - J_2\left(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2\lambda_n}\right) \geq -Ch(1)$$

and in the intervals such that $u'_n < S$ either on $(i\lambda_n, (i+1)\lambda_n)$ or $((i+1)\lambda_n, (i+2)\lambda_n)$, where

$$J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - J_2\left(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2\lambda_n}\right) \geq -C$$

as J_2 is bounded from below. In the remaining cases we have $u'_n = \tilde{u}'_n$ in $(i\lambda_n, (i+2)\lambda_n)$. Hence from inequality (38) we obtain

$$H_n(u_n) - H_n(\tilde{u}_n) \geq h(1)(J_1(S) - J_1(K) - C) - Ch(1),$$

where C does not depend on n and on S .

Notice in addition that

$$h(1) = \lambda_n \# \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} < S \right\}.$$

Hence

$$\limsup_n \frac{H_n(u_n) - H_n(\tilde{u}_n)}{\lambda_n} \geq [J_1(S) - J_1(K) - C] \limsup_n \# \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} < S \right\}. \quad (39)$$

As we supposed that (13) does not hold, one has that

$$\liminf_{n \rightarrow \infty} \min_{i \in \{0, \dots, n-1\}} \frac{u_n^{i+1} - u_n^i}{\lambda_n} = 0.$$

This implies that for every $S > 0$ it holds

$$\limsup_n \# \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} < S \right\} \geq 1. \quad (40)$$

By extracting a subsequence from $(u_n)_n$ (denoted again by u_n) we can suppose that the lim sup in (40) and

$$\limsup_n \frac{H_n(u_n) - H_n(\tilde{u}_n)}{\lambda_n}$$

are both realized. Then

$$\begin{aligned}
\liminf_n H_{1,n}^\ell(u_n) &\geq \liminf_n \frac{H_n(u_n) - H_n(\tilde{u}_n)}{\lambda_n} + \liminf_n H_{1,n}^\ell(\tilde{u}_n) \\
&\geq \liminf_n \frac{H_n(u_n) - H_n(\tilde{u}_n)}{\lambda_n} - M \\
&= \lim_n \frac{H_n(u_n) - H_n(\tilde{u}_n)}{\lambda_n} - M,
\end{aligned} \tag{41}$$

where we used (33) in the proof of the part A) of Theorem 11 to estimate $H_{1,n}^\ell(\tilde{u}_n)$ from below by $-M$. We remark that M is independent of the sequence \tilde{u}_n and more precisely of S . Finally choosing S small enough in (39) and using hypothesis [H5] and the equiboundedness of $H_{1,n}^\ell(u_n)$ in combination with (40) and (41) we reach a contradiction. \square

Proof of Proposition 12. In order to prove the convergence properties of u_n we first observe that with the same argument as in the proof of Proposition 4 one proves that $\|u_n\|_{BV(0,1)} \leq C$ uniformly in n . Therefore there exists a (not relabelled) subsequence $(u_n)_n$ and $u \in BV^\ell([0,1])$ such that $u_n \rightharpoonup u$ weakly* in BV . In particular we have that $u_n \rightarrow u$ strongly in L^1 . Notice in addition that, thanks to assumption [H5] and the equiboundedness of the energy, $(u_n^{i+2} - u_n^i)/\lambda_n > 0$ for every i and n .

We describe in details the arguments for n even, as for n odd the modifications are straightforward. Consider

$$I_n := \left\{ i \in \{0, \dots, n-2\} : \frac{u_n^{i+2} - u_n^i}{2\lambda_n} > \sqrt{n} \right\}$$

and define the following function:

$$v_n(x) := \begin{cases} u_n(x) & x \in [i\lambda_n, (i+2)\lambda_n), i \notin I_n \\ u_n(i\lambda_n) & x \in [i\lambda_n, (i+2)\lambda_n), i \in I_n. \end{cases}$$

Let us prove that $v_n \rightarrow u$ in L^1 as $n \rightarrow +\infty$. Indeed by construction

$$\int_0^1 |u_n - v_n| dx = \sum_{i \in I_n} \int_{i\lambda_n}^{(i+2)\lambda_n} |u_n - u_n(i\lambda_n)| dx \leq \sum_{i \in I_n} \lambda_n (u_n((i+2)\lambda_n) - u_n(i\lambda_n)) \leq \lambda_n \ell.$$

Defining

$$\mathcal{H}_n(u_n) = \sum_{i=1}^{n-2} \left[J_0 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) - J_0^{**} \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) \right]$$

we have, thanks to (33), that $\sup_n \mathcal{H}_n(u_n) < C$ and therefore $\sup_n \#I_n < M$ for $M > 0$. Hence we can suppose that S_{v_n} converges to a finite set that we denote by $\{x_1, \dots, x_m\} \subset [0,1]$. As the nature of the following argument is local, we can assume without loss of generality that $S = \{x_0\}$. Define the following sequence of functions:

$$w_n(x) = \begin{cases} v_n(0) + \int_0^x v_n'(t) dt & x \leq x_0 \\ v_n(0) + \int_0^{0,x} v_n'(t) dt + \sum_{t \in S_{v_n}} [v_n(t)] & x > x_0. \end{cases}$$

Let us prove first that $w_n \rightarrow u$ almost everywhere in $(0, 1)$. Indeed for every $\varepsilon > 0$ there exists n_0 such that for $n > n_0$ we have $\text{dist}(S_{v_n}, x_0) < \varepsilon$. Hence $w_n = v_n$ in $(x_0 - \varepsilon, x_0 + \varepsilon)$. As ε is arbitrary it follows that v_n and w_n have the same pointwise limit.

Notice that by construction $w'_n = v'_n$; moreover $v'_n = u'_n$ for $x \in (i\lambda_n, (i+2)\lambda_n)$ with $i \notin I_n$ and $v'_n = 0$ otherwise. Hence one deduces that there exists $c_1, c_2 > 0$ such that

$$c_1 \int_0^1 |v'_n|^2 dx - c_2 \leq \mathcal{H}_n(u_n) < C. \quad (42)$$

Indeed, given $C > 0$, by the construction of v_n , we have

$$\int_0^1 |v'_n|^2 dx = \int_{\{v'_n \leq \gamma + C\}} |v'_n|^2 dx + \int_{\{v'_n > \gamma + C\}} |v'_n|^2 dx \leq (\gamma + C)^2 + n|\{v'_n > \gamma + C\}|,$$

while on the other hand calling $I_n^C := \{i : v'_n > \gamma + C \text{ in } (i\lambda_n, (i+2)\lambda_n)\}$, there exists $\tilde{C} > 0$ such that (see hypothesis [H4])

$$\begin{aligned} \sum_{i=0}^{n-2} J_0 \left[\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) - J_0^{**} \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) \right] &\geq \sum_{i \in I_n^C} \left[J_0 \left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) - J_0(\gamma) \right] \geq \tilde{C} \# I_n^C \\ &= \tilde{C} n |\{v'_n > \gamma + C\}|. \end{aligned}$$

Therefore (42) holds with the right choice of the constants c_1 and c_2 .

Equation (42) implies that $\|w'_n\|_{L^2((0,1))} = \|v'_n\|_{L^2((0,1))} < C$ and, applying Poincaré's inequality on the interval $(0, x_0)$ and $(x_0, 1)$, we infer that w_n is uniformly bounded in $W^{1,2}((0, 1) \setminus \{x_0\})$. Hence $u \in W^{1,2}((0, 1) \setminus \{x_0\})$ and, up to subsequences, $w'_n \rightharpoonup u'$ weakly in $L^2((0, 1))$. In addition to that, from the definition of w it follows that

$$\lim_{n \rightarrow +\infty} [w_n](x_0) = [u](x_0).$$

Finally we define the new potential $\tilde{J}_0(z) := J_0(z) - J_0^{**}(z)$ for $z > 0$ and the rescaled (and extended) ones:

$$F_n(z) = \begin{cases} \frac{\tilde{J}_0(z)}{\lambda_n} & 0 < z \leq \sqrt{n} \\ +\infty & \text{otherwise,} \end{cases} \quad (43)$$

and

$$G_n(z) = \begin{cases} \tilde{J}_0 \left(\frac{z}{\lambda_n} \right) & 0 < z \leq \frac{1}{\sqrt{n}} \\ +\infty & \text{otherwise.} \end{cases} \quad (44)$$

We observe that

$$\begin{aligned} \mathcal{H}_n(u_n) &= \sum_{i \notin I_n} \tilde{J}_0 \left(\frac{v_n^{i+2} - v_n^i}{2\lambda_n} \right) + \sum_{i \in I_n} \tilde{J}_0 \left(\frac{[v_n]((i+2)\lambda_n)}{\lambda_n} \right) \\ &= \int_a^b F_n(v'_n) dx + \sum_{t \in S_{v_n}} G_n[v_n](t). \end{aligned}$$

By classical results of gamma convergence (see for example Proposition 2.2 in [5]) and generalizing for and arbitrary number of discontinuity we obtain

$$C > \liminf_n \mathcal{H}_n(u_n) \geq \int_0^1 F(u') dx + \sum_{t \in S_u} G([u](t)) \quad \text{if } u \in SBV((0, 1))$$

where

$$F(z) = \begin{cases} 0 & 0 < z \leq \gamma \\ +\infty & \text{otherwise} \end{cases}$$

and

$$G(w) = \begin{cases} J_0(+\infty) - J_0(\gamma) & w \geq \gamma \\ +\infty & w \leq 0 \\ 0 & \text{otherwise.} \end{cases}$$

Moreover $\liminf_n \mathcal{H}_n(u_n) = +\infty$ if $u \in L^1(0, 1) \setminus SBV((0, 1))$.

Hence we deduce that $u \in SBV((0, 1))$, $[u] > 0$ and $u' \leq \gamma$ almost everywhere and, thanks to hypothesis [H5], that $\#S_u < +\infty$. □

Proof of Proposition 14. We will show that given a minimizer u , we may construct a minimizer \tilde{u} such that $\tilde{u}' = \min\{u', \gamma\}$ holds and such that $D^s \tilde{u}$ is concentrated on the set of points where $\frac{\partial \Phi}{\partial u}$ changes sign.

We have supposed that $\frac{\partial \Phi}{\partial u}$ changes sign at $x_1 < x_2 < \dots < x_{M-1}$ for some $M \in \mathbb{N}$. Set $x_0 = 0$ and $x_M = 1$. Then define

$$\tilde{u}(x) := \int_{x_i}^x \min\{u'(y), \gamma\} dy + a_i \tag{45}$$

for $x \in (x_i, x_{i+1})$, where we choose

$$a_i := u(x_{i+1})$$

if $\Phi(x, w)$ is nondecreasing in w for $x \in (x_i, x_{i+1})$ and

$$a_i := u(x_{i+1}) + \int_{x_i}^{x_{i+1}} (u'(y) - \gamma)_+ dy + |D^s u|((x_i, x_{i+1}))$$

if $\Phi(x, w)$ is nonincreasing in w for $x \in (x_i, x_{i+1})$. We have $\tilde{u}(x) \leq u(x)$ on (x_i, x_{i+1}) if $\Phi(x, w)$ is nondecreasing in w and the reverse estimate if $\Phi(x, w)$ is nonincreasing in w . Hence

$$H(u) - H(\tilde{u}) = \sum_{i=0}^{M-1} \int_{x_i}^{x_{i+1}} \Phi(x, u(x)) - \Phi(x, \tilde{u}(x)) dx \geq 0.$$

So, $\tilde{u} \in BV^\ell([0, 1])$ is also a minimizer of H . □

Acknowledgements

This project was partially supported through grants SCHL 1706/2-1 and SCHL 1706/4-1 of the German Science Foundation. All authors acknowledge the stimulating working conditions at ESI Vienna during a workshop.

References

- [1] L. Ambrosio, N. Fusco, and D. Pallara. *Functions of bounded variation and free discontinuity problems*. Oxford Mathematical Monographs. The Clarendon Press, Oxford University Press, New York, 2000.

- [2] G. Anzellotti and S. Baldo. Asymptotic development by Γ -convergence. *Appl. Math. Optim.*, 27:105–123, 1993.
- [3] A. Braides. *Gamma-convergence for beginners*. Oxford University Press, 2002.
- [4] A. Braides and M. Cicalese. Surface energies in nonconvex discrete systems. *Mathematical Models and Methods in Applied Sciences*, 17:985–1037, 2007.
- [5] A. Braides and M. S. Gelli. Continuum limits of discrete systems without convexity hypotheses. *Math. Mech. Solids*, 7(1):41–66, 2002.
- [6] A. Braides and M. S. Gelli. The passage from discrete to continuous variational problems: a nonlinear homogenization process. *Nonlinear Homogenization and its Applications to Composites, Polycrystals and Smart Materials*, pages 45–63, 2004.
- [7] A. Braides and M. S. Gelli. Analytical treatment for the asymptotic analysis of microscopic impenetrability constraints for atomistic systems. *ESAIM Math. Model. Numer. Anal.*, 51(5):1903–1929, 2017.
- [8] A. Braides, A. J. Lew, and M. Ortiz. Effective cohesive behavior of layers of interatomic planes. *Arch. Ration. Mech. Anal.*, 180(2):151–182, 2006.
- [9] A. Braides, G. D. Maso, and A. Garroni. Variational Formulation of Softening Phenomena in Fracture Mechanis: the One-Dimensional Case. *Archive for Rational Mechanics and Analysis*, 146:23–58, 1999.
- [10] A. Braides and L. Truskinovsky. Asymptotic expansions by Γ -convergence. *Continuum Mech. Thermodyn.*, 20:21–62, 2008.
- [11] C. S. Casari, M. Tommasini, R. R. Tykwinski, and A. Milani. Carbon-atom wires: 1-d systems with tunable properties. *Nanoscale*, 8:4414–4435, 2016.
- [12] A. Chambolle. Image segmentation by variational methods: Mumford and Shah functional and the discrete approximations. *SIAM J. Appl. Math.*, 55(3):827–863, 1995.
- [13] M. Charlotte and L. Truskinovsky. Linear elastic chain with a hyper-pre-stress. *J. Mech. Phys. Solids*, 50(2):217–251, 2002.
- [14] M. Charlotte and L. Truskinovsky. Towards multi-scale continuum elasticity theory. *Contin. Mech. Thermodyn.*, 20(3):133–161, 2008.
- [15] B. Dacorogna. *Direct Methods in the Calculus of Variations*. Springer Science+Business Media, LLC, second edition, 2008.
- [16] G. A. Francfort and J.-J. Marigo. Revisiting brittle fracture as an energy minimization problem. *J. Mech. Phys. Solids*, 46(8):1319–1342, 1998.
- [17] M. Friedrich and B. Schmidt. An atomistic-to-continuum analysis of crystal cleavage in a two-dimensional model problem. *J. Nonlinear Sci.*, 24(1):145–183, 2014.
- [18] M. Friedrich and B. Schmidt. An analysis of crystal cleavage in the passage from atomistic models to continuum theory. *Arch. Ration. Mech. Anal.*, 217(1):263–308, 2015.
- [19] T. Hudson and C. Ortner. On the stability of Bravais lattices and their Cauchy-Born approximations. *ESAIM Math. Model. Numer. Anal.*, 46(1):81–110, 2012.

- [20] L. Lauerbach, M. Schäffner, and A. Schlömerkemper. On continuum limits of heterogeneous discrete systems modelling cracks in composite materials. *GAMM-Mitt.*, 40(3):184–206, 2018.
- [21] C. M. Lieber. One-dimensional nanostructures: Chemistry, physics and applications. *Solid State Communications*, 107(11):607 – 616, 1998.
- [22] L. Scardia, A. Schlömerkemper, and C. Zanini. Boundary layer energies for nonconvex discrete systems. *Mathematical Models and Methods in Applied Sciences*, 21(4):777–817, 2011.
- [23] L. Scardia, A. Schlömerkemper, and C. Zanini. Towards uniformly Γ -equivalent theories for nonconvex discrete systems. *Discrete Contin. Dyn. Syst. Ser. B*, 17(2):661–686, 2012.
- [24] M. Schäffner and A. Schlömerkemper. On a Γ -convergence analysis of a quasicontinuum method. *Multiscale Model. Simul.*, 13(1):132–172, 2015.
- [25] M. Schäffner and A. Schlömerkemper. On Lennard-Jones systems with finite range interactions and their asymptotic analysis. *Netw. Heterog. Media*, 13(1):95–118, 2018.
- [26] L. Truskinovsky. Fracture as a phase transition. *Math. Mech. Solids Contemporary research in the mechanics and mathematics of materials*, 322-332, pages 322–332, 1996.