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External Forces in the Continuum Limit of Discrete Systems with Non-Convex Interaction Potentials: Compactness for a Γ-Development

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This paper is concerned with equilibrium configurations of one-dimensional particle systems 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 and thus may model dead as well as live loads. Our result is based on a new technique for deriving compactness results which are required for calculating the first-order Γ-limit in the presence of external forces: 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. The paper is complemented with the study of the minimizers of the Γ-limit.

Keywords: Discrete-to-continuum limit, fracture, external force, Lennard-Jones potential.

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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.

In this article we focus on one-dimensional systems, which have served as toy-models by themselves in engineering and mathematical physics, see, e.g. [13, 22] and references therein. In particular, one-dimensional systems have the advantage of a

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monotonic ordering of the particles that makes the mathematical modeling simpler, cf. [8, 10]. In nanomaterials research, one-dimensional particle systems have recently gained interest, for instance as carbon atom wires [12, 26, 33] or one-dimensional systems of silicon [25]. One-dimensional surface nanostructures on semiconductor surfaces such as chains of gold atoms on certain substrates, see, e.g., [30], raise the interest of mechanical properties of such chains depending on the forces exerted by the substrate since the electronic properties strongly depend on the lattice constants. Similarly, chains of fullerenes in carbon nanotubes experience external forces which influence the chain's mechanical properties, see, e.g., [31]. Our analysis yields a first insight into the effective behaviour due to particle interactions and external forces.

Following [4, 27], 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. We additionally allow for external forces, including 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 includes many physically interesting potentials that are strongly repulsive at short distances and mildly attractive at long distances, cf. Section 3 for more details. The classical Lennard-Jones potential (even without a cut-off) is just one example. Other expamples include interaction potentials typically used in molecular dynamics like the Gay-Berne potentials for fixed geometries of the molecules in liquid crystals [32] or the Girifalco potentials derived for the interaction of fullerene molecules [19].

Our aim is to derive continuum energy functionals from models in the discrete setting as the number of particles tends to infinity. We do so in the context of Γ-convergence techniques. Related mathematical results known for higher-dimensional fracture problems and the derivation of surface energies in the passage from discrete to continuous systems can be found in [8, 17, 18, 23]. For literature on the variational modeling of fracture in the continuum setting we refer to the introduction of [16] and the references therein.

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, 11, 28]. We note that this first approach, which we follow here, allows for large deformations, cf. also [4, 27]. For a discussion of the importance of allowing for large deformations see [16]. (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. [9, 11, 24, 28, 29]. Moreover, there are studies of one-dimensional systems with different scalings for the convex and the concave part of the internal potentials, cf. [5, 6, 7]. For other mathematical approaches to discrete to continuum analysis for fracture mechanics and surface energies we refer to [13, 14, 20, 21, 22].

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

$$H^{\ell}_{1,n}(u_n) := n(H_n(u_n) - \inf_u H(u)) \tag{1}$$

with the goal of determining a Γ-limit for $H^{\ell}_{1,n}$, 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 of $H^{\ell}_{1,n}$ 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 $H^{\ell}_{1,n}(u_n)$. 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 $\mathscr{A}$ 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 occour. 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 [5], where the special case of a dead load $\Phi(x,u) = -f(x)u(x)$ is considered.

In Section 2.3 we state the main results concerning the compactness estimates for the first order Γ-limit: in Theorem 2.11 (a) we prove that sequences of configurations that keep $H^\ell_{1,n}$ 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, 27]. 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 2.11 (b) we provide a more precise information on the magnitude of $(u'_n - \gamma)_+$. Finally, in Theorem 2.11 (c) we prove that the ratio of compression of the material remains uniformly bounded along sequences that keep the rescaled energies $H^\ell_{1,n}$ 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 $\mathscr{A}$) 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 2.1). 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 $u_n : \lambda_n\mathbb{Z}\cap[0,1] \to \mathbb{R}$, where we abbreviate $\lambda_n := \frac{1}{n}$, $n \in \mathbb{N}$. As it is customary, we call the set of all possible configurations $\mathcal{A}_n(0,1)$ and we identify it with the set of all piecewise affine interpolations on $[0,1]$:

$$\mathcal{A}_n(0,1) = \left\{ u\colon [0,1] \to \mathbb{R} : \begin{array}{l} u \in C([0,1]),\ u(x) \text{ is affine in} \\ (i\lambda_n, (i+1)\lambda_n)\ \forall i = 0,\dots,n-1 \end{array} \right\}.$$

We also denote by $u^i_n := u(i\lambda_n)$ 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 Φ : $[0,1] \times \mathbb{R} \to \mathbb{R}$, 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 2.1. We assume the potential Φ to be in $C^2([0,1] \times \mathbb{R})$ throughout the paper. Moreover the assumptions on J_j for $j = 1,2$ are quite classical for the usual convex-concave interaction potentials; they are satisfied, e.g., 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 $\mathscr{A}$. 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 strong convexity of J_1 and J_2, see [H0] in Assumption $\mathscr{A}$ for details.

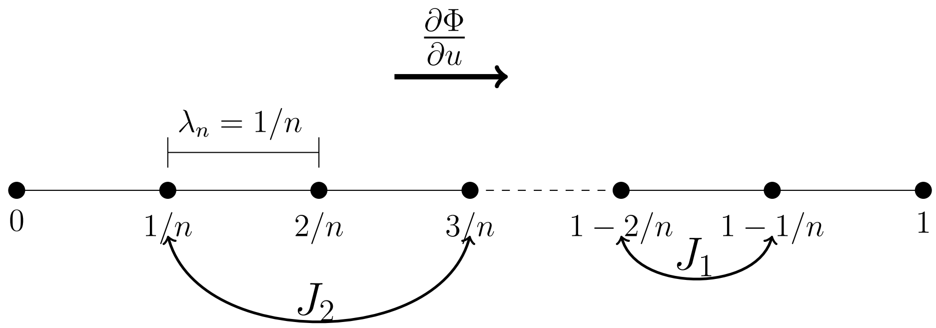

Figure 2.1: A chain of $n+1$ atoms with interactions given by the potentials J_1 and J_2 and the external potential Φ.

Example 2.2. (i) If the external force f depends only on the Lagrangian coordinate, i.e., describes a dead load, the potential simply is

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

(ii) If the external force f also depends on the Eulerian coordinate, which models what is sometimes called live loads and is, e.g., of interest in the case of a chain of atoms that is placed on a substrate [30], the potential reads

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

We define the energy associated with a configuration u_n by

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

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

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

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

$[B1]$ $\quad u_n^1 = \lambda_n\theta_0$ 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 [27] where additionally $[B1]$ is imposed. The Dirichlet conditions $[B0]$ and $[B1]$ correspond to the situation of a *hard loading* *device.* As remarked in [13, 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
$$H_n^\ell(u_n) = \begin{cases} H_n(u_n) & \text{if } u_n \in \mathcal{A}_n^\ell(0,1)\,, \\ +\infty & \text{otherwise}\,. \end{cases} \tag{4}$$

Endowing $\mathcal{A}_n^\ell(0,1)$ with the L^1 topology we define the (zeroth-order) Γ-limit of H_n^ℓ for $n \to +\infty$ as
$$H := \Gamma - \lim_{n\to+\infty} H_n^\ell$$
in the L^1 topology (see [3] for an introduction to 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.
$$J_0(z) := \inf\left\{ J_2(z) + \frac{1}{2}\left(J_1(z_1) + J_1(z_2)\right) : \frac{1}{2}(z_1 + z_2) = z \right\}. \tag{5}$$
Its minimizer is denoted by γ, see Assumption $\mathscr{A}$. Further, J_0^{**} is the lower convex envelope of J_0, cf. (16). We also denote the set of all functions $u \in BV((a-1, b+1))$ that are equal to 0 on $(a-1, a)$ and equal to $\ell > 0$ on $(b, b+1)$ by $BV^\ell([a,b])$. Similarly we define the space $SBV^\ell([a,b])$. 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. Finally, given $x \in [0,1]$ and $u \in BV^\ell([0,1])$ we denote by $u(x-)$ and $u(x+)$ the left and the right limit of u in x, respectively.

Proposition 2.3. *Suppose that Assumption $\mathscr{A}$ is satisfied. Then the Γ-limit of $(H_n^\ell)_n$ with respect to the $L^1(0,1)$ topology is given by*
$$H(u) := \begin{cases} \displaystyle\int_0^1 J_0^{**}(u') + \Phi(x,u)\, dx & \textit{if } u \in BV^\ell([0,1]) \textit{ and } D^s u \geq 0 \\ +\infty & \textit{else}\,. \end{cases} \tag{6}$$

The derivation of the zeroth-order Γ-limit for functionals of the type of (3) is classical and it has been established in [27] in case $\Phi \equiv 0$ (see also [4, Theorem 4.2] and [7, 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, 11]). More precisely, one considers the sequence of functionals
$$H_{1,n}^\ell(u_n) := \frac{H_n^\ell(u_n) - \inf_u H(u)}{\lambda_n}$$
with the goal of determining a Γ-limit for $H_{1,n}^\ell$, called *first order* Γ*-limit* of H_n.

The following 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 2.4. *Suppose that Assumption $\mathscr{A}$ is satisfied. Then the functional $H : L^1(0,1) \to (-\infty, +\infty]$ 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 (1) 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.

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 vanish outside some set determined by the external potential Φ.

Proposition 2.5. *Suppose that Assumption $\mathscr{A}$ is satisfied. Let $u \in BV^\ell([0,1])$ be a minimizer of H. Let $F : [0,1] \to \mathbb{R}$ 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 the domain $(0,1)$ and at the boundary, as well as a derivative that is strictly bigger than γ. The first example deals with the case of absence of external forces, while the second one is an instance of external forces depending only on Lagrangian coordinates, i.e., it deals with dead loads.

Example 2.6. Let $\Phi(x,w) = 0$ for every x, w. Then $M = [0,1]$ and it is clear from (16) 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 [27]. □

Example 2.7. 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 in Proposition 2.5 has a global maximum in x_0, i.e., if $f(x_0) = 0$. Secondly, in the case $f(x) < 0$ for all $x \in (0,1)$ and $\ell > \gamma$, we have $M = \{1\}$. Assume that $u \in BV^\ell([0,1])$ is a minimizer of H. If we modify it by defining $\widetilde{u} \in BV^\ell([0,1])$ as

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

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

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 2.8. *Suppose that Assumption $\mathscr{A}$ 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*

$$\Phi(x_0, u(x_0-)) = \Phi(x_0, u(x_0+)) = \min_{w \in [u(x_0-), u(x_0+)]} \Phi(x_0, w) \tag{7}$$

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

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

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 2.9. *Suppose that Assumption $\mathscr{A}$ is satisfied. Then any minimizer $u \in BV^\ell([0,1])$ of H satisfies* $\operatorname{essinf}_{x \in [0,1]} u'(x) > 0$.

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

Proposition 2.10. *Suppose that Assumption $\mathscr{A}$ is satisfied. Any minimizer u of H is a solution to the Euler-Lagrange-Equation*

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

Moreover u' is continuous on the open set

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

Next we consider the compactness properties of the Γ-limit of first order. The proofs of the above propositions are given in Section 4.

2.3. Compactness

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

Theorem 2.11. *Suppose that Assumption $\mathscr{A}$ is satisfied. Let $(u_n) \subset \mathcal{A}^\ell_n(0,1)$ be a sequence of configurations such that $\sup_n H^\ell_{1,n}(u_n) < +\infty$. Then the following statements hold:*

(a) *For every $\varepsilon > 0$ there exists a constant $C = C(\varepsilon) > 0$ independent of n such that*

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

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

(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*

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

(c) *There holds:* $$\liminf_{n\to+\infty} \min_{i\in\{0,\ldots,n-1\}} \frac{u_n^{i+1} - u_n^i}{\lambda_n} > 0\,. \tag{13}$$

Some comments are in order.

Part (a) of Theorem 2.11 shows that sequences of configurations that keep the rescaled energies $H^\ell_{1,n}$ 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, 27] 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 $H^\ell_{1,n}$ are bounded. This is the asymptotic counterpart of Proposition 2.9. 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 2.11 can be found in Sections 5.1, 5.2 and 5.3, respectively.

As a consequence of Theorem 2.11 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 [6] (see also [4]); it can be found in Section 5.3.

Proposition 2.12. *Suppose that Assumption* $\mathscr{A}$ *is satisfied. Let* $(u_n)_n \subset \mathcal{A}^\ell_n(0,1)$ *be a sequence of configurations such that* $\sup_{n\to+\infty} H^\ell_{1,n}(u_n) < +\infty$. *Then, up to a subsequence,* $u_n \to u$ *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 2.12, 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 2.13. Consider an arbitrary function $\widetilde{w} \in C^2(0,1)$ such that $\widetilde{w}(0) = 0$, $\widetilde{w}(1) = \ell$ and $\widetilde{w}'(x) > \gamma$ for every $x \in (0,1)$. Then, choosing $\Phi(x,u) = (u - \widetilde{w})^2$, we obtain that the function $u = \widetilde{w}$ is the unique minimizer of H. Hence for this choice of the potential Φ all the minimizers of H have slope bigger than γ everywhere. From Theorem 2.12 (iii) it follows that the first order Γ-limit is infinite and so it does not provide additional information on the behaviour of the system. □

In particular, this result demonstrates the further complexity that external forces add to the problem. In this case the study of the first order Γ-limit provides no additional information on the crack formation of the system and an additional analysis is required. 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. Examples of potentials satisfying these conditions are $\Phi(x,u) = (u-\widetilde{w})_+^4$ or $\Phi(x,u) = (u-\widetilde{w})_-^4$ with $\widetilde{w}$ as in Example 2.13.

Proposition 2.14. *Suppose that Assumption $\mathscr{A}$ is satisfied. Assume in addition that for any $x \in [0,1]$*

$$\operatorname{sign} \frac{\partial \Phi}{\partial u}(x,w) \quad \textit{is independent of } w \in \mathbb{R}, \tag{14}$$

and that $\operatorname{sign} \frac{\partial \Phi}{\partial u}$ only changes its value at finitely many points in $[0,1]$. 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 $|D^c u|([0,1]) = 0$.

2.4. First order Γ-limit: discussion and perspectives

The ultimate goal of the present analysis is to derive a first order Γ-limit for the energies H_n, that is to characterize the Γ-limit of the rescaled energies

$$H_{1,n}^\ell(u_n) := \frac{H_n(u_n) - \inf_u H(u)}{\lambda_n}\,. \tag{15}$$

Such complete analysis is postponed to a future work. However, we discuss in this section how Theorem 2.11 and Proposition 2.12 can be employed to characterize the first order Γ-limit of the energies H_n and which difficulties arise in the Γ-liminf and Γ-limsup estimates for $H_{1,n}^\ell$. Theorem 2.11 and Proposition 2.12 describe asymptotic properties of sequences of configurations u_n such that the rescaled energies $H_{1,n}^\ell(u_n)$ are equibounded. In particular, Proposition 2.12 is the counterpart of classical compactness results for convex-concave potentials (see for instance Proposition 4.3 in [4] and Proposition 4.2 in [27]). In case of absence of external forces, the sequence $(u_n)_n$ is converging in L^1, up to subsequences, to a special function of bounded variation u such that $u' = \gamma$ almost everywhere. In our case, however, we can only ensure that $u' \leq \gamma$ almost everywhere. This difference shows that external forces act on the system in a non-trivial way. It also reflects the fact that in our setting we cannot rely on an explicit characterization of the minimum value for H, whereas in [4, 27], it holds

$$\min H = \begin{cases} J_0(\ell) & \text{if } \ell \leq \gamma \\ J_0(\gamma) & \text{if } \ell > \gamma\,. \end{cases}$$

The lack of such characterization makes the derivation of the Γ-liminf and the Γ-limsup for $H_{1,n}^\ell(u_n)$ much more involved. Moreover, as highlighted by Example 2.13, Proposition 2.12 shows that for a specific choice of the external force it can happen that the first order Γ-limit is infinite and thus, in this case, a first order analysis on the energy is not suitable to study crack formation. As a consequence, we plan to restrict the derivation of the first order Γ-limit to external forces for which there exists a minimizer of H satisfying $u'(x) \leq \gamma$ almost everywhere and $|D^c u|([0,1]) = 0$ (see also Proposition 2.14). In this case, we plan to employ a strategy similar to the proof of Theorem 2.11 defining suitable competitors able to provide control of

$H^{\ell}_{1,n}(u_n)$ without relying on an explicit formula for the minimum value for H, but just on the properties of the minimizers on the cracks and on the elastic region, c.f. Section 2.2. In doing so we would be able to characterize boundary-layer energies related to the elastic behaviour and to internal fractures of the material [4, 27], showing how they depend on the external forces applied to the system.

2.5. Extension to higher dimensions

In this work, we have limited our analysis to 1-dimensional models. Of course, this is a severe drawback since the understanding of cracks formation in 2 and 3 dimensions would have important consequences for several applications to materials science. However, the generalization of our results to higher dimensions is not straightforward. The key point is that in one-dimensional systems the atoms are monotonically ordered and, consequently, the cracks of the materials disconnect the domain. Such a property is heavily used in most of our proofs. In particular, in the compactness results for the first order Γ-limit (see Theorem 2.11 and Theorem 2.12), our proof is based on constructing $v_{1,n}$ and $v_{2,n}$, suitable competitors for H, 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 $H^{\ell}_{1,n}(u_n)$. The competitors $v_{1,n}$ and $v_{2,n}$ are constructed from the even/odd interpolations of u_n by truncating the slopes and introducing jumps in suitably chosen points of the domain. Such construction is purely 1-dimensional: indeed, in more dimensions, it is unclear how to define proper interpolating functions and high dimensional cracks to preserve the boundary conditions and the non-interprenetration assumption. A strategy based on a slicing argument could be helpful to extend the results to higher dimensions; however it is possible that additional assumptions on the boundary conditions, on the interactions between each atom, and on the external forces are needed. We also remark that the positive result provided by Proposition 2.14 is also specific to a 1-dimensional model due to the assumptions made on sign $\frac{\partial \Phi}{\partial u}$ and to the strategy of the proof that is based on a 1-dimensional constructive argument. We believe that only additional hypotheses on the external forces would allow to obtain information on the first order Γ-limit in higher dimensions.

3. Assumption $\mathscr{A}$ on interaction potentials and external forces

We say that Assumption $\mathscr{A}$ 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 [Φ1] stated as follows:

[H0] (strong convexity on a bounded interval) There exist $\gamma^c \in (0, +\infty)$ and $c > 0$ such that J_j is strongly 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 $z \in (0, \gamma^c)$

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

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

[H3] (behaviour at infinity) There exists $\lim_{z\to+\infty} J_j(z) \in \mathbb{R}$ denoted by $J_j(\infty)$ 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 $z \le 0$ and $J_j(z) \to +\infty$ as $z \to 0$ for $j = 1, 2$.

We remark that assumption [H0] about the strong convexity of J_1 up to γ^c is needed in part (b) of Theorem 2.11. The other hypotheses are classical in the context of one-dimensional, non-convex discrete to continuum theory (see for example [4, 27]).

Our assumption on the potential Φ is as follows:

[Φ1] $\Phi \in C^2([0,1] \times \mathbb{R})$.

Remark 3.1. Assumptions [H0] and [H4] imply that

$$J_0^{**}(z) := \begin{cases} J_0(z) & z < \gamma\,, \\ J_0(\gamma) & z \ge \gamma\,. \end{cases} \tag{16}$$

Remark 3.2. (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 [H0]–[H5] (see Remark 4.1 in [27] for the detailed computation).

4. Proofs for Proposition 2.3 and Section 2.2

Proof of Proposition 2.3. As the result for $\Phi \equiv 0$ has already been proved in [27] it is enough to show the convergence of the force term for any converging sequence $(u_n)_n \subset \mathcal{A}_n^\ell(0,1)$.

Let $(u_n)_n \subset \mathcal{A}_n^\ell(0,1)$ 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 $(n_k)_k$ such that $u_{n_k}'(x) \le 0$ in an interval, then $H(u_{n_k}) = +\infty$ for every k and $H(u) = +\infty$ thanks to assumption [H5]. Thus we have

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

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

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

$$\lim_{n\to+\infty} \sum_{i=0}^{n-1} \int_{i\lambda_n}^{(i+1)\lambda_n} |u_n(y) - u_n(i\lambda_n)|\, dy = 0\,. \tag{17}$$

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

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

that yields (17). $\square$

Proof of Proposition 2.4. By Proposition 2.3, 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 $u_k \to u$ 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]). $\square$

Proof of Proposition 2.5. Assume that the conclusion 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 conclusion does not hold, then the support of λ would not be contained in M. Choose a point $m \in M$ and set

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

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

$$u(x) = \int_0^x u'(y)\; dy + D^s u([0,x]), \quad x \in [0,1]\,. \tag{18}$$

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

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

where δ_m denotes the Dirac measure concentrated in the point m. Obviously we have $\widetilde{u} \in BV^\ell([0,1])$. We have $u' = \widetilde{u}'$ outside the set $\{u' > \gamma\}$, inside of which we have $\widetilde{u}' = \gamma$. Since by (16) $J_0^{**}(v) = J_0^{**}(\gamma)$ for $v \geq \gamma$, for $\mu \in [0,1]$ we calculate

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

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

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

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 suppλ is not a subset of M, it follows that

$$\frac{d}{d\mu}H((1-\mu)u + \mu\widetilde{u})\Big|_{\mu=0} < 0\,,$$

which yields that u is not a minimizer of H. □

Proof of Proposition 2.8. We argue by contraposition. 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 $\widetilde{u}_\varepsilon(x) \in BV^\ell([0,1])$ as

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

We have
$$\int_0^1 J_0^{**}(u')\,dx = \int_0^1 J_0^{**}(\widetilde{u}'_\varepsilon)\,dx \tag{19}$$
and
$$\int_0^1 \Phi(x, \widetilde{u}_\varepsilon(x)) - \Phi(x, u(x))\,dx = \int_{x_0-\varepsilon}^{x_0} \Phi(x, u(x)+w-u(x_0-)) - \Phi(x, u(x))\,dx\,. \tag{20}$$

As $x \nearrow x_0$, we have $u(x) \to u(x_0-)$ and thus $u(x) + w - u(x_0-) \to w$. Hence by continuity of Φ, (19) and (20), we obtain that

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

Hence u is not a minimizer of H, which finishes the proof. □

Proof of Proposition 2.9. Let u be a minimizer of H. Suppose by contradiction that u satisfies $\operatorname{essinf}_{x\in[0,1]} u'(x) = 0$. Fix $m, n \in \mathbb{N}$ such that $m < n$ and set

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

As $\operatorname{essinf}_{x\in[0,1]} u'(x) = 0$, for every $n \in \mathbb{N}$ one has that $|A_n| > 0$. Moreover
$$\lim_{n\to+\infty} |A_n| = 0\,, \tag{21}$$
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 $u_{m,n}$ 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

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

It turns out that $u_{m,n} \in BV^\ell([0,1])$. Notice in addition that
$$u'_{m,n}(x) = u'(x) \quad \text{for a.e. } x \in [0,1] \setminus (C_m \cup A_n)\,. \tag{22}$$

By the above definition of $u_{m,n}$ and Equation (18), we obtain for any $x \in [0,1]$

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

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

$$\sup_{x\in[0,1]} |u(x) - u_{m,n}(x)| \leq \frac{2|A_n|}{m}\,. \tag{23}$$

Moreover, by [H1] and [H3] we know that J_0^{**} is Lipschitz continuous on $[\frac{1}{2m}, +\infty)$ for every $m > 0$. Thus, using (21) and (23), 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 following inequality holds:

$$|J_0^{**}(u'_{m,n}(x)) - J_0^{**}(u'(x))| \leq C(m)\frac{|A_n|}{m}.$$

This yields for any n large enough, using [Φ1] as well as Equations (22) and (23),

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

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

Proof of Proposition 2.10. Let u be a minimizer of H. For every test function $\phi \in C_0^\infty([0,1])$ consider $u + \lambda\phi$ for $\lambda \in \mathbb{R}$. Thanks to the minimality of u we have

$$\frac{H(u+\lambda\phi) - H(u)}{\lambda} \geq 0\,. \tag{24}$$

By Proposition 2.9, for λ small enough, $u'(x)+\lambda\phi'(x) > 0$ for almost every $x \in [0,1]$. Therefore, letting $\lambda \to 0$ in (24) and using assumptions [Φ1], [H1] and [H3] to differentiate under the integral sign, we obtain that

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

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 u is bounded as it is a one-dimensional BV function. Hence, $\frac{\partial\Phi}{\partial u}(x,u)$ is bounded as well. The Euler-Lagrange equation (8) therefore entails that $J_0^{**\prime}(u')$ is Lipschitz. Notice that the preimage of $\{0\}$ of the continuous map $J_0^{**\prime}(u')$ equals $\{x \in [0,1] : u'(x) \geq \gamma\}$ by the strict monotonicity of $J_0^{**\prime}(z)$ for $z \leq \gamma$ (assumption [H0]) and the fact that $J_0^{**\prime}(z)$ 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 $J_0^{**\prime}(u')$, the strict monotonicity of $J_0^{**\prime}$ also implies the continuity of u' on M_γ. □

5. Proofs for Section 2.3

In what follows we use extensively the following quantity:

$$R(z_1, z_2) := \frac{1}{2}\left[J_1(z_1) + J_1(z_2)\right] + J_2\left(\frac{z_1 + z_2}{2}\right) - J_0\left(\frac{z_1 + z_2}{2}\right). \tag{25}$$

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 2.11.

Lemma 5.1. *Let* [H0]–[H5] *be satisfied. Then there exists* $C > 0$ *such that*

$$R(z_1, z_2) \geq C\,|z_1 - z_2|^2 \quad \text{for all } 0 < z_1, z_2 < \gamma^c. \tag{26}$$

Proof. By strong 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 (26) follows. □

We are in position to prove the main theorem. In the next sections we prove separately part (a), (b) and (c) of Theorem 2.11.

5.1. Proof of part (a) of Theorem 2.11

Proof. Let $(u_n) \subset \mathcal{A}_n^\ell(0,1)$ be a sequence of configurations such that we have $\sup_n H_{1,n}^\ell(u_n) < +\infty$. The first step of the proof of the compactness result for the Γ-limit of first order is the novel 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 $\frac{1}{\lambda_n}\left(H_n^\ell(u_n) - \frac{1}{2}(H(v_{1,n}) + H(v_{2,n}))\right)$ 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 $v_{2,n}$

Define first $\widetilde{v}_{1,n} : [0,1] \to \mathbb{R}$ on the even atoms (and on the n-th one) as follows:

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

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

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

$$\frac{1}{2}J_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)+\frac{1}{2}J_1\left(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\right)+J_2\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right)$$
$$=J_0\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right)+R\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n},\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\right) \tag{27}$$

(see (25) for the definition of R) in order to compare $\frac{1}{2}H(\widetilde{v}_{1,n})+\frac{1}{2}H(\widetilde{v}_{2,n})$ with $H_n(u_n)$. However, due to the presence of a force term Φ this does not work directly, as the affine interpolation involved in the definition of $\widetilde{v}_{i,n}$ may lead to a large difference between u_n and $\widetilde{v}_{i,n}$ at some points (see Figure 5.1). We thus need to modify the functions $\widetilde{v}_{i,n}$ accordingly.

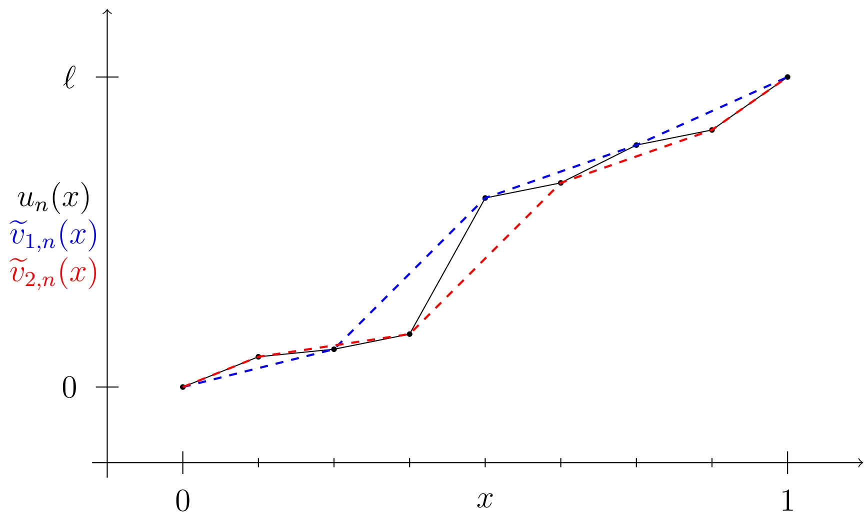

Figure 5.1: A configuration of the discrete chain (black) and the corresponding naive even-odd interpolators $\widetilde{v}_{1,n}$, $\widetilde{v}_{2,n}$ (dashed lines, blue, red)

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

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

Then, we extend it to $(2k\lambda_n,(2k+2)\lambda_n)$ not by affine interpolation but we instead impose $\overline{v}_{1,n}$ to have slope γ almost everywhere on the interval $(2k\lambda_n,(2k+2)\lambda_n)$. In this way we are forced to 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. Figure 5.2).

Finally, we possibly perform a translation to $\overline{v}_{1,n}$ 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 $\overline{v}_{1,n}$ 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. Figures 5.3 and 5.4). 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 $\overline{v}_{1,n}$ being larger than γ on $(2k\lambda_n, (2k+2)\lambda_n)$.

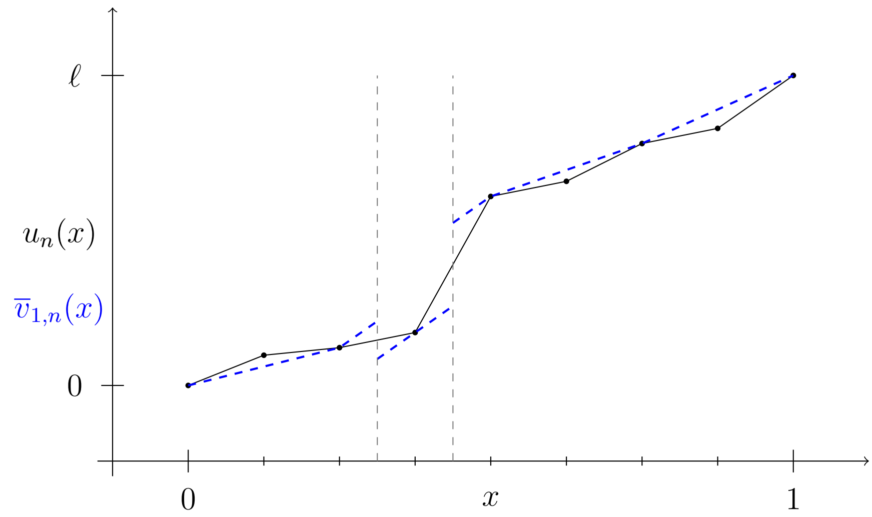

Figure 5.2: A configuration of the discrete chain (black) and the corresponding adjusted even-odd interpolating function $\overline{v}_{1,n}$ before the final translation step (dashed line, blue)

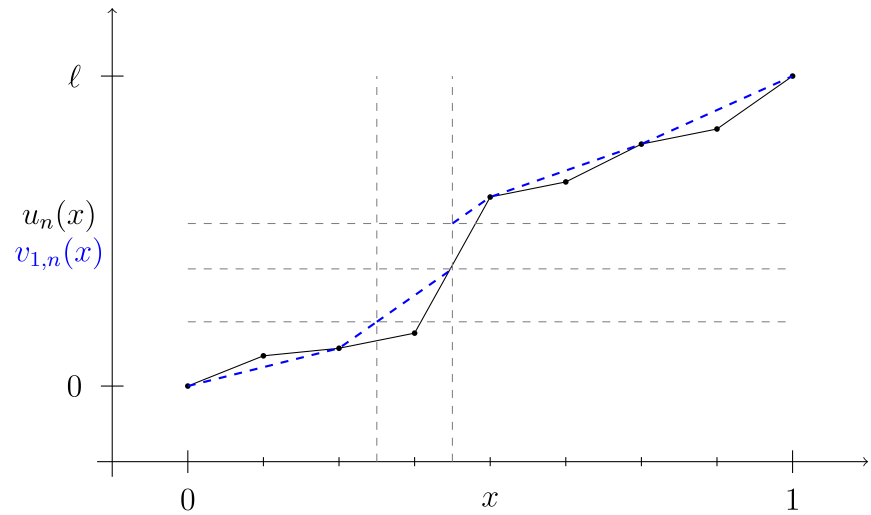

Figure 5.3: A configuration of the discrete chain (black) and the corresponding adjusted even-odd interpolating function $v_{1,n}$ after the final translation step (dashed line, blue); the left discontinuity has been fixed during the translation step

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 the same procedure to $\widetilde{v}_{2,n}$ used to construct $v_{1,n}$ from $\widetilde{v}_{1,n}$.

Step 2. Compactness estimates

Now we are in a position to prove the statements of part (a) of Theorem 2.11. By (27) and the definition of $\widetilde{v}_{1,n}$ above, the following equality holds for any even $0 \le i \le n-2$:

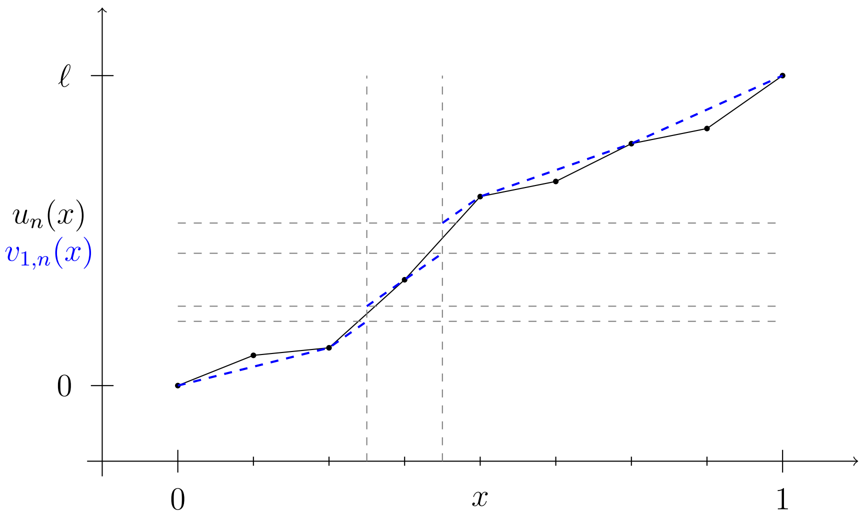

Figure 5.4: A slightly different configuration of the discrete chain (black) and the corresponding adjusted even-odd interpolating function $v_{1,n}$ (dashed line, blue); here no translation was required as no "backward" jump occurred as a result of the modification of $\widetilde{v}_{1,n}$ and consequently $v_{1,n}$ remains discontinuous at two points.

$$\begin{aligned}&\frac{1}{2}J_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)+\frac{1}{2}J_1\left(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\right)+J_2\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right)\\&=\frac{1}{2\lambda_n}\int_{i\lambda_n}^{(i+2)\lambda_n}J_0(\widetilde{v}_{1,n}')\,dx+R\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n},\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\right).\end{aligned}\tag{28}$$

An analogous equality holds for i odd and $\widetilde{v}_{2,n}$. Taking the sum with respect to i ranging from 0 to $n-2$ and multiplying by λ_n, we therefore obtain

$$\begin{aligned}&\sum_{i=0}^{n-1}\lambda_nJ_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)+\sum_{i=0}^{n-2}\lambda_nJ_2\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right)\\&=\frac{1}{2}\int_0^1J_0(\widetilde{v}_{1,n}')\,dx+\frac{1}{2}\int_0^1J_0(\widetilde{v}_{2,n}')\,dx+\sum_{i=0}^{n-2}\lambda_nR\left(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n},\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)\\&\quad+\frac{\lambda_n}{2}\left[J_1\left(\frac{u_n^1-u_n^0}{\lambda_n}\right)+J_1\left(\frac{u_n^n-u_n^{n-1}}{\lambda_n}\right)-J_0\left(\frac{u_n^1-u_n^0}{\lambda_n}\right)-J_0\left(\frac{u_n^n-u_n^{n-1}}{\lambda_n}\right)\right],\end{aligned}\tag{29}$$

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

$$\begin{aligned}&\sum_{i=0}^{n-1}\lambda_nJ_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)+\sum_{i=0}^{n-2}\lambda_nJ_2\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right)\\&\geq\frac{1}{2}\int_0^1J_0(\widetilde{v}_{1,n}')\,dx+\frac{1}{2}\int_0^1J_0(\widetilde{v}_{2,n}')\,dx+\sum_{i=0}^{n-2}\lambda_nR\left(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n},\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)-C\lambda_n\,.\end{aligned}\tag{30}$$

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 $[\Phi1]$), we infer

$$\frac{1}{\lambda_n}\int\limits_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} \Phi(x, v_{1,n}(x))\, dx - \Phi(i\lambda_n, u_n^i) \leq \frac{1}{\lambda_n}\int\limits_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} \left|\Phi(x, v_{1,n}(x)) - \Phi(i\lambda_n, u_n^i)\right|\, dx$$

$$\leq C\lambda_n + \frac{C}{\lambda_n}\int\limits_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} |v_{1,n}(x) - u_n^i|\, dx \leq C\lambda_n\,. \tag{31}$$

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 $v_{1,n}(i\lambda_n) = \widetilde{v}_{1,n}(i\lambda_n) = \frac{u_n^{i+1}+u_n^{i-1}}{2}$. In this case as well it is easy to check that $|u_n^i - v_{1,n}(i\lambda_n)| \leq C\lambda_n$. Hence, due to assumption [Φ1], we infer

$$\frac{1}{\lambda_n}\int\limits_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} \Phi(x, v_{1,n}(x))\, dx - \Phi(i\lambda_n, u_n^i)$$

$$\leq \frac{1}{\lambda_n}\int\limits_{(i-\frac{1}{2})\lambda_n}^{(i+\frac{1}{2})\lambda_n} |\Phi(x, v_{1,n}(x)) - \Phi(i\lambda_n, v_{1,n}(i\lambda_n))|\, dx + \left|\Phi(i\lambda_n, v_{1,n}(i\lambda_n) - \Phi(i\lambda_n, u_n^i)\right|$$

$$\leq C\lambda_n\,. \tag{32}$$

Analogous estimates hold for $v_{2,n}$. Then, multiplying inequalities (31) and (32) by $\lambda_n/2$ and summing from 1 to $n-1$, we obtain

$$\begin{aligned}
&\sum_{i=0}^{n} \lambda_n \Phi(i\lambda_n, u_n^i) \\
&\geq \frac{1}{2}\int_0^1 \Phi(x, v_{1,n})\, dx + \frac{1}{2}\int_0^1 \Phi(x, v_{2,n})\, dx + \lambda_n\Phi(0,0) + \lambda_n\Phi(1,\ell) \\
&\quad - \frac{1}{2}\int_0^{\frac{\lambda_n}{2}} \Phi(x, v_{1,n}) + \Phi(x, v_{2,n})\, dx - \frac{1}{2}\int_{1-\frac{\lambda_n}{2}}^1 \Phi(x, v_{1,n}) + \Phi(x, v_{2,n})\, dx - C\lambda_n \\
&\geq \frac{1}{2}\int_0^1 \Phi(x, v_{1,n})\, dx + \frac{1}{2}\int_0^1 \Phi(x, v_{2,n})\, dx - C\lambda_n\,,
\end{aligned} \tag{33}$$

where in the last inequality we used assumption [Φ1]. Putting together estimates (33) and (5.1), we infer

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

where we have used $J_0^{**}(v'_{i,n}) = J_0^{**}(\widetilde{v}'_{i,n})$, as $\widetilde{v}'_{i,n}$ 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 have precisely the value $\frac{1}{2}H(v_{1,n}) + \frac{1}{2}H(v_{2,n})$. Subtracting this term from both sides of the equation and dividing by λ_n, we obtain that

$$\begin{aligned} H^\ell_{1,n}(u_n) &= \frac{H^\ell_n(u_n) - \inf H(u)}{\lambda_n} \geq \frac{H^\ell_n(u_n) - \frac{1}{2}H(v_{1,n}) - \frac{1}{2}H(v_{2,n})}{\lambda_n} \\ &\geq \frac{1}{2\lambda_n}\int_0^1 (J_0 - J_0^{**})(\widetilde{v}'_{1,n})\,dx + \frac{1}{2\lambda_n}\int_0^1 (J_0 - J_0^{**})(\widetilde{v}'_{2,n})\,dx \\ &\quad + \sum_{i=0}^{n-2} R\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) - C\,. \end{aligned} \tag{34}$$

Notice that the constant C in (34) does not depend on the sequence $(u_n)_n$.

We now prove (10) by contradiction. For a given $0 < \varepsilon < \frac{\gamma^c - \gamma}{2}$ define

$$I_n := \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} \geq \gamma + \varepsilon \right\} \quad \text{and} \quad J_n := \left\{ i : \frac{u_n^{i+2} - u_n^i}{2\lambda_n} \geq \gamma + \varepsilon/2 \right\}. \tag{35}$$

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

$$\limsup_{n\to+\infty} \#I_n = +\infty\,. \tag{36}$$

First we prove that (36) implies that

$$\limsup_{n\to+\infty} \#J_n = +\infty\,. \tag{37}$$

Indeed, using (34) and the equiboundedness of the rescaled energy, we obtain

$$\sum_{i=0}^{n-2} R\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) \leq C\,. \tag{38}$$

We introduce the notation

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

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 $i \in \mathfrak{I}_n$

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

Hence from (38) we infer

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

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

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

As $\#\mathfrak{I}_n < C(\varepsilon)$, we conclude that $\#(I_n \cap J_n^c) < C(\varepsilon)$. Then (37) follows as a consequence of (36). Finally, using the inequality (34) we obtain

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

By the definition of J_n in (35) we have

$$\sum_{i\in J_n}\left(J_0\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right) - J_0(\gamma)\right) \geq \sum_{i\in J_n}\left(\min_{z\geq\gamma+\varepsilon/2} J_0\left(z\right) - J_0(\gamma)\right).$$

Hence assumption [H4] and (37) yield a contradiction. In an analogous way it is possible to obtain (11). □

5.2. Proof of part (b) of Theorem 2.11

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 2.11, we deduce that for all $i \in \mathcal{I}_n$ but a finite number of indices (independent of n) one has that

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

where γ^c is the constant defined in assumption [H0]. Therefore, combining this fact with Lemma 5.1 and inequality (34) 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

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

hence, thanks to (10) in Theorem 2.11, its cardinality is finite and independent of n. Therefore

$$\sum_{i \in \mathcal{I}_n} \left(\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma \right)_+^2 \leq 2 \sum_{i \in \mathfrak{I}_n^c} \left(\frac{u_n^{i+1} - u_n^{i-1}}{2\lambda_n} - \gamma \right)_+^2 + C \,. \tag{39}$$

Finally, using the strong convexity of J_0 in $(0, \gamma^c + c)$ (see hypothesis [H0]), we obtain from (39) that

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

where in the last inequality we used (34) and the equiboundedness of the rescaled energy. □

5.3. Proofs of Theorem 2.11, part (c), and Propositions 2.12 and 2.14

Proof of part (c) of Theorem 2.11. Assume that (13) was not 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 $u_n \to u$ with $u_n' > 0$. Set $0 < S < \widetilde{S}$ and define

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

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

$$\widetilde{u}_n(x) := u_n(x) + K h(x) - \frac{K h(1) w(x)}{w(1)} \,.$$

One can easily check that $\widetilde{u}_n \in \mathcal{A}_n^\ell(0, 1)$ and for $x \in (\lambda_n, 1 - \lambda_n)$

$$\widetilde{u}_n'(x) = u_n'(x) + K \chi_{\{u_n' < S\}} - \frac{K h(1) \chi_{\{u_n' > \widetilde{S}\}}}{w(1)} \,.$$

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

Hence choosing S small enough such that $Kh(1)/w(1) \leq \widetilde{S}/2$ we ensure that we have $\widetilde{u}_n'(x) > 0$. Moreover

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

This implies, thanks to assumption [Φ1] that

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

Therefore

$$\begin{aligned} H_n(u_n) - H_n(\widetilde{u}_n) \geq & \sum_{i=0}^{n-1} \lambda_n \left[J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) - J_1\left(\frac{\widetilde{u}_n^{i+1} - \widetilde{u}_n^i}{\lambda_n}\right)\right] \\ & + \sum_{i=0}^{n-2} \lambda_n \left[J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - J_2\left(\frac{\widetilde{u}_n^{i+2} - \widetilde{u}_n^i}{2\lambda_n}\right)\right] - Ch(1)\,. \end{aligned} \tag{40}$$

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

$$J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) - J_1\left(\frac{\widetilde{u}_n^{i+1} - \widetilde{u}_n^i}{\lambda_n}\right) \geq -Ch(1)\,. \tag{41}$$

On the other hand, if $u_n' < S$ on $(i\lambda_n, (i+1)\lambda_n)$, then $K < \widetilde{u}_n' < K + S$ 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

$$J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) - J_1\left(\frac{\widetilde{u}_n^{i+1} - \widetilde{u}_n^i}{\lambda_n}\right) \geq J_1(S) - J_1(K) \tag{42}$$

on these segments.

Regarding the next-to-nearest neighbour potentials, we split the sum (40) into the sum of the intervals $(i\lambda_n, (i+1)\lambda_n)$ such that $u_n' \geq \widetilde{S}$ either on $(i\lambda_n, (i+1)\lambda_n)$ or $((i+1)\lambda_n, (i+2)\lambda_n)$. If $u_n' \geq \widetilde{S}$ we obviously get $|\widetilde{u}_n' - u_n'| \leq Kh(1)/w(1) \leq \widetilde{S}/2$ for n big enough. Hence, using again hypothesis [H1], we obtain

$$J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - J_2\left(\frac{\widetilde{u}_n^{i+2} - \widetilde{u}_n^i}{2\lambda_n}\right) \geq -Ch(1)\,. \tag{43}$$

On the other hand, consider the intervals $(i\lambda_n, (i+1)\lambda_n)$ such that $u_n' < S$ either on $(i\lambda_n, (i+1)\lambda_n)$ or $((i+1)\lambda_n, (i+2)\lambda_n)$.

As $K < \widetilde{u}_n' < K + S$ whenever $u_n' < S$, we deduce that

$$J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - J_2\left(\frac{\widetilde{u}_n^{i+2} - \widetilde{u}_n^i}{2\lambda_n}\right) \geq -C \tag{44}$$

as J_2 is bounded from below. In the remaining cases we have $u_n' = \widetilde{u}_n'$ in the interval $(i\lambda_n, (i+2)\lambda_n)$. Note now that

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

Hence from inequality (40), using (41)–(44), we obtain

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

where C does neither depend on n nor on S. Hence

$$\limsup_n \frac{H_n(u_n) - H_n(\widetilde{u}_n)}{\lambda_n} \geq \Big[J_1(S) - J_1(K) - C \Big] \limsup_n \# \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} < S \right\} . \tag{45}$$

As we assume that (13) does not hold, we have that

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

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

$$\limsup_n \# \left\{ i : \frac{u_n^{i+1} - u_n^i}{\lambda_n} < S \right\} \geq 1\,. \tag{46}$$

By extracting a subsequence from $(u_n)_n$ (denoted again by u_n), we can suppose that the $\limsup$ in (46) and

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

are both realized. Then

$$\begin{aligned} \liminf_n H_{1,n}^\ell(u_n) &\geq \liminf_n \frac{H_n(u_n) - H_n(\widetilde{u}_n)}{\lambda_n} + \liminf_n H_{1,n}^\ell(\widetilde{u}_n) \\ &\geq \liminf_n \frac{H_n(u_n) - H_n(\widetilde{u}_n)}{\lambda_n} - M = \lim_n \frac{H_n(u_n) - H_n(\widetilde{u}_n)}{\lambda_n} - M\,, \end{aligned} \tag{47}$$

where we used (34) in the proof of the part a) of Theorem 2.11 to estimate $H_{1,n}^\ell(\widetilde{u}_n)$ from below by $-M$ (notice that in (34) all the terms on the right side of the inequality are positive). We remark that the constant M provided by the estimate (34) is independent of the sequence $(\widetilde{u}_n)$ and more precisely of S. Combining (45), (46) and (47), we then obtain

$$\liminf_n H_{1,n}^\ell(u_n) \geq \Big[J_1(S) - J_1(K) - C \Big] - M\,.$$

So, choosing S small enough and using hypothesis [H5] we reach a contradiction to the equiboundedness of $H_{1,n}^\ell$. □

Proof of Proposition 2.12. Before we show the convergence properties of u_n, we observe that, with the same argument as in the proof of Proposition 2.4, one obtains that $\|u_n\|_{BV(0,1)} \leq C$ uniformly in n. Therefore, there exists a subsequence (again denoted by) $(u_n)_n$ and $u \in BV^\ell([0,1])$ such that $u_n \rightharpoonup u$ weakly* in BV. In particular, we have that $u_n \to u$ strongly in L^1. Notice in addition that, thanks to assumption [H5] and the equiboundedness of the energy, $(u_n^{i+1} - u_n^i)/\lambda_n > 0$ for every i and n.

We describe in details the arguments for n even; the modifications for n odd 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 $v_n \to u$ in L^1 as $n \to +\infty$. 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 $\displaystyle \mathcal{H}_n(u_n) = \sum_{i=1}^{n-2} \left[J_0\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) - J_0^{\star\star}\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n} \right) \right]$,

we have, thanks to (34), 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:

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

First we prove that $w_n \to u$ almost everywhere in $(0,1)$. Indeed, for every $\varepsilon > 0$ there exists an n_0 such that for all $n > n_0$ we have $\mathrm{dist}(S_{v_n}, x_0) < \varepsilon$. 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 $w_n' = v_n'$ by construction; moreover $v_n'(x) = u_n'(x)$ for $x \in (i\lambda_n, (i+2)\lambda_n)$ with $i \notin I_n$ and $v_n' = 0$ otherwise. This allows to deduce that there exist $c_1, c_2 > 0$ such that

$$c_1 \int_0^1 |v_n'|^2\, dx - c_2 \leq \mathcal{H}_n(u_n) < C\,. \tag{48}$$

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

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

Now, set $I_n^C := \{i : v_n' > \gamma + C \text{ in } (i\lambda_n, (i+2)\lambda_n)\}$. Then there exists $\widetilde{C} > 0$ such that (see hypothesis [H4])

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

Therefore (48) holds with the right choice of the constants c_1 and c_2.

Equation (48) implies that $\|w_n'\|_{L^2(0,1)} = \|v_n'\|_{L^2(0,1)} < C$ and, applying Poincaré's inequality on the intervals $(0, x_0)$ and $(x_0, 1)$, we infer that w_n is uniformly bounded in $W^{1,2}((0,1)\backslash\{x_0\})$. Hence $u \in W^{1,2}((0,1)\backslash\{x_0\})$ and, up to subsequences, $w_n' \rightharpoonup u'$ weakly in $L^2(0,1)$. In addition, the definitions of v_n, w_n yield that

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

Finally, following [6], we define the new potential $\widetilde{J}_0(z) := J_0(z) - J_0^{\star\star}(z)$ for $z > 0$ and the rescaled (and extended) ones:

$$
F_n(z) = \begin{cases} \dfrac{\widetilde{J}_0(z)}{\lambda_n} & 0 < z \leq \sqrt{n}\,, \\ +\infty & \text{otherwise}\,, \end{cases} \quad \text{and} \quad G_n(z) = \begin{cases} \widetilde{J}_0\left(\dfrac{z}{\lambda_n}\right) & z \geq \dfrac{1}{\sqrt{n}}\,, \\ +\infty & \text{otherwise}\,. \end{cases} \tag{49}
$$

We observe that

$$
\begin{aligned}
\mathcal{H}_n(u_n) &= \sum_{i \notin I_n} \widetilde{J}_0 \left(\frac{v_n^{i+2} - v_n^i}{2\lambda_n} \right) + \sum_{i \in I_n} \widetilde{J}_0 \left(\frac{[v_n]((i+2)\lambda_n)}{2\lambda_n} \right) \\
&= \int_0^1 F_n(v_n')\, dx + \sum_{t \in S_{v_n}} G_n([v_n](t)) \,.
\end{aligned}
$$

By classical results of Γ-convergence, see for example [6, Proposition 2.2], generalized for an arbitrary number of discontinuities, we obtain

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

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 $u \in L^1(0,1) \setminus SBV^\ell([0,1])$.

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

Proof of Proposition 2.14. By Proposition 2.4 we know that a minimizer u of H exists. We show that we may construct a minimizer $\widetilde{u}$ such that $\widetilde{u}' = \min\{u', \gamma\}$ holds and such that $D^s \widetilde{u}$ is concentrated on the set of points where $\frac{\partial \Phi}{\partial u}$ changes sign and at the boundary of the interval $(0,1)$.

By assumption, $\frac{\partial\Phi}{\partial u}$ changes sign at at most finitely many points, which we denote by $x_1 < x_2 < \ldots < x_{M-1}$ for some $M \in \mathbb{N}$. Set $x_0 = 0$ and $x_M = 1$. Then define

$$\widetilde{u}(x) := \int_{x_i}^{x} \min\{u'(y), \gamma\}\, dy + a_i \tag{50}$$

for $x \in (x_i, x_{i+1})$, $i = 0, \ldots, M-1$, where we set $a_i := u(x_i+)$ if $\Phi(x, w)$ is nondecreasing in w for $x \in (x_i, x_{i+1})$, and

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

if $\Phi(x, w)$ is nonincreasing in w for $x \in (x_i, x_{i+1})$. Additionally, we add jumps at the boundary of the interval $(0, 1)$ in order to match the boundary conditions. We have $\widetilde{u}(x) \le u(x)$ 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

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

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

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