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by

Lucia Scardia, Anja Schlömerkemper, and Chiara Zanini

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Lucia Scardia*, Anja Schlömerkemper† and Chiara Zanini‡

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Abstract

In this work we consider a one-dimensional chain of atoms which interact through nearest and next-to-nearest neighbour interactions of Lennard-Jones type. We impose Dirichlet boundary conditions and in addition prescribe the deformation of the second and last but one atoms of the chain. This corresponds to prescribing the slope at the boundary of the discrete setting. We compute the Γ-limits of zero and first order, where the latter leads to the occurrence of boundary layer contributions to the energy. These contributions depend on whether the chain behaves elastically close to the boundary or whether there is a crack. This in turn depends on the given boundary data. We also analyse the location of fracture in dependence on the prescribed discrete slopes.

1 Introduction

Devices in engineering become smaller and smaller. The applicability of classical continuum theories reaches its limit in the modelling of the physical properties of such devices. On the other hand purely atomistic models are often still too complex to handle. To capture discreteness effects and still to be able to model and analyse physical properties, we start from a discrete system and derive its continuum limit. This approach is by now established in the literature and has been successfully applied to different settings. Moreover, there are mathematically rigorous derivations of discrete-to-continuum limits; see e.g. [BLBL02, BG06, BT08, Sch06] in the context of elasticity, [BC07, BDMG99] for fracture mechanics and [Sch05, SS09] for magnetic materials.
In this work we focus on a model that describes fracture. The first important work on a discrete-to-continuum derivation in this area is Truskinovsky's article [Tru96]. Truskinovsky's approach consists of starting from a one-dimensional chain of atoms which interact by Lennard-Jones potentials and to scale the strain in the region close to a crack differently than the strain in the region far away from the crack. This yields a continuum theory which contains a small parameter with the scale of length, which is thus able to reflect the fact that fracture is a size-dependent phenomenon. Truskinovsky obtains a bulk energy as well as a contribution due to the crack. The latter energy contribution depends on the crack opening and is formulated in the sense of Barenblatt [Bar62].

*Eindhoven University of Technology, PO Box 513, WH 4.10, 5600 MB Eindhoven, The Netherlands, email: L.Scardia@tue.nl

†Department of Mathematics, University of Erlangen-Nürnberg, Martensstr. 3, 91058 Erlangen, Germany, email: schloemerk@am.uni-erlangen.de

‡Department of Mathematics, University of Erlangen-Nürnberg, Martensstr. 3, 91058 Erlangen, Germany, email: zanini@am.uni-erlangen.de

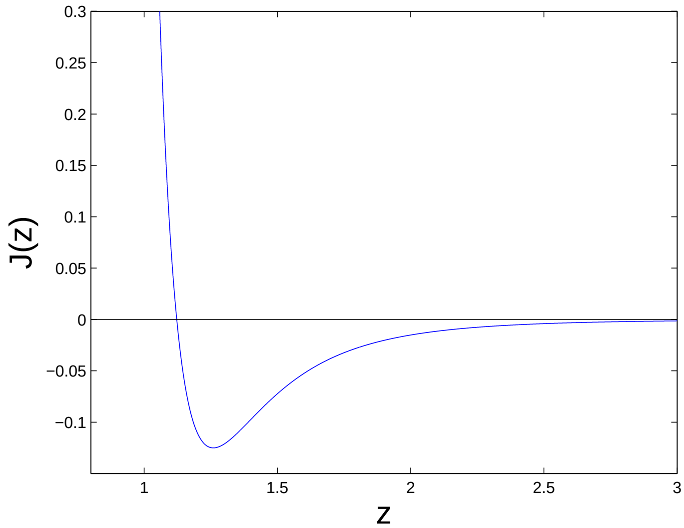

Figure 1: A typical example of a Lennard-Jones potential.

In [BDMG99] Braides, Dal Maso and Garroni provide a first mathematical result related to fracture mechanics by using Γ-convergence methods (see [Bra02] and [DM93] for a comprehensive introduction to Γ-convergence). While Braides, Dal Maso and Garroni assume different scaling behaviour of the Lennard-Jones potential in the convex and concave regions, respectively, we follow Braides and Cicalese [BC07] and derive an asymptotic expansion for the limiting continuum energy up to the first order via Γ-convergence. This is motivated by Braides and Truskinovsky's work [BT08], in which uniformly Γ-equivalent theories are developed in order to obtain a mathematical justification of Truskinovsky's earlier work [Tru96], among others. As we outline in more detail below, one of our future goals is to derive a uniformly Γ-equivalent theory for the setting which we treat in this paper.

As in [BC07] we consider next-to-nearest neighbour interactions in addition to the nearest neighbour interactions between the atoms in the energy functional (see also [CT02]). This leads to boundary layer contributions to the limit energy and thus allows to describe fracture, as will be extensively shown in this article. Throughout we assume that the interaction potentials between nearest and next-to-nearest neighbouring atoms are of Lennard-Jones type. See Figure 1 for an example of a Lennard-Jones potential, and see below for details. Note that our class of Lennard-Jones type potentials also contains typical other interaction potentials of physical relevance, such as Morse potentials or double Yukawa potentials, see Remark 4.1.

Since we deal with nearest and next-to-nearest neighbour interactions, we impose Dirichlet boundary conditions (corresponding to a hard device) not only at the endpoints of the chain, as in [BC07], but also at the second and last but one atoms, in agreement with [CT02]. We notice that this further constraint can be equivalently interpreted as prescribing the discrete slopes at the boundary of the chain. Imposing these additional natural boundary conditions results in new definitions of the occurring boundary layer energies, see (4.13), (4.27) and (4.29), where we relate these with the corresponding ones in [BC07]. For earlier treatments of boundary layer energies see [BLBL02] in the case of pointwise limits using higher gradients and [CT08] using internal variables.

It turns out that the Γ-limit of our discrete energy yields a bulk energy, cf. Theorem 3.1. The bulk energy density is the convexification of a potential, J_0, obtained by combining the Lennard-Jones type potentials between consecutive atoms and between next-to-nearest neighbour atoms through an inf-convolution, cf. (3.3) for details. In order to capture boundary layer contributions, we then compute the first-order Γ-limit in Section 4. We distinguish the cases of elasticity ($\ell \leq \gamma$, Subsection 4.1) and the case of the occurrence of fracture ($\ell > \gamma$, Subsection 4.2), which depend on the parameter of the boundary value ℓ, and on the minimum point γ of the potential J_0.

Therefore our results for the first-order Γ-limit depend on the Dirichlet boundary condition, i.e., on whether $\ell > \gamma$ or not, cf. Theorems 4.3 and 4.8. In other words, the limiting functional is not uniform in ℓ. One of our future goals is to find an energy functional which is uniform in ℓ in the sense of Braides and Truskinovsky [BT08]. Moreover, the limiting functional contains an explicit dependence on the boundary slopes, and it is in general different to the one obtained in [BC07] even if $\ell = \gamma$, cf. Remark 4.5. We point out that the presence of these additional parameters in the boundary layer energy allows us to describe a wider range of possible limiting behaviours for the discrete chain. In particular it turns out that prescribing appropriate discrete slopes at the boundary yields a continuum model which allows for internal cracks for minimal energy configurations, cf. Theorem 5.3 and the end of Section 5 for a corresponding discussion including a multiple scales aspect. On the contrary, fixing only the first and last boundary atoms leads to a location of fracture at the boundary always, as shown in [BC07, Theorem 5.2].

This issue is of particular interest having in mind as application the derivation of a model of cracks using the quasicontinuum method. This method was developed to combine advantages of continuum as well as of discrete descriptions (see [KO01, MTPO98, SMT$^+$98]). The idea is to use the continuum description away from the crack tip and to model the neighbourhood of a crack tip by an atomistic model.
A first step to verify earlier works mathematically was done by Blanc, Le Bris and Legoll [BLBL05]. They consider nearest neighbour interactions, introduce an artificial scaling in the continuum energy in terms of the lattice parameter in order to avoid an unnatural behaviour of the system, and they compute a pointwise limit of the energy functional. Instead of dealing with this modified energy we intend to consider the expansion obtained in the present work by Γ-convergence methods since this contains the lattice parameter naturally.

We finally observe that, as in most of the related mathematical literature we consider a one-dimensional model. This is of course a drawback since we head for a model of fracture in three-dimensional materials, but for now it is not clear how to overcome the related mathematical difficulties. However we hope that this one-dimensional model case will contribute to a better understanding of three-dimensional fracture mechanics. Moreover the one-dimensional model can be regarded as a model for trusses or a model for cleavage. In the latter case, the material breaks along crystalline planes so that a model describing cleavage can be reduced to a one-dimensional one by symmetry, cf. [BLO06, NO02].

2 Setting of the problem

The discrete model which we take as the starting point for the derivation of a continuum energy functional describing the occurrence of fracture is as follows, cf. also Figure 2. We start from a one-dimensional chain of $n+1$ atoms in $[0, 1]$ and consider the limit as $n \to \infty$. For convenience we often

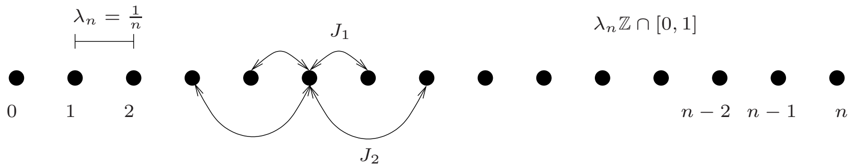

Figure 2: A chain of n atoms.

set $\lambda_n = \frac{1}{n}$. The deformation from the reference configuration is a function $u : \lambda_n\mathbb{Z} \cap [0,1] \to \mathbb{R}$, and u^i is shorthand for $u(i\lambda_n)$. Note that for a function $v : \mathbb{Z} \to \mathbb{R}$ we write $v^i = v(i)$ as shorthand. The Lennard-Jones type potentials J_1 and J_2 describe the interactions between nearest neighbours and next-to-nearest neighbours, respectively. Exact assumptions for both potentials are given in Theorem 3.1 and in $[H1]$–$[H5]$ below. The discrete energy reads

$$H_n(u) = \sum_{i=0}^{n-1} \lambda_n J_1\left(\frac{u^{i+1} - u^i}{\lambda_n}\right) + \sum_{i=0}^{n-2} \lambda_n J_2\left(\frac{u^{i+2} - u^i}{2\lambda_n}\right) \tag{2.1}$$

and is defined on $\mathcal{A}_n(0,1)$, the set of all functions $u : \lambda_n\mathbb{Z} \cap [0,1] \to \mathbb{R}$, which we identify with their piecewise affine interpolations. Thus

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

As in [BC07] we impose Dirichlet boundary conditions on the first and last atoms. In addition we also fix the second and last but one atoms of the one-dimensional chain of atoms under consideration. That is, for given ℓ, $u_0^{(1)}$, $u_1^{(1)} > 0$ we set

$$\begin{aligned} u(0) &= u^0 = 0, & u(1) &= u^n = \ell, \\ u(\lambda_n) &= u^1 = \lambda_n u_0^{(1)}, & u(1-\lambda_n) &= u^{n-1} = \ell - \lambda_n u_1^{(1)}. \end{aligned} \tag{2.2}$$

Note that it is natural to have four boundary conditions in the case of next-to-nearest neighbour interactions, cf. e.g. [CT02, CT08]. Since in nature cracks also occur in the interior of materials, we head for a model that allows for a location of cracks in the interior. By imposing conditions on the first and second as well as on the last and last but one atoms we obtain a model which allows to have fracture in the interior in special cases, see Theorem 5.3.

Remark 2.1. We notice that prescribing the discrete boundary slope does not translate in the continuum picture into prescribing the slope at 0 and 1. On the other hand, its effect is a penalisation in terms of the energy, described by new boundary layer energies with respect to [BC07], cf. (4.13) and (4.27)–(4.29).

Since we require physical configurations u to satisfy the boundary conditions, we incorporate the boundary conditions in the definition of the functional. For given ℓ, $u_0^{(1)}$, $u_1^{(1)} > 0$ we consider the functional $H_n^\ell : \mathcal{A}_n(0,1) \to (-\infty, +\infty]$ defined by

$$H_n^\ell(u) = \begin{cases} H_n(u) & \text{if } u^0 = 0, \ u^1 = \lambda_n u_0^{(1)}, \ u^{n-1} = \ell - \lambda_n u_1^{(1)}, \ u^n = \ell, \\ +\infty & \text{else.} \end{cases} \tag{2.3}$$

It turns out that the zero and first-order Γ-limits of this functional depend on ℓ (cf. Theorems 3.1, 4.3 and 4.8 below). For this reason we make the ℓ-dependence also visible in the notation of the energy in the discrete setting.

3 Zero-order Γ-limit of the discrete energy

The zero-order Γ-limit is the same as the Γ-limit of the discrete energy in (2.3) and yields the bulk contribution of the energy. We derive the Γ-limit in Theorem 3.1, which is based on [BG04, Theorem 3.2] and [BC07, Theorem 4.2]. The bulk energy density identifying the limiting functional is a convexification of a potential that is obtained by combining the nearest neighbour and next-to-nearest neighbour interaction potentials. The combination of the potentials is done by an inf-convolution, see (3.3).

For given $\ell > 0$ we denote by $BV^\ell(0,1)$ the space of functions u with bounded variation defined on $(0,1)$ and satisfying the Dirichlet boundary conditions $u(0) = 0$ and $u(1) = \ell$. We point out that when 0 (resp. 1) is a jump point of u, the Dirichlet boundary condition is replaced by $u(0-) = 0$ (resp. $u(1+) = \ell$). In other words $BV^\ell(0,1)$ can be identified with the space of functions $u \in BV_{\mathrm{loc}}(\mathbb{R})$ such that $u = 0$ on $(-\infty, 0)$ and $u = \ell$ on $(1, +\infty)$. The space of special functions with bounded variation $SBV^\ell(0,1)$ is defined correspondingly. Moreover, for a function $u \in BV^\ell(0,1)$ (or in $SBV^\ell(0,1)$) we denote by S_u the jump set of u in $[0,1]$, and for $t \in S_u$ we set $[u(t)] = u(t+) - u(t-)$.

Theorem 3.1. *Let $J_j : \mathbb{R} \to (-\infty, +\infty]$ be Borel functions bounded from below, for $j = 1, 2$. Suppose that there exists a convex function $\Psi : \mathbb{R} \to [0, +\infty]$ such that*

$$\lim_{z \to -\infty} \frac{\Psi(z)}{|z|} = +\infty \tag{3.1}$$

and there exist constants $c_1^j, c_2^j > 0$ for $j = 1, 2$ such that

$$c_1^j(\Psi(z) - 1) \le J_j(z) \le c_2^j \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}, \quad j = 1, 2. \tag{3.2}$$

Let ℓ, $u_0^{(1)}$, $u_1^{(1)} > 0$. Then the Γ-limit of H_n^ℓ with respect to the L^1-topology is the functional H^ℓ defined by

$$H^\ell(u) = \begin{cases} \displaystyle\int_0^1 J_0^{**}(u'(t))\,dt & \text{if } u \in BV^\ell(0,1), [u] > 0 \text{ on } S_u, \\ +\infty & \text{else} \end{cases}$$

on $L^1(0,1)$. Here J_0^{**} denotes the convexification of the function

$$J_0(z) = J_2(z) + \frac{1}{2} \inf\{J_1(z_1) + J_1(z_2) : z_1 + z_2 = 2z\} \tag{3.3}$$

defined for all $z \in \mathbb{R}$.

Proof. **Compactness.** For fixed $u_0^{(1)}, u_1^{(1)} > 0$, let (u_n) be a sequence with equibounded energy H_n^ℓ. By [BG04, Theorem 1.2, Theorem 3.2] we have that $u_n \in BV^\ell(0,1)$ and that there exists $u \in BV(0,1)$ such that u_n converges weakly to u in $BV(0,1)$. It remains to verify that the limit function u satisfies the boundary conditions in 0 and in 1. Since $u_n^0 = 0$ and $u_n^n = \ell$ for every n, we can define the extension $\widetilde{u}_n \in BV_{\mathrm{loc}}(\mathbb{R})$ as

$$\widetilde{u}_n^i = \begin{cases} 0 & \text{if } i \le 0, \\ u_n^i & \text{if } 0 \le i \le n, \\ \ell & \text{if } i \ge n. \end{cases}$$

Then we have that $\widetilde{u}_n$ converges weakly in $BV_{\rm loc}(\mathbb{R})$ to the extension $\widetilde{u}$ of u and from this we deduce that

$$u(0-) = \lim_{t\to 0^-} \widetilde{u}(t) = 0 \quad \text{and} \quad u(1+) = \lim_{t\to 1^+} \widetilde{u}(t) = \ell.$$

Liminf inequality. It can be proved in the same way as in [BG04, Theorem 3.2].

Limsup inequality. Let $u \in BV^\ell(0,1)$, with $[u] > 0$. Then [BG04, Theorem 3.2] provides a recovery sequence (u_n) which does not satisfy the Dirichlet boundary conditions (2.2). Therefore we define the sequence $\hat{u}_n$ as the affine interpolation of the following discrete values

$$\hat{u}_n^i = \begin{cases} 0 & \text{if } i = 0, \\ \lambda_n u_0^{(1)} & \text{if } i = 1, \\ u_n^i & \text{if } 2 \le i \le n-2, \\ \ell - \lambda_n u_1^{(1)} & \text{if } i = n-1, \\ \ell & \text{if } i = n. \end{cases}$$

Clearly $\hat{u}_n$ converges to u, since we modify the recovery sequence only at a microscopic level. Moreover the change in the energy is of order λ_n, therefore $\hat{u}_n$ is a recovery sequence for u. □

4 First-order Γ-limit of the discrete energy

In order to obtain a continuum energy functional that contains boundary layer energies we are interested in the first-order Γ-limit of H_n^ℓ. That is, we compute the Γ-limit of the functional $H_{1,n}^\ell$ defined by

$$H_{1,n}^\ell(u) = \frac{H_n^\ell(u) - \min H^\ell}{\lambda_n}. \tag{4.1}$$

With respect to deriving an asymptotic expansion of the limiting functional of $H_{1,n}^\ell$ in terms of λ_n, we remark that the first-order Γ-limit yields the second term of such an (formal) expansion, i.e., the term of order λ_n. More precisely, the minimisers of the first-order Γ-limit are the second term of an asymptotic expansion of the minimisers of the original functional in terms of λ_n, see [AB93].

First of all we state the assumptions on J_1, J_2 and J_0 under which the convergence result is obtained.

$[H1]$ (strict convexity of J_0 in its convexity points).

$$\{z : J_0(z) = J_0^{**}(z)\} \cap \{z : J_0 \text{ is affine near } z\} = \emptyset.$$

$[H2]$ (uniqueness of minimal energy configurations).

$$\#M^z = 1 \quad \text{for every } z \in \mathbb{R} : J_0(z) = J_0^{**}(z),$$

where the set M^z describes the minimising pairs for J_1, i.e.,

$$M^z = \left\{ (z_1, z_2) : z_1 + z_2 = 2z,\ J_0(z) = J_2(z) + \frac{1}{2}\big(J_1(z_1) + J_1(z_2)\big) \right\}. \tag{4.2}$$

Thus $M^z = \{(z,z)\}$, which implies that

$$J_0(z) = J_1(z) + J_2(z) \quad \text{for every } \; z \in \mathbb{R} : J_0(z) = J_0^{**}(z). \tag{4.3}$$

$[H3]$ (regularity and behaviour at $+\infty$). $J_1, J_2 : \mathbb{R} \to (-\infty, +\infty]$ be in $C^{1,\alpha}$, $0 < \alpha \leq 1$, on their domains, i.e., on $\{z \in \mathbb{R} : J_j(z) < +\infty\}$, $j = 1, 2$, and such that $J_0 \in C^1$ on its domain. The following limits exist in $\mathbb{R}$

$$\lim_{z \to +\infty} J_j(z) = 0, \; j = 1, 2 \quad \text{and} \quad \lim_{z \to +\infty} J_0(z) = J_0(+\infty).$$

$[H4]$ (structure of J_1, J_2 and J_0). J_1, J_2 are such that there exists a convex function $\Psi : \mathbb{R} \to [0, +\infty]$ and constants $c_1^j, c_2^j > 0$ for $j = 1, 2$ such that (3.1) and (3.2) are satisfied. J_j has a unique minimum point δ_j and it is strictly convex in $(-\infty, \delta_j)$ on its domain for $j = 1, 2$. Moreover J_0 has a unique minimum point γ, with $J_0(\gamma) < J_0(+\infty)$.

$[H5]$ (additional condition on J_0 in the case $\ell < \gamma$). $J_0(z) = J_0^{**}(z)$ for all $z \leq \gamma$.

Assumption $[H5]$ is used in Proposition 4.2 and Subsection 4.1, see Theorem 4.3, which is in fact the only result where we apply the $C^{1,\alpha}$-regularity of $[H3]$.

Note that, assumption $[H2]$ rules out the possibility that the Lennard-Jones type potentials J_1 and J_2 have several wells. Our choice is due to the intention of focusing on the effect of prescribed discrete slopes on the limiting functional, rather than presenting our results under more general assumptions for the interaction potentials, cf. [BC07] for related work on the latter topic. Analogous to [BC07] we could easily relax the assumption of $J_1(+\infty) = J_2(+\infty) = 0$.

Remark 4.1. The above conditions are satisfied by typical physical interaction potentials. The main example that we have in mind is the Lennard-Jones potential, which is why we call potentials satisfying $[H1] - [H5]$ potentials of Lennard-Jones type. The classical Lennard-Jones potentials are defined, for some k_1, k_2 being positive constants, by

$$J_1(z) = \frac{k_1}{z^{12}} - \frac{k_2}{z^6}, \quad J_2(z) = J_1(2z) \quad \text{for } z > 0 \tag{4.4}$$

and extended to $+\infty$ on $(-\infty, 0]$, see Figure 1 for a plot. $[H1] - [H4]$ are clear from the definition. To prove $[H5]$, we first note that

$$\frac{1}{2} \inf \{J_1(z_1) + J_1(z_2) : z_1 + z_2 = 2z\} = \frac{1}{2} \inf \{J_1(z_1) + J_1(2z - z_1) : z_1\}.$$

Setting the first derivative of this equal to zero, yields the condition $J_1'(z_1) = J_1'(2z - z_1)$. Now observe that $J_1'(z)$ is injective and $J_1'(z) \leq 0$ for all $0 < z \leq \delta_1$ with δ_1 being the minimum point of J_1, and $J_1'(z) > 0$ for all $z > \delta_1$. Moreover note that $z \leq \delta_1$ implies that at least one of z_1 and $2z - z_1$ is less than or equal to δ_1. Hence the properties of the first derivative yield $z_1 = 2z - z_1$, i.e., $z_1 = z$ for all $z \leq \delta_1$. Therefore, for Lennard-Jones potentials as defined in (4.4) we have

$$J_0(z) = J_1(z) + J_2(z) \quad \text{for all } 0 < z \leq \delta_1. \tag{4.5}$$

An elementary calculation reveals that $J_1(z) + J_2(z)$ has non-negative second derivative for all $z \leq \left(\frac{13}{7}\right)^{\frac{1}{6}} \gamma$ with γ being the minimum point of the effective energy J_0 and

$$\gamma = \left(\frac{1 + 2^{-12}}{1 + 2^{-6}}\right)^{\frac{1}{6}} \delta_1 = \left(\frac{1 + 2^{-12}}{1 + 2^{-6}}\right)^{\frac{1}{6}} \left(\frac{2k_1}{k_2}\right)^{\frac{1}{6}} \tag{4.6}$$

as proven in [BC07, Example 4.1]. From $\gamma < \left(\frac{13}{7}\right)^{\frac{1}{6}} \gamma$ and $\gamma < \delta_1$, we deduce $[H5]$.
Since the double Yukawa potential, cf. [FA81], has a similar shape as the Lennard-Jones potential, we expect that it also satisfies $[H1] - [H5]$.
Another example is the so-called Morse-potential where for some $\delta_1, k_1, k_2 > 0$, the potential is defined by $J_1(z) = k_1 \left(1 - e^{-k_2(z-\delta_1)}\right)^2 - k_1$ for $z \geq 0$, and $J_2(z) = J_1(2z)$. This is finite at 0, but the structure is the same: the potential is strictly convex up to an inflection point, where it becomes concave and approaches 0 as $z \to \infty$, i.e., we have $[H1] - [H4]$. To prove $[H5]$, one may proceed as for the Lennard-Jones potential using properties of the first derivative of J_1.

We notice that, by Jensen's inequality, $\min H^\ell = J_0^{**}(\ell)$ for every ℓ. More explicitly,

$$\min H^\ell = \begin{cases} J_0(\ell) & \text{if } \ell \leq \gamma, \\ J_0(\gamma) & \text{if } \ell > \gamma. \end{cases} \tag{4.7}$$

Indeed, $[H1] - [H4]$ imply $J_0^{**}(z) = J_0(\gamma)$ for every $z \geq \gamma$. Moreover, in the case $\ell \leq \gamma$, assumption $[H5]$ entails in particular $J_0(\ell) = J_0^{**}(\ell)$.

For what follows it is useful to rearrange the terms in the expression of the energy $H_{1,n}^\ell$ in (4.1). For given $\ell, u_0^{(1)}, u_1^{(1)} > 0$ let (u_n) be a sequence of functions satisfying the boundary conditions (2.2) for each n. Then by (2.1)

$$\begin{aligned} H_{1,n}^\ell(u_n) =& \sum_{i=0}^{n-1} J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) + \sum_{i=0}^{n-2} J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) - \frac{\min H^\ell}{\lambda_n} \\ =& \frac{1}{2} J_1\left(\frac{u_n^1 - u_n^0}{\lambda_n}\right) + \sum_{i=0}^{n-2} \left\{ J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) + \frac{1}{2} J_1\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\right) \right. \\ & \left. + \frac{1}{2} J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) \right\} + \frac{1}{2} J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) - \frac{\min H^\ell}{\lambda_n} \\ =& \frac{1}{2} J_1\left(\frac{u_n^1 - u_n^0}{\lambda_n}\right) + \sum_{i=0}^{n-2} \sigma_n^i + \frac{1}{2} J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) - \min H^\ell, \end{aligned} \tag{4.8}$$

where we set for $i = 0, \dots, n-2$

$$\sigma_n^i = J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) + \frac{1}{2}\left(J_1\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\right) + J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right)\right) - \min H^\ell. \tag{4.9}$$

The following compactness result states that for $\ell \leq \gamma$ functions u_n with equibounded energy $H_{1,n}^\ell$ converge necessarily to the function $u(t) = \ell t$, while if $\ell > \gamma$, the limit function u has a finite number of jumps and is such that $u' = \gamma$ a.e. We recall that S_u is the jump set of u.

Proposition 4.2. *1. Let $0 < \ell \leq \gamma$ and suppose that hypotheses $[H1] - [H5]$ hold. Let $u_0^{(1)}$, $u_1^{(1)} > 0$. If (u_n) is a sequence of functions such that*

$$\sup_n H_{1,n}^\ell(u_n) < +\infty, \tag{4.10}$$

then there exists a finite set $S \subset [0,1]$ such that, up to subsequences, $u_n \to u$ in $W^{1,\infty}_{\text{loc}}((0,1) \setminus S)$ with $u(t) = \ell t$, $t \in [0,1]$.

2. *Let $\ell > \gamma$ and suppose that hypotheses $[H1] - [H4]$ hold. Let $u_0^{(1)}$, $u_1^{(1)} > 0$. If (u_n) is a sequence of functions such that (4.10) is satisfied, then, up to subsequences, $u_n \to u$ in $L^1(0,1)$, where $u \in SBV^\ell(0,1)$ is such that*

   (i) $0 < \#S_u < +\infty$;

   (ii) $[u] > 0$ *on* S_u;

   (iii) $u' = \gamma$ *a.e.;*

   (iv) there exists a finite set $S \subset [0,1]$ such that, up to subsequences, $u_n \to u$ in $W^{1,\infty}_{\rm loc}((0,1)\setminus S)$.

Proof. The first result of the proposition follows from [BC07, Propositions 3.1 and 4.2], see also below. The results $(i) - (iii)$ for $\ell > \gamma$ follow directly from [BC07, Proposition 4.2], since our approximating functionals are finite on a smaller set than the corresponding ones in [BC07]. Statement (iv) follows again from [BC07, Proposition 3.1], which we outline in the following; the corresponding result for the case $\ell \le \gamma$ in 1. can be obtained in a similar way. In the case $\ell > \gamma$ we have (4.8) with $\min H^\ell = J_0(\gamma)$. From (4.10) there exists $C > 0$ such that

$$\sup_n \sum_{i=0}^{n-2} \sigma_n^i \le C < +\infty,$$

where σ_n^i is defined as in (4.9). Hence, for every fixed $\eta > 0$, setting $I_n := \big\{ i \in \{0, \dots, n-2\} : \sigma_n^i > \eta \big\}$, there exists a constant $C(\eta)$ such that

$$\sup \#I_n \le C(\eta) < +\infty.$$

Let $i \in \{0, \dots, n-2\}$ be such that $i \notin I_n$, i.e.,

$$\sigma_n^i = J_2\left(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\right) + \frac{1}{2} J_1\left(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\right) + \frac{1}{2} J_1\left(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\right) - J_0(\gamma) \le \eta. \tag{4.11}$$

Since $J_0(z) \ge J_0(\gamma)$ for every z, from (3.3) and (4.11) we have

$$0 \le J_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \frac{1}{2} J_1\Big(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\Big) + \frac{1}{2} J_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - J_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) \le \eta,$$

and moreover, using the definition of J_0, (4.11) implies that

$$0 \le J_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) - J_0(\gamma) \le \eta.$$

Let $\varepsilon = \varepsilon(\eta) > 0$ be such that if

$$\begin{aligned} &0 \le J_2(z) + \frac{1}{2} J_1(z_1) + \frac{1}{2} J_1(z_2) - J_0(z) \le \eta \quad \text{with } z_1 + z_2 = 2z \\ &0 \le J_0(z) - J_0(\gamma) \le \eta \end{aligned}$$

then $|z_1 - \gamma| + |z_2 - \gamma| < \varepsilon$. Therefore if $i \notin I_n$ then

$$\Big|\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n} - \gamma\Big| < \varepsilon \quad \text{and} \quad \Big|\frac{u_n^{i+1} - u_n^i}{\lambda_n} - \gamma\Big| < \varepsilon. \tag{4.12}$$

Let M_n be the maximal number of indices i in I_n and let $I_n := \{i_1^n, \dots, i_{M_n}^n\}$ with $0 \le i_k^n \le i_{k+1}^n \le n-2$, $k = 1, \dots, M_n - 1$. Note that $\sum_{i=0}^{n-2} \sigma_n^i \ge C(\eta) M_n$, and therefore (4.10) implies that $\sup_n C(\eta) M_n < +\infty$. Therefore we may assume $M_n = M$ and observe that, up to subsequences, for every $k = 1, \dots, M$ there exists $x_k \in [0,1]$ with $\lambda_n i_k^n \to x_k$. Let $S = \{x_1, \dots, x_M\}$ and, for fixed $\omega > 0$, $S_\omega = \bigcup_k (x_k - \omega, x_k + \omega)$. Hence, by identifying u_n with its piecewise affine interpolation, we get from (4.12) for n large enough

$$\sup_{t \in (0,1) \setminus S_\omega} |u_n'(t) - \gamma| < \varepsilon.$$

Since $u' = \gamma$ a.e.,we conclude by (iii), due to the arbitrariness of ω, that up to a further subsequence $u_n \to u$ in $W^{1,\infty}_{\mathrm{loc}}((0,1) \setminus S)$. □

For simplicity of notation we define for $\ell > \gamma$

$$SBV_c^\ell(0,1) = \left\{ u \in SBV^\ell(0,1) : \text{conditions } (i) - (iii) \text{ are satisfied} \right\}.$$

4.1 The case $\ell \le \gamma$

First of all we consider the case $\ell \le \gamma$, where we recall that ℓ denotes the Dirichlet condition imposed on the last atom of the chain and γ denotes the minimum point of J_0. For $\ell \le \gamma$ we have elastic behaviour and therefore no fracture occurs. We compute the discrete-to-continuum limit of the discrete energy of first order $H_{1,n}^\ell$ in terms of Γ-convergence. This yields in particular that our limiting functional depends on the prescribed slopes $u_0^{(1)}$ and $u_1^{(1)}$, see Theorem 4.3.

For any $0 < \ell \le \gamma$ and $\theta > 0$ we define the boundary layer energy $B(\theta, \ell)$ as

$$\begin{aligned} B(\theta, \ell) = \inf_{N \in \mathbb{N}} \min \Bigg\{ & \frac{1}{2} J_1 \left(v^1 - v^0\right) + \sum_{i \ge 0} \Bigg\{ J_2 \left(\frac{v^{i+2} - v^i}{2} \right) \\ & + \frac{1}{2} \left(J_1 \left(v^{i+2} - v^{i+1}\right) + J_1 \left(v^{i+1} - v^i\right) \right) - J_0(\ell) - J_0'(\ell) \left(\frac{v^{i+2} - v^i}{2} - \ell \right) \Bigg\} : \\ & v : \mathbb{N} \to \mathbb{R}, v^0 = 0, v^1 - v^0 = v^1 = \theta, v^{i+1} - v^i = \ell \text{ if } i \ge N \Bigg\}. \end{aligned} \tag{4.13}$$

In what follows $\theta = u_0^{(1)}$ or $\theta = u_1^{(1)}$, so the constraint $v^1 - v^0 = \theta$ is due to the boundary conditions imposed on the first and on the last two atoms of the chain, respectively. Hence, $B(\theta, \ell)$ represents the *elastic boundary layer energy*. The expression involving $-J_0'(\ell)$ is crucial here to ensure, together with (4.3), that the terms in the sums are non-negative and thus that the boundary layer energy is bounded from below. Indeed, by the definition of J_0 and since $J_0(\ell) = J_0^{**}(\ell)$ for $\ell \le \gamma$ by $[H5]$,

$$\begin{aligned} & J_2 \left(\frac{v^{i+2} - v^i}{2} \right) + \frac{1}{2} \left(J_1 \left(v^{i+2} - v^{i+1}\right) + J_1 \left(v^{i+1} - v^i\right) \right) - J_0(\ell) - J_0'(\ell) \left(\frac{v^{i+2} - v^i}{2} - \ell \right) \\ & \ge J_0 \left(\frac{v^{i+2} - v^i}{2} \right) - J_0(\ell) - J_0'(\ell) \left(\frac{v^{i+2} - v^i}{2} - \ell \right) \ge 0, \end{aligned}$$

where the latter inequality follows from the fact that $J_0(x) - J_0(\ell) - J_0'(\ell)(x - \ell) \ge J_0^{**}(x) - J_0^{**}(\ell) - (J_0^{**})'(\ell)(x - \ell) \ge 0$ for all $x \in \mathbb{R}$; thus in particular $J_0(\gamma) - J_0(\ell) - J_0'(\ell)(\gamma - \ell) \ge 0$.

For the definition of the corresponding boundary layer energy in the case $\ell > \gamma$ see (4.29).

Theorem 4.3. *Suppose that hypotheses* $[H1]-[H5]$ *hold and let* $0<\ell\leq\gamma$ *and* $u_0^{(1)}$, $u_1^{(1)}>0$. *Then* $H^\ell_{1,n}$ Γ*-converges with respect to the* L^∞*-topology to the functional* H^ℓ_1 *defined by*

$$H_1^\ell(u)=\begin{cases}B\left(u_0^{(1)},\ell\right)+B\left(u_1^{(1)},\ell\right)-J_0(\ell)-J_0'(\ell)\left(\frac{u_0^{(1)}+u_1^{(1)}}{2}-\ell\right) & \text{if } u(t)=\ell t,\\ +\infty & \text{else}\end{cases}$$

on $W^{1,\infty}(0,1)$.

In Figure 3 we give an intuitive picture of the location of the occurring boundary layers in the elastic case, i.e., for $\ell\leq\gamma$.

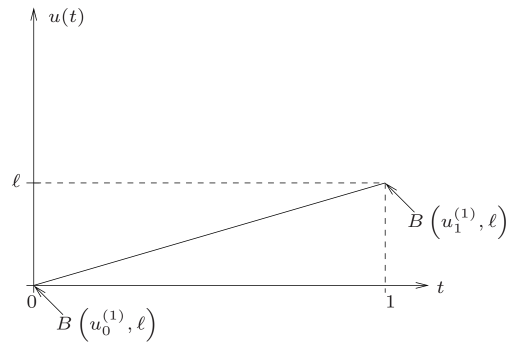

Figure 3: An intuitive picture of the location of boundary layers for $\ell\leq\gamma$.

Proof. **Liminf inequality.** We show that for any sequence $u_n\to u$ in $L^\infty(0,1)$ with equibounded energy $H^\ell_{1,n}$ we have

$$\liminf_{n\to\infty}H^\ell_{1,n}(u_n)\geq B\left(u_0^{(1)},\ell\right)+B\left(u_1^{(1)},\ell\right)-J_0(\ell)-J_0'(\ell)\left(\frac{u_0^{(1)}+u_1^{(1)}}{2}-\ell\right).$$

From Proposition 4.2 we have that $u(t)=\ell t$ for all $t\in[0,1]$ and that there exists a finite set S with, up to subsequences, $u_n\to u$ in $W^{1,\infty}_{\rm loc}((0,1)\setminus S)$. This allows us to choose a sequence of integer numbers $h_n\in\mathbb{N}$ such that $\lambda_nh_n\to\frac12$ as $n\to\infty$ (note that without loss of generality we may assume that $\frac12\notin S$, since otherwise we may pick another point in $(0,1)$ which does not belong to S) and moreover

$$\lim_{n\to\infty}\frac{u_n^{h_n+2}-u_n^{h_n+1}}{\lambda_n}=\ell. \tag{4.14}$$

We write $H^\ell_{1,n}(u_n)$ as in (4.8), where we make use of (4.7). Then we add and subtract the term

$J_0'(\ell)\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right)$ in the sum to obtain

$$\begin{aligned} H_{1,n}^{\ell}(u_n) =& \frac{1}{2}J_1\left(\frac{u_n^1-u_n^0}{\lambda_n}\right) + \sum_{i=0}^{n-2}\Bigg\{J_2\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right) + \frac{1}{2}\Bigg(J_1\left(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\right) \\ &+ J_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)\Bigg) - J_0(\ell) - J_0'(\ell)\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n} - \ell\right)\Bigg\} \\ &+ \sum_{i=0}^{n-2} J_0'(\ell)\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n} - \ell\right) + \frac{1}{2}J_1\left(\frac{u_n^n-u_n^{n-1}}{\lambda_n}\right) - J_0(\ell). \end{aligned} \tag{4.15}$$

Since $\sum_{i=0}^{n-1}(u_n^{i+1}-u_n^i) = u_n^n - u_n^0 = \ell$ by construction, we have

$$\sum_{i=0}^{n-2}\left(u_n^{i+2}-u_n^i\right) = 2\sum_{i=0}^{n-1}\left(u_n^{i+1}-u_n^i\right) - \left(u_n^1-u_n^0\right) - \left(u_n^n-u_n^{n-1}\right) = 2\ell - \lambda_n\left(u_0^{(1)}+u_1^{(1)}\right).$$

Thus

$$\sum_{i=0}^{n-2} J_0'(\ell)\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n} - \ell\right) = J_0'(\ell)\left(\frac{\ell}{\lambda_n} - \frac{u_0^{(1)}+u_1^{(1)}}{2} - (n-1)\ell\right) = -J_0'(\ell)\left(\frac{u_0^{(1)}+u_1^{(1)}}{2} - \ell\right) \tag{4.16}$$

and we already have the last term in the finite limiting energy $H_1^{\ell}(u)$. By (4.15) and (4.16) the energy $H_{1,n}^{\ell}(u_n)$ reads

$$H_{1,n}^{\ell}(u_n) = \frac{1}{2}J_1\left(\frac{u_n^1-u_n^0}{\lambda_n}\right) + \sum_{i=0}^{n-2} s_n^i + \frac{1}{2}J_1\left(\frac{u_n^n-u_n^{n-1}}{\lambda_n}\right) - J_0(\ell) - J_0'(\ell)\left(\frac{u_0^{(1)}+u_1^{(1)}}{2} - \ell\right), \tag{4.17}$$

where for $i = 0, \dots, n-2$ we define

$$\begin{aligned} s_n^i =& J_2\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\right) + \frac{1}{2}\left(J_1\left(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\right) + J_1\left(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\right)\right) - J_0(\ell) \\ &- J_0'(\ell)\left(\frac{u_n^{i+2}-u_n^i}{2\lambda_n} - \ell\right). \end{aligned} \tag{4.18}$$

Note that, for $\ell = \gamma$, s_n^i is the same as σ_n^i defined in (4.9) since $J_0'(\gamma) = 0$ by $[H4]$. We define the sequence $v_n : \mathbb{N} \to \mathbb{R}$ as

$$v_n^i = \begin{cases} \frac{u_n^i}{\lambda_n} & \text{if } 0 \le i \le h_n + 2, \\ \ell(i - (h_n+2)) + \frac{u_n^{h_n+2}}{\lambda_n} & \text{if } i \ge h_n + 2. \end{cases} \tag{4.19}$$

Then, in terms of v_n we have

$$\begin{aligned}\sum_{i=0}^{h_n} s_n^i &= \sum_{i=0}^{h_n} \left\{ J_2\left(\frac{v_n^{i+2}-v_n^i}{2}\right) + \frac{1}{2}\left(J_1\left(v_n^{i+2}-v_n^{i+1}\right) + J_1\left(v_n^{i+1}-v_n^i\right)\right) - J_0(\ell) \right.\\ &\quad \left. - J_0'(\ell)\left(\frac{v_n^{i+2}-v_n^i}{2} - \ell\right)\right\}\\ &= \sum_{i\geq 0} \left\{ J_2\left(\frac{v_n^{i+2}-v_n^i}{2}\right) + \frac{1}{2}\left(J_1\left(v_n^{i+2}-v_n^{i+1}\right) + J_1\left(v_n^{i+1}-v_n^i\right)\right) - J_0(\ell) \right.\\ &\quad \left. - J_0'(\ell)\left(\frac{v_n^{i+2}-v_n^i}{2} - \ell\right)\right\} - \omega(n),\end{aligned}$$

where $\omega(n)$ denotes an infinitesimal function for $n \to \infty$ specified below. The last equality follows observing that, by (4.19) and (4.3), the terms of the sum are identically 0 for every $i \geq h_n + 2$, while by (4.14) and (4.3) we have that the term corresponding to $i = h_n + 1$ satisfies

$$\begin{aligned}s_n^{h_n+1} &= J_2\left(\frac{u_n^{h_n+2}-u_n^{h_n+1}}{2\lambda_n} + \frac{\ell}{2}\right) + \frac{1}{2}\left(J_1(\ell) + J_1\left(\frac{u_n^{h_n+2}-u_n^{h_n+1}}{\lambda_n}\right)\right) - J_0(\ell)\\ &\quad - J_0'(\ell)\left(\frac{u_n^{h_n+2}-u_n^{h_n+1}}{2\lambda_n} + \frac{\ell}{2} - \ell\right)\\ &= \omega(n) \to 0 \quad \text{as } n \to \infty.\end{aligned}$$

Observe that $v_n^0 = \frac{u_n^0}{\lambda_n} = 0$, $v_n^1 - v_n^0 = \frac{u_n^1}{\lambda_n} = u_0^{(1)}$ and $v_n^{i+1} - v_n^i = \ell$ for $i \geq h_n + 2$. Hence v_n is a competitor for the minimum problem defining $B\left(u_0^{(1)}, \ell\right)$, cf. (4.13). Therefore

$$\begin{aligned}&\frac{1}{2}J_1\left(\frac{u_n^1-u_n^0}{\lambda_n}\right) + \sum_{i=0}^{h_n} s_n^i\\ &= \frac{1}{2}J_1(v_n^1 - v_n^0) + \sum_{i\geq 0}\left\{J_2\left(\frac{v_n^{i+2}-v_n^i}{2}\right) + \frac{1}{2}\left(J_1\left(v_n^{i+2}-v_n^{i+1}\right) + J_1\left(v_n^{i+1}-v_n^i\right)\right)\right.\\ &\quad \left. - J_0(\ell) - J_0'(\ell)\left(\frac{v_n^{i+2}-v_n^i}{2} - \ell\right)\right\} - \omega(n)\\ &\geq B\left(u_0^{(1)}, \ell\right) - \omega(n).\end{aligned} \tag{4.20}$$

In order to estimate the remaining part in the energy in (4.17), we observe that

$$\begin{aligned}B(\theta,\ell) = \inf_{N\in\mathbb{N}} \min &\left\{ \frac{1}{2}J_1(w^0 - w^{-1}) + \sum_{i\leq 0}\left\{J_2\left(\frac{w^i - w^{i-2}}{2}\right)\right.\right.\\ &\left. + \frac{1}{2}\left(J_1\left(w^i - w^{i-1}\right) + J_1\left(w^{i-1}-w^{i-2}\right)\right) - J_0(\ell) - J_0'(\ell)\left(\frac{w^i - w^{i-2}}{2} - \ell\right)\right\} :\\ &\left. w : -\mathbb{N} \to \mathbb{R}, w^0 = 0, w^0 - w^{-1} = -w^{-1} = \theta, w^i - w^{i-1} = \ell \text{ if } i \leq -N\right\},\end{aligned} \tag{4.21}$$

as one can easily see setting $v^j =: -w^{-j}$ in (4.13) and $i := -j$. We define $w_n : -\mathbb{N} \to \mathbb{R}$ as

$$w_n^j = \begin{cases} \frac{u_n^{n+j}}{\lambda_n} - \frac{\ell}{\lambda_n} & \text{if } h_n - n + 1 \leq j \leq 0,\\ \ell(j - (h_n - n + 1)) - \frac{\ell}{\lambda_n} + \frac{u_n^{h_n+1}}{\lambda_n} & \text{if } j \leq h_n - n + 1.\end{cases} \tag{4.22}$$

Then, in terms of w_n we have

$$\begin{aligned}\sum_{i=h_n+1}^{n-2} s_n^i = &\sum_{j=h_n-n+3}^{0} \Bigg\{ J_2\left(\frac{w_n^j - w_n^{j-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w_n^j - w_n^{j-1}\right) + J_1\left(w_n^{j-1} - w_n^{j-2}\right)\right) - J_0(\ell) \\ &- J_0'(\ell)\left(\frac{w_n^j - w_n^{j-2}}{2} - \ell\right)\Bigg\} \\ =&\sum_{j\le 0} \Bigg\{ J_2\left(\frac{w_n^j - w_n^{j-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w_n^j - w_n^{j-1}\right) + J_1\left(w_n^{j-1} - w_n^{j-2}\right)\right) - J_0(\ell) \\ &- J_0'(\ell)\left(\frac{w_n^j - w_n^{j-2}}{2} - \ell\right)\Bigg\} - \omega(n),\end{aligned}$$

where now $\omega(n)$ denotes the term corresponding to $j = h_n - n + 2$ in the sum, which is infinitesimal by (4.14) and (4.3).

Since $w_n^0 = \frac{u_n^n - \ell}{\lambda_n} = 0$, $w_n^0 - w_n^{-1} = \frac{u_n^n - u_n^{n-1}}{\lambda_n} = u_1^{(1)}$, $w_n^j - w_n^{j-1} = \ell$ for $j \le h_n - n + 1$, we deduce that w_n is a competitor for the minimum problem defining $B\left(u_1^{(1)}, \ell\right)$, cf. (4.21). Therefore

$$\begin{aligned}&\frac{1}{2}J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) + \sum_{i=h_n+1}^{n-2} s_n^i \\ &= \frac{1}{2}J_1(w_n^0 - w_n^{-1}) + \sum_{i\le 0}\Bigg\{ J_2\left(\frac{w_n^i - w_n^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w_n^i - w_n^{i-1}\right) + J_1\left(w_n^{i-1} - w_n^{i-2}\right)\right) \\ &- J_0(\ell) - J_0'(\ell)\left(\frac{w_n^i - w_n^{i-2}}{2} - \ell\right)\Bigg\} - \omega(n) \\ &\ge B\left(u_1^{(1)}, \ell\right) - \omega(n). \end{aligned} \tag{4.23}$$

In summary, from (4.17), (4.20) and (4.23) we obtain the desired liminf inequality.

Limsup inequality. By the definition of $H_1^\ell(u)$ it is sufficient to consider the case $u(t) = \ell t$. We construct a sequence (u_n) converging to u in $L^\infty(0,1)$ satisfying (2.2) and such that

$$\limsup_{n\to\infty} H_{1,n}^\ell(u_n) \le B\left(u_0^{(1)}, \ell\right) + B\left(u_1^{(1)}, \ell\right) - J_0(\ell) - J_0'(\ell)\left(\frac{u_0^{(1)} + u_1^{(1)}}{2} - \ell\right).$$

Let $\eta > 0$. Then, by the definition of $B\left(u_0^{(1)}, \ell\right)$, we can find $v : \mathbb{N} \to \mathbb{R}$ and $N_1 \in \mathbb{N}$ such that $v^0 = 0$, $v^1 - v^0 = u_0^{(1)}$, $v^{i+1} - v^i = \ell$ for $i \ge N_1$ and

$$\begin{aligned}&\frac{1}{2}J_1\left(v^1 - v^0\right) + \sum_{i\ge 0}\Bigg\{ J_2\left(\frac{v^{i+2} - v^i}{2}\right) + \frac{1}{2}\left(J_1\left(v^{i+2} - v^{i+1}\right) + J_1\left(v^{i+1} - v^i\right)\right) - J_0(\ell) \\ &- J_0'(\ell)\left(\frac{v^{i+2} - v^i}{2} - \ell\right)\Bigg\} \\ &\le B\left(u_0^{(1)}, \ell\right) + \eta. \end{aligned} \tag{4.24}$$

In the same way, by (4.21), there exist $w : -\mathbb{N} \to \mathbb{R}$ and $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^0 - w^{-1} = u_1^{(1)}$, $w^i - w^{i-1} = \ell$ if $i \leq -N_2$, such that

$$\begin{aligned}&\frac{1}{2}J_1(w^0 - w^{-1}) + \sum_{i\leq 0}\Bigg\{J_2\left(\frac{w^i - w^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w^i - w^{i-1}\right) + J_1\left(w^{i-1} - w^{i-2}\right)\right) - J_0(\ell)\\ &\quad - J_0'(\ell)\left(\frac{w^i - w^{i-2}}{2} - \ell\right)\Bigg\}\\ &\leq B\left(u_1^{(1)}, \ell\right) + \eta. \end{aligned} \tag{4.25}$$

We construct a recovery sequence for u by means of the functions v and w. Indeed, we set

$$u_n^i = \begin{cases} \lambda_n v^i & \text{if } 0 \leq i \leq N_1 + 2,\\ \lambda_n v^{N_1+2} + \frac{\ell + \lambda_n (w^{-N_2-2} - v^{N_1+2})}{n - N_1 - N_2 - 4}(i - N_1 - 2) & \text{if } N_1 + 2 \leq i \leq n - N_2 - 2,\\ \ell + \lambda_n w^{i-n} & \text{if } n - N_2 - 2 \leq i \leq n. \end{cases}$$

We note that, for each n, u_n satisfies the boundary conditions (2.2). We write $H_{1,n}^{\ell}(u_n)$ as in (4.17) and thus only need to show that the first three terms on the right-hand side of (4.17) yield $B\left(u_0^{(1)}, \ell\right)$ and $B\left(u_1^{(1)}, \ell\right)$ in order to prove that $H_{1,n}^{\ell}(u_n)$ converges to $H_1^{\ell}(u)$. To this end we split the sum as follows

$$\sum_{i=0}^{n-2} s_n^i = \sum_{i=0}^{N_1} s_n^i + \sum_{i=N_1+1}^{n-N_2-3} s_n^i + \sum_{i=n-N_2-2}^{n-2} s_n^i.$$

We observe that

$$\begin{aligned}\frac{1}{2}J_1\left(\frac{u_n^1 - u_n^0}{\lambda_n}\right) + \sum_{i=0}^{N_1} s_n^i = \frac{1}{2}J_1\left(v^1 - v^0\right) + \sum_{i=0}^{N_1}\Bigg\{J_2\left(\frac{v^{i+2} - v^i}{2}\right) + \frac{1}{2}\big(J_1\left(v^{i+2} - v^{i+1}\right)\\ + J_1\left(v^{i+1} - v^i\right)\big) - J_0(\ell) - J_0'(\ell)\left(\frac{v^{i+2} - v^i}{2} - \ell\right)\Bigg\},\end{aligned}$$

where we can replace the sum of the right-hand side with the same sum up to $+\infty$ since $v^{i+1} - v^i = \ell$ for $i \geq N_1$. Hence, by (4.24) we obtain the upper bound $B\left(u_0^{(1)}, \ell\right) + \eta$. Similarly,

$$\begin{aligned}&\frac{1}{2}J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) + \sum_{i=n-N_2-2}^{n-2} s_n^i\\ &= \frac{1}{2}J_1(w^0 - w^{-1}) + \sum_{i\leq 0}\Bigg\{J_2\left(\frac{w^i - w^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w^i - w^{i-1}\right) + J_1\left(w^{i-1} - w^{i-2}\right)\right) - J_0(\ell)\\ &\quad - J_0'(\ell)\left(\frac{w^i - w^{i-2}}{2} - \ell\right)\Bigg\},\end{aligned}$$

which is less or equal than $B\left(u_1^{(1)}, \ell\right) + \eta$ by construction, see (4.25). Thus it remains to prove that $\sum_{i=N_1+1}^{n-N_2-3} s_n^i$ is infinitesimal as $n \to \infty$. For $N_1 + 2 \leq i \leq n - N_2 - 3$ we have

$$\frac{u_n^{i+1} - u_n^i}{\lambda_n} = \frac{\ell + \lambda_n\left(w^{-N_2-2} - v^{N_1+2}\right)}{\lambda_n(n - N_1 - N_2 - 4)} = \frac{\ell}{1 - \lambda_n(N_1 + N_2 + 4)} + \frac{w^{-N_2-2} - v^{N_1+2}}{n - N_1 - N_2 - 4},$$

which is of the order of $\ell + \frac{c}{n}$ for some constant c. Hence by continuity

$$s_n^i \simeq J_2\left(\ell + \frac{c}{n}\right) + J_1\left(\ell + \frac{c}{n}\right) - J_0(\ell) - J_0'(\ell)\frac{c}{n}$$

for $N_1 + 2 \leq i \leq n - N_2 - 4$. Now, since $J_0'(\ell) = J_1'(\ell) + J_2'(\ell)$ by (4.3) and $[H3]$

$$\begin{aligned} s_n^i &\simeq J_2\left(\ell + \frac{c}{n}\right) + J_1\left(\ell + \frac{c}{n}\right) - J_1(\ell) - J_2(\ell) - J_1'(\ell)\frac{c}{n} - J_2'(\ell)\frac{c}{n} \\ &= \left(J_2'\left(\xi_{2,n}\right) - J_2'(\ell)\right)\frac{c}{n} + \left(J_1'\left(\xi_{1,n}\right) - J_1'(\ell)\right)\frac{c}{n} \end{aligned}$$

for some $\xi_{1,n}$ and $\xi_{2,n}$ between ℓ and $\ell + \frac{c}{n}$. Hence, by $[H3]$, for a possibly different constant c,

$$\sum_{i=N_1+2}^{n-N_2-4} s_n^i \leq \sum_{i=N_1+2}^{n-N_2-4} |s_n^i| \leq \sum_{i=1}^{n} \frac{c}{n^{1+\alpha}} = \frac{c}{n^\alpha} \to 0 \quad \text{as } n \to \infty.$$

It remains to estimate the terms for $i = N_1 + 1$ and $i = n - N_2 - 3$. Note that

$$\begin{aligned} \frac{u_n^{N_1+3} - u_n^{N_1+1}}{2\lambda_n} &= \frac{1}{2}\left(v^{N_1+2} + \frac{\ell + \lambda_n(w^{-N_2-2} - v^{N_1+2})}{\lambda_n(n - N_1 - N_2 - 4)}\right) - \frac{1}{2}v^{N_1+1} \\ &= \frac{v^{N_1+2} - v^{N_1+1}}{2} + \frac{\ell}{2 - 2\lambda_n(N_1 + N_2 + 4)} + \frac{w^{-N_2-2} - v^{N_1+2}}{2(n - N_1 - N_2 - 4)} \\ &\simeq \frac{\ell}{2} + \frac{\ell}{2} + \frac{c}{2n} \longrightarrow \ell. \end{aligned}$$

Hence $s_n^{N_1+1}$ converges to 0 as $n \to \infty$ by (4.3). Similarly,

$$\begin{aligned} &\frac{u_n^{n-N_2-1} - u_n^{n-N_2-3}}{2\lambda_n} \\ &= \frac{1}{2}\left(\frac{\ell}{\lambda_n} + w^{-N_2-1} - v^{N_1+2} - \frac{\ell + \lambda_n(w^{-N_2-2} - v^{N_1+2})}{\lambda_n(n - N_1 - N_2 - 4)}(n - N_2 - 3 - N_1 - 2)\right) \\ &\longrightarrow \ell \end{aligned}$$

since $\frac{n-N_2-3-N_1-2}{\lambda_n(n-N_1-N_2-4)}$ is of order $\frac{1}{\lambda_n} - 1$ and $w^{-N_2-1} - w^{-N_2-2} = \ell$. Hence, again by (4.3), $s_n^{n-N_2-3}$ converges to 0 as n tends to infinity, which proves the convergence of the energy. Moreover, since the discrete derivative of u_n converges to ℓ, we have in particular that (u_n) converges to $u(t) = \ell t$ in $L^\infty(0,1)$. □

Next we discuss a special case: let $\ell = \gamma$ and $\theta = \gamma$. Then it is immediate to notice that $(\gamma i, 0)$ is a minimiser, hence the boundary layer energy takes the simple explicit form

$$B(\gamma, \gamma) = \frac{1}{2}J_1(\gamma). \tag{4.26}$$

The following corollary is then a consequence of Theorem 4.3.

Corollary 4.4. *Suppose that hypotheses $[H1] - [H5]$ hold and let $\ell = \gamma$ and $u_0^{(1)} = u_1^{(1)} = \gamma$. The sequence of functionals $H_{1,n}^\gamma$ Γ-converges with respect to the L^∞-topology to the functional H_1^γ given by*

$$H_1^\gamma(u) = \begin{cases} J_1(\gamma) - J_0(\gamma) = -J_2(\gamma) & \text{if } u(t) = \gamma t, \\ +\infty & \text{else} \end{cases}$$

on $W^{1,\infty}(0,1)$.

Remark 4.5. Notice that if the Dirichlet boundary conditions for the second and last but one atoms are not prescribed, then the limit functional is $2B(\gamma) - J_0(\gamma)$ [BC07, Theorem 4.4], see also (4.28) for a definition of $B(\gamma)$. By Proposition 5.4 below we know that $B(\gamma) < \frac{1}{2}J_1(\gamma)$ in some relevant examples, more precisely for the classical Lennard-Jones potentials as defined in (4.4). Hence, at least for these examples, prescribing the second and last but one atoms leads to a different limiting functional even for $\ell = \gamma$.

Remark 4.6. Proving directly the assertion of Corollary 4.4 shows that assumption $[H5]$ is not needed.

4.2 The case $\ell > \gamma$

According to the compactness result in Proposition 4.2, we have fracture in the case $\ell > \gamma$. To this end we define boundary layer energies due to the presence of a crack at the boundary or in the interior of the chain. When a fracture occurs at a boundary point, the corresponding boundary layer energy is given, for $\theta > 0$, by

$$\begin{aligned} B_b(\theta) = \inf_{k\in\mathbb{N}} \min \Bigg\{ \frac{1}{2} J_1\left(\widehat{v}^1 - \widehat{v}^0\right) + \sum_{i=0}^{k-1} \Bigg\{ J_2\left(\frac{\widehat{v}^{i+2} - \widehat{v}^i}{2}\right) \\ + \frac{1}{2}\left(J_1\left(\widehat{v}^{i+2} - \widehat{v}^{i+1}\right) + J_1\left(\widehat{v}^{i+1} - \widehat{v}^i\right)\right) - J_0(\gamma)\Bigg\} : \\ \widehat{v} : \mathbb{N} \to \mathbb{R}, \widehat{v}^{k+1} = 0, \widehat{v}^{k+1} - \widehat{v}^k = -\widehat{v}^k = \theta \Bigg\}. \end{aligned} \tag{4.27}$$

Remark 4.7. We point out that the boundary layer energy $B_b(\theta)$ yields the optimal position, at a microscopic scale, of a fracture that occurs at the boundary at a macroscopic scale. See the end of Section 5 for examples about the optimal position of microscopic cracks. In this case we use again (3.3) and that J_0 has a unique minimum point γ to deduce that the terms in the sums are non-negative.

Next we recall the definition of $B(\gamma)$, which is the *boundary layer energy of a free boundary*, occurring in the case of an internal fracture, and was introduced in [BC07].

$$\begin{aligned} B(\gamma) = \inf_{N\in\mathbb{N}} \min \Bigg\{ \frac{1}{2} J_1\left(\widetilde{u}^1 - \widetilde{u}^0\right) + \sum_{i\geq 0} \Bigg\{ J_2\left(\frac{\widetilde{u}^{i+2} - \widetilde{u}^i}{2}\right) \\ + \frac{1}{2}\left(J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^{i+1}\right) + J_1\left(\widetilde{u}^{i+1} - \widetilde{u}^i\right)\right) - J_0(\gamma)\Bigg\} : \\ \widetilde{u} : \mathbb{N} \to \mathbb{R}, \widetilde{u}^0 = 0, \widetilde{u}^{i+1} - \widetilde{u}^i = \gamma \text{ if } i \geq N \Bigg\}. \end{aligned} \tag{4.28}$$

In the case of an internal fracture, the *elastic boundary layer energy* at the endpoints due to the prescribed boundary conditions is similar to the one defined in the elastic case $\ell \leq \gamma$, see (4.13).

More precisely, we define, for $\theta > 0$,

$$B(\theta,\gamma) = \inf_{N\in\mathbb{N}} \min \left\{ \frac{1}{2} J_1\left(v^1 - v^0\right) + \sum_{i\geq 0} \left\{ J_2\left(\frac{v^{i+2}-v^i}{2}\right) \right.\right.$$
$$\left. + \frac{1}{2}\left(J_1\left(v^{i+2}-v^{i+1}\right) + J_1\left(v^{i+1}-v^i\right)\right) - J_0(\gamma) \right\} :$$
$$\left. v:\mathbb{N}\to\mathbb{R}, v^0 = 0, v^1 - v^0 = v^1 = \theta, v^{i+1} - v^i = \gamma \text{ if } i \geq N \right\}. \tag{4.29}$$

Theorem 4.8. *Suppose that hypotheses $[H1]-[H4]$ hold and let $\ell > \gamma$ and $u_0^{(1)}$, $u_1^{(1)} > 0$. Then $H_{1,n}^{\ell}$ Γ-converges with respect to the L^1-topology to the functional H_1^{ℓ} defined by*

$$H_1^{\ell}(u) = \begin{cases} B\left(u_0^{(1)},\gamma\right)(1 - \#(S_u \cap \{0\})) & \\ +B\left(u_1^{(1)},\gamma\right)(1 - \#(S_u \cap \{1\})) - J_0(\gamma) + B_{IJ}\#(S_u \cap (0,1)) & \\ +B_{BJ}\left(u_0^{(1)}\right)\#(S_u \cap \{0\}) + B_{BJ}\left(u_1^{(1)}\right)\#(S_u\cap\{1\}) & \text{if } u \in SBV_c^{\ell}(0,1), \\ +\infty & \text{else,} \end{cases}$$

on $L^1(0,1)$, where, for $\theta > 0$,

$$B_{BJ}(\theta) = \frac{1}{2}J_1(\theta) + B_b(\theta) + B(\gamma) - 2J_0(\gamma), \tag{4.30}$$

is the boundary layer energy due to a jump at the boundary, *while*

$$B_{IJ} = 2B(\gamma) - 2J_0(\gamma) \tag{4.31}$$

is the boundary layer energy due to a jump at an internal point *of* $(0,1)$.

In Figures 4 and 5 we give an intuitive picture of the location of occurring boundary layers in the case of a crack in 0 and in the interior, respectively.

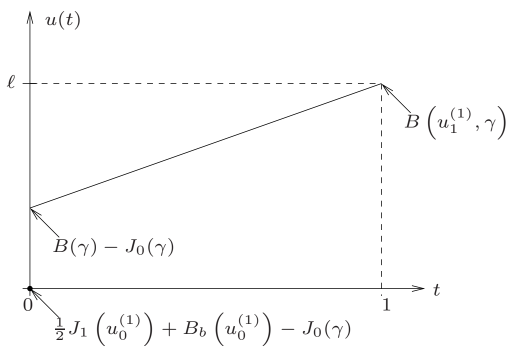

Figure 4: An intuitive picture of the location of boundary layers for a crack in 0.

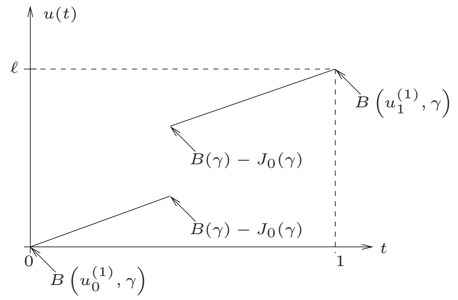

Figure 5: An intuitive picture of the location of boundary layers for a crack in the interior.

Proof. **Liminf inequality.** Without loss of generality we can assume that there is only one jump point, i.e., $\#S_u = 1$. In the following we consider the case of having a jump at the boundary or in the interior separately. Since the jumps at 0 and 1, respectively, are similar due to symmetry, we only treat the boundary jump at 0.

Jump at 0. Assume that $S_u = \{0\}$ and let (u_n) be a sequence such that $\sup_n H^\ell_{1,n}(u_n) < +\infty$. By Proposition 4.2 we know that $u_n \to u$ in $L^1(0,1)$ with

$$u(t) = \begin{cases} 0 & \text{if } t = 0, \\ \gamma t + (\ell - \gamma) & \text{if } t \in (0,1]. \end{cases} \tag{4.32}$$

Moreover, there exists a finite set S such that $u_n \to u$ in $W^{1,\infty}_{\text{loc}}((0,1)\setminus S)$. We prove that

$$\liminf_n H^\ell_{1,n}(u_n) \geq \frac{1}{2}J_1\left(u_0^{(1)}\right) + B_b\left(u_0^{(1)}\right) + B(\gamma) - 2J_0(\gamma) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma). \tag{4.33}$$

Let $k_n^1 \in \mathbb{N}$ with $\lambda_n k_n^1 \to \frac{3}{4}$ be such that

$$\lim_{n\to\infty} \frac{u_n^{k_n^1+2} - u_n^{k_n^1+1}}{\lambda_n} = \gamma, \tag{4.34}$$

note that without loss of generality we may assume $\frac{3}{4} \notin S$. We start from (4.8) and decompose the sum into a sum from 0 to k_n^1 and a sum from k_n^1+1 to $n-2$. In the following we adapt parts of the proof of Theorem 4.3; note that σ_n^i defined in (4.9) is the same as s_n^i defined in (4.18) for $\ell = \gamma$. Instead of (4.22) we set

$$w_n^j = \begin{cases} \frac{u_n^{n+j}}{\lambda_n} - \frac{\ell}{\lambda_n} & \text{if } k_n^1 - n + 1 \leq j \leq 0, \\ \gamma(j - (k_n^1 - n + 1)) - \frac{\ell}{\lambda_n} + \frac{u_n^{k_n^1+1}}{\lambda_n} & \text{if } j \leq k_n^1 - n + 1. \end{cases}$$

and then can prove analogously to (4.23) that

$$\frac{1}{2}J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) + \sum_{i=k_n^1+1}^{n-2} \sigma_n^i \geq B\left(u_1^{(1)},\gamma\right) - \omega(n) \tag{4.35}$$

with an appropriate function ω converging to 0 as $n \to \infty$. Therefore, in order to obtain (4.33) we focus now on the sum of the terms σ_n^i for i ranging between 0 and k_n^1.

Since, by assumption, $u_n \to u$ and $S_u = \{0\}$, we have that there exists $h_n \in \mathbb{N}$ with $\lambda_n h_n \to 0$ such that

$$\lim_{n\to\infty} \frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} = +\infty. \tag{4.36}$$

Indeed, since u_n converges to u almost everywhere, for every $\varepsilon > 0$ there exists some $q_n \in \mathbb{N}$ such that $\lambda_n q_n \to 0$ and $u_n^{q_n} = u_n(\lambda_n q_n) := a_n \geq \ell - \gamma + \gamma\lambda_n q_n - \varepsilon$, for n large enough. We set $r_n := \gamma\lambda_n q_n - \varepsilon$. Therefore, we have for n large enough

$$\frac{u_n^{q_n} - u_n^1}{\lambda_n} = \frac{a_n}{\lambda_n} - u_0^{(1)} \geq \frac{\ell - \gamma + r_n}{\lambda_n} - u_0^{(1)} \to +\infty.$$

Observe that there are two cases: either the discrete slope of u_n is constant in $[\lambda_n, \lambda_n q_n]$ or not. If such a slope is constant, then we have that for every $j = 1, \dots, q_n - 1$

$$\frac{u_n^{j+1} - u_n^j}{\lambda_n} = \frac{a_n - \lambda_n u_0^{(1)}}{\lambda_n q_n} \to +\infty.$$

Therefore, the claim (4.36) follows choosing $h_n = q_n - 1$ for example, or choosing $h_n = j$ for some $j \in \{1, \dots, q_n - 1\}$.

If the slope is not constant, then there exists $\widehat{h} \in \{1, \dots, q_n - 1\}$ such that

$$\frac{u_n^{\widehat{h}+1} - u_n^{\widehat{h}}}{\lambda_n} \geq \frac{a_n - \lambda_n u_0^{(1)}}{\lambda_n q_n} \to +\infty,$$

and (4.36) follows choosing $h_n = \widehat{h}$.

We then split the sum, by isolating the terms $i = h_n - 1$ and $i = h_n$ which contain terms as in (4.36):

$$\sum_{i=0}^{k_n^1} \sigma_n^i = \sum_{i=0}^{h_n-2} \sigma_n^i + \sigma_n^{h_n-1} + \sigma_n^{h_n} + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i. \tag{4.37}$$

According to (4.36), since $J_1(+\infty) = J_2(+\infty) = 0$, we have that some terms in $\sigma_n^{h_n-1}$ and in $\sigma_n^{h_n}$ are infinitesimal. We collect them in the function $r_1(n)$ defined by

$$r_1(n) = J_2\left(\frac{u_n^{h_n+1} - u_n^{h_n-1}}{2\lambda_n}\right) + J_2\left(\frac{u_n^{h_n+2} - u_n^{h_n}}{2\lambda_n}\right) + J_1\left(\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n}\right)$$

and converging to 0 as $n \to \infty$. Hence, from (4.37) we have

$$\sum_{i=0}^{k_n^1} \sigma_n^i = \frac{1}{2}J_1\left(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n}\right) + \sum_{i=0}^{h_n-2} \sigma_n^i + \frac{1}{2}J_1\left(\frac{u_n^{h_n+2} - u_n^{h_n+1}}{\lambda_n}\right) + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i - 2J_0(\gamma) + r_1(n). \tag{4.38}$$

We show that

$$\frac{1}{2}J_1\left(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n}\right) + \sum_{i=0}^{h_n-2} \sigma_n^i \geq B_b\left(u_0^{(1)}\right), \tag{4.39}$$

$$\frac{1}{2}J_1\left(\frac{u_n^{h_n+2} - u_n^{h_n+1}}{\lambda_n}\right) + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i \geq B(\gamma) + r_2(n), \tag{4.40}$$

with $r_2(n) \to 0$ as $n \to \infty$, see below for details. Indeed, (4.39)–(4.40) together with (4.35) and (4.38) then give (4.33).

Let us start by proving the inequality in (4.39). We observe that (4.27) can be phrased equivalently for test functions defined on $-\mathbb{N}$, in the same way as (4.21) was derived from (4.13). We define for $j = -h_n + 2, \dots, 0$

$$\widehat{w}_n^j = \frac{u_n^{j+h_n}}{\lambda_n}.$$

Then

$$\begin{aligned}\frac{1}{2}J_1\left(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n}\right) + \sum_{i=0}^{h_n-2} \sigma_n^i =& \frac{1}{2}J_1\left(\widehat{w}_n^0 - \widehat{w}_n^{-1}\right) + \sum_{j=-h_n+2}^{0} \left\{ J_2\left(\frac{\widehat{w}_n^j - \widehat{w}_n^{j-2}}{2}\right) \right. \\ & \left. + \frac{1}{2}\left(J_1(\widehat{w}_n^j - \widehat{w}_n^{j-1}) + J_1(\widehat{w}_n^{j-1} - \widehat{w}_n^{j-2})\right) - J_0(\gamma) \right\}\end{aligned}$$

and, moreover, $\widehat{w}_n^{-h_n} = 0$, $\widehat{w}_n^{1-h_n} - \widehat{w}_n^{-h_n} = u_0^{(1)}$, which means that $\widehat{w}_n$ is an admissible test for $B_b\left(u_0^{(1)}\right)$ and thus (4.39) holds true.

It remains to prove (4.40). We define, for $j \geq 0$

$$\widetilde{u}_n^j = \begin{cases} \dfrac{u_n^{h_n+1+j}}{\lambda_n} - \dfrac{u_n^{h_n+1}}{\lambda_n} & \text{if } j \leq k_n^1 - h_n + 1, \\ \gamma\left(j - k_n^1 + h_n - 1\right) + \dfrac{u_n^{k_n^1+2}}{\lambda_n} - \dfrac{u_n^{h_n+1}}{\lambda_n} & \text{if } j \geq k_n^1 - h_n + 1. \end{cases}$$

Therefore, we find

$$\begin{aligned}\frac{1}{2}J_1\left(\frac{u_n^{h_n+2} - u_n^{h_n+1}}{\lambda_n}\right) + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i =& \frac{1}{2}J_1\left(\widetilde{u}_n^1 - \widetilde{u}_n^0\right) + \sum_{j\geq 0} \left\{ J_2\left(\frac{\widetilde{u}_n^{j+2} - \widetilde{u}_n^j}{2}\right) \right. \\ & \left. + \frac{1}{2}\left(J_1\left(\widetilde{u}_n^{j+2} - \widetilde{u}_n^{j+1}\right) + J_1\left(\widetilde{u}_n^{j+1} - \widetilde{u}_n^j\right)\right) - J_0(\gamma) \right\} - r_2(n),\end{aligned}$$

where $r_2(n)$ corresponds to the term $j = k_n^1 - h_n$, and we can consider an infinite sum since the terms for $j \geq k_n^1 - h_n + 1$ are identically 0. We observe that

$$r_2(n) = J_2\left(\frac{1}{2}\left(\gamma + \frac{u_n^{k_n^1+2} - u_n^{k_n^1+1}}{\lambda_n}\right)\right) + \frac{1}{2}\left(J_1(\gamma) + J_1\left(\frac{u_n^{k_n^1+2} - u_n^{k_n^1+1}}{\lambda_n}\right)\right) - J_0(\gamma) \to 0$$

as $n \to \infty$, since, by (4.34), $\frac{u_n^{k_n^1+2} - u_n^{k_n^1+1}}{\lambda_n} \to \gamma$, and $J_2(\gamma) + J_1(\gamma) = J_0(\gamma)$ by (4.3). Note that $\widetilde{u}_n^0 = 0$, $\widetilde{u}_n^{j+1} - \widetilde{u}_n^j = \gamma$ for all $j \geq k_n^1 - h_n + 1$. According to the definition of $B(\gamma)$ recalled in (4.28), we thus obtain (4.40), which concludes the proof of (4.33).

Internal jump. Assume that $S_u = \{\bar{t}\}$, where $\bar{t} \in (0,1)$. Without loss of generality we consider $\bar{t} = \frac{1}{2}$. Let (u_n) be a sequence converging to u such that $\sup_n H_{1,n}^\ell(u_n) < +\infty$. Then Proposition 4.2 implies that $u_n \to u$ in $L^1(0,1)$ with

$$u(t) = \begin{cases} \gamma t & \text{if } 0 \leq t \leq \frac{1}{2}, \\ (\ell - \gamma) + \gamma t & \text{if } \frac{1}{2} < t \leq 1. \end{cases} \tag{4.41}$$

Moreover, there exists a finite set S such that $u_n \to u$ in $W^{1,\infty}_{\rm loc}((0,1)\setminus S)$. We prove

$$\liminf_n H^\ell_{1,n}(u_n) \geq B\left(u_0^{(1)},\gamma\right) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma) + 2B(\gamma) - 2J_0(\gamma). \tag{4.42}$$

Without loss of generality we may assume $\frac{1}{4}, \frac{3}{4} \notin S$. Let k_n^0, k_n^1, h_n be integers with $\lambda_n k_n^0 \to \frac{1}{4}$, $\lambda_n k_n^1 \to \frac{3}{4}$, $\lambda_n h_n \leq \frac{1}{2}$ and $\lambda_n h_n \to \frac{1}{2}$ such that

$$\frac{u_n^{k_n^0+2} - u_n^{k_n^0+1}}{\lambda_n} \to \gamma, \ \frac{u_n^{k_n^1+2} - u_n^{k_n^1+1}}{\lambda_n} \to \gamma, \ \frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n} \to +\infty \quad \text{as } n \to \infty. \tag{4.43}$$

By using again the definition of σ_n^i, $i = 0, \dots, n-2$, given in (4.9), we decompose the energy $H^\ell_{1,n}(u_n)$ as follows to extract the occurring boundary layer energies.

$$\begin{aligned} H^\ell_{1,n}(u_n) = &\frac{1}{2} J_1\left(\frac{u_n^1 - u_n^0}{\lambda_n}\right) + \sum_{i=0}^{k_n^0} \sigma_n^i + \sum_{i=k_n^0+1}^{h_n-2} \sigma_n^i + \sigma_n^{h_n-1} + \sigma_n^{h_n} + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i + \sum_{i=k_n^1+1}^{n-2} \sigma_n^i \\ &+ \frac{1}{2} J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) - J_0(\gamma). \end{aligned} \tag{4.44}$$

As in (4.35) we have

$$\frac{1}{2} J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) + \sum_{i=k_n^1+1}^{n-2} \sigma_n^i \geq B\left(u_1^{(1)},\gamma\right) - \omega(n). \tag{4.45}$$

In a similar way (see also (4.20)) we get

$$\frac{1}{2} J_1\left(\frac{u_n^1 - u_n^0}{\lambda_n}\right) + \sum_{i=0}^{k_n^0} \sigma_n^i \geq B\left(u_0^{(1)},\gamma\right) - \omega(n) \tag{4.46}$$

for some (in general different) functions $\omega(n)$, see above, converging to 0 as $n \to \infty$. Therefore, in order to obtain (4.42), we focus on

$$\Sigma = \sum_{i=k_n^0+1}^{h_n-2} \sigma_n^i + \sigma_n^{h_n-1} + \sigma_n^{h_n} + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i.$$

According to the third limit in (4.43), since $J_1(+\infty) = J_2(+\infty) = 0$, we deduce (as in the case of boundary jumps) that some terms defining $\sigma_n^{h_n-1}$ and $\sigma_n^{h_n}$ are infinitesimal. Therefore, rearranging the terms, we can rewrite Σ as follows:

$$\Sigma = \frac{1}{2} J_1\left(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n}\right) + \sum_{i=k_n^0+1}^{h_n-2} \sigma_n^i + \frac{1}{2} J_1\left(\frac{u_n^{h_n+2} - u_n^{h_n+1}}{\lambda_n}\right) + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i - 2J_0(\gamma) + \omega(n), \tag{4.47}$$

where

$$\omega(n) = J_2\left(\frac{u_n^{h_n+1} - u_n^{h_n-1}}{2\lambda_n}\right) + \frac{1}{2} J_1\left(\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n}\right) + J_2\left(\frac{u_n^{h_n+2} - u_n^{h_n}}{2\lambda_n}\right) + \frac{1}{2} J_1\left(\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n}\right)$$

converges to 0 as $n \to \infty$. It remains to prove that

$$\frac{1}{2} J_1 \left(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n} \right) + \sum_{i=k_n^0+1}^{h_n-2} \sigma_n^i \geq B(\gamma) + r_1(n), \tag{4.48}$$

$$\frac{1}{2} J_1 \left(\frac{u_n^{h_n+2} - u_n^{h_n+1}}{\lambda_n} \right) + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i \geq B(\gamma) + r_2(n), \tag{4.49}$$

with $r_i(n) \to 0$, for $i = 1, 2$, as $n \to \infty$. Indeed, (4.48)–(4.49) together with (4.44), (4.47) will then give (4.42). We start by proving (4.48). We define $\widetilde{u}_n : \mathbb{N} \to \mathbb{R}$ as

$$\widetilde{u}_n^j = \begin{cases} \dfrac{u_n^{h_n} - u_n^{h_n-j}}{\lambda_n} & \text{if } 0 \leq j \leq h_n - k_n^0 - 1, \\ \gamma(j - h_n + k_n^0 + 1) + \dfrac{u_n^{h_n} - u_n^{k_n^0+1}}{\lambda_n} & \text{if } j \geq h_n - k_n^0 - 1. \end{cases}$$

We observe that $\widetilde{u}_n^0 = 0$, $\widetilde{u}_n^{j+1} - \widetilde{u}_n^j = \gamma$ for all $j \geq h_n - k_n^0 - 1$. The idea is to rewrite the left-hand side in (4.48) as an infinite sum involving $\widetilde{u}_n^j$ as follows

$$\begin{aligned} \frac{1}{2} J_1 \left(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n} \right) + \sum_{i=k_n^0+1}^{h_n-2} \sigma_n^i =& \frac{1}{2} J_1 \left(\widetilde{u}_n^1 - \widetilde{u}_n^0 \right) + \sum_{j\geq 0} \left\{ J_2 \left(\frac{\widetilde{u}_n^{j+2} - \widetilde{u}_n^j}{2} \right) \right. \\ & \left. + \frac{1}{2} \left(J_1 \left(\widetilde{u}_n^{j+2} - \widetilde{u}_n^{j+1} \right) + J_1 \left(\widetilde{u}_n^{j+1} - \widetilde{u}_n^j \right) \right) - J_0(\gamma) \right\} - r_1(n), \end{aligned}$$

where $r_1(n)$ is an infinitesimal term corresponding to $j = h_n - k_n^0 - 2$; we can consider the sum as an infinite sum since the terms for $j \geq h_n - k_n^0 - 1$ are identically 0. According to the definition of $B(\gamma)$ given by (4.28), we thus obtain (4.48).

We pass now to (4.49). We define another test function $\widetilde{u}_n : \mathbb{N} \to \mathbb{R}$, again denoted by $\widetilde{u}_n$, such that

$$\widetilde{u}_n^j = \begin{cases} \dfrac{u_n^{j+h_n+1} - u_n^{h_n+1}}{\lambda_n} & \text{if } 0 \leq j \leq k_n^1 - h_n + 1, \\ \gamma(j + h_n - k_n^1 - 1) + \dfrac{u_n^{k_n^1+2} - u_n^{h_n+1}}{\lambda_n} & \text{if } j \geq k_n^1 - h_n + 1. \end{cases}$$

Thus, $\widetilde{u}_n^0 = 0$ and $\widetilde{u}_n^{j+1} - \widetilde{u}_n^j = \gamma$ for $j \geq k_n^1 - h_n + 1$. We can rewrite the left-hand side of (4.49) in terms of an infinite sum involving $\widetilde{u}_n^j$:

$$\begin{aligned} \frac{1}{2} J_1 \left(\frac{u_n^{h_n+2} - u_n^{h_n+1}}{\lambda_n} \right) + \sum_{i=h_n+1}^{k_n^1} \sigma_n^i =& \frac{1}{2} J_1 \left(\widetilde{u}_n^1 - \widetilde{u}_n^0 \right) + \sum_{j\geq 0} \left\{ J_2 \left(\frac{\widetilde{u}_n^{j+2} - \widetilde{u}_n^j}{2} \right) \right. \\ & \left. + \frac{1}{2} \left(J_1 \left(\widetilde{u}_n^{j+2} - \widetilde{u}_n^{j+1} \right) + J_1 \left(\widetilde{u}_n^{j+1} - \widetilde{u}_n^j \right) \right) - J_0(\gamma) \right\} - r_2(n), \end{aligned}$$

where $r_2(n)$ corresponds to the term $j = k_n^1 - h_n$ and converges to 0 as $n \to \infty$ by (4.43) and by (4.3). Thus (4.49) follows, and this concludes the proof of the liminf inequality.

Limsup inequality. As before, we distinguish between the different situations.

Jump at 0. We assume that $S_u = \{0\}$ where u is given by (4.32). We need to prove that there exists a sequence (u_n) converging to u in $L^1(0,1)$, satisfying (2.2) and such that

$$\limsup_n H^\ell_{1,n}(u_n) \le \frac{1}{2}J_1\left(u_0^{(1)}\right) + B_b\left(u_0^{(1)}\right) + B(\gamma) - 2J_0(\gamma) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma). \tag{4.50}$$

Let us fix $\eta > 0$. Then, by the definition of $B(\gamma)$ (see (4.28)), we can find $\widetilde{u} : \mathbb{N} \to \mathbb{R}$ and $\widetilde{N} \in \mathbb{N}$ such that $\widetilde{u}^0 = 0, \widetilde{u}^{i+1} - \widetilde{u}^i = \gamma$ if $i \ge \widetilde{N}$ and

$$\frac{1}{2}J_1\left(\widetilde{u}^1 - \widetilde{u}^0\right) + \sum_{i\ge 0}\left\{J_2\left(\frac{\widetilde{u}^{i+2} - \widetilde{u}^i}{2}\right) + \frac{1}{2}\left(J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^{i+1}\right) + J_1\left(\widetilde{u}^{i+1} - \widetilde{u}^i\right)\right) - J_0(\gamma)\right\}$$
$$\le B(\gamma) + \eta. \tag{4.51}$$

In the same way, by the definition of $B\left(u_1^{(1)}, \gamma\right)$ given in (4.29) and the observation that this can be phrased equivalently for test functions defined on $-\mathbb{N}$, there exist $w : -\mathbb{N} \to \mathbb{R}$ and $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^0 - w^{-1} = -w^{-1} = u_1^{(1)}$, $w^i - w^{i-1} = \gamma$ if $i \le -N_2$, such that

$$\frac{1}{2}J_1(w^0 - w^{-1}) + \sum_{i\le 0}\left\{J_2\left(\frac{w^i - w^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w^i - w^{i-1}\right) + J_1\left(w^{i-1} - w^{i-2}\right)\right) - J_0(\gamma)\right\}$$
$$\le B\left(u_1^{(1)}, \gamma\right) + \eta. \tag{4.52}$$

Analogously, by the definition of $B_b(\theta)$ given in (4.27), there exist $\widehat{w} : -\mathbb{N} \to \mathbb{R}$ and $\widehat{k}_0 \in \mathbb{N}$ such that $\widehat{w}^{-\widehat{k}_0-1} = 0$, $\widehat{w}^{-\widehat{k}_0} - \widehat{w}^{-\widehat{k}_0-1} = \widehat{w}^{-\widehat{k}_0} = u_0^{(1)}$ and

$$\frac{1}{2}J_1\left(\widehat{w}^0 - \widehat{w}^{-1}\right) + \sum_{i=-\widehat{k}_0+1}^{0}\left\{J_2\left(\frac{\widehat{w}^i - \widehat{w}^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(\widehat{w}^i - \widehat{w}^{i-1}\right) + J_1\left(\widehat{w}^{i-1} - \widehat{w}^{i-2}\right)\right) - J_0(\gamma)\right\}$$
$$\le B_b\left(u_0^{(1)}\right) + \eta. \tag{4.53}$$

Let $\{k_n^1\}$ be a sequence of integers with $\lambda_n k_n^1 \to \frac{3}{4}$ as $n \to \infty$ such that

$$k_n^1 - (\widehat{k}_0 + 2) \ge \widetilde{N} \quad \text{and} \quad k_n^1 - n + 2 \le -N_2 \quad \text{for all } n \in \mathbb{N}. \tag{4.54}$$

We construct the sequence (u_n) by means of the functions $\widetilde{u}$, w and $\widehat{w}$. Indeed, we define

$$u_n^i = \begin{cases} \lambda_n \widehat{w}^{i-\widehat{k}_0-1} & \text{if } 0 \le i \le \widehat{k}_0 + 1, \\ \ell + \lambda_n\left(w^{k_n^1+1-n} + \widetilde{u}^{i-(\widehat{k}_0+2)} - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)}\right) & \text{if } \widehat{k}_0 + 2 \le i \le k_n^1 + 1, \\ \ell + \lambda_n w^{i-n} & \text{if } k_n^1 + 1 \le i \le n. \end{cases}$$

Note that the sequence (u_n) satisfies the boundary conditions

$$u_n^0 = \lambda_n \widehat{w}^{-\widehat{k}_0-1} = 0, \qquad u_n^n = \ell + \lambda_n w^0 = \ell,$$
$$u_n^1 = \lambda_n \widehat{w}^{-\widehat{k}_0} = \lambda_n u_0^{(1)}, \qquad u_n^n - u_n^{n-1} = \lambda_n(w^0 - w^{-1}) = \lambda_n u_1^{(1)},$$

and satisfies $u_n^{i+1} - u_n^i = \gamma$ for $\widetilde{N} + \widehat{k}_0 + 2 \le i \le k_n^1$ and for $k_n^1 + 1 \le i \le n - 1 - N_2$ by definition. Moreover we have that

$$u_n^{\widehat{k}_0+2} - u_n^{\widehat{k}_0+1} \to \ell - \gamma. \tag{4.55}$$

Indeed, by using the facts that $\widetilde{u}^{i+1} - \widetilde{u}^i = \gamma$ if $i \geq \widetilde{N}$ and $w^i - w^{i-1} = \gamma$ if $i \leq -N_2$, together with (4.54) we obtain

$$\begin{aligned} u_n^{\widehat{k}_0+2} - u_n^{\widehat{k}_0+1} &= \ell + \lambda_n \left(w^{k_n^1+1-n} + (\widetilde{u}^0 - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)}) - \widehat{w}^0 \right) \\ &= \ell + \lambda_n \left((w^{k_n^1+1-n} - w^{-N_2}) + w^{-N_2} + (\widetilde{u}^{\widetilde{N}} - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)}) - \widetilde{u}^{\widetilde{N}} - \widehat{w}^0 \right) \\ &= \ell + \lambda_n \left(\gamma(k_n^1 + 1 - n + N_2) + w^{-N_2} - \gamma(k_n^1 + 1 - (\widehat{k}_0 + 2) - \widetilde{N}) - \widetilde{u}^{\widetilde{N}} - \widehat{w}^0 \right) \\ &= \ell - \gamma n \lambda_n + \lambda_n \left(\gamma(N_2 + (\widehat{k}_0 + 2) + \widetilde{N}) + w^{-N_2} - \widetilde{u}^{\widetilde{N}} - \widehat{w}^0 \right) \longrightarrow \ell - \gamma. \end{aligned}$$

Hence $u_n \to u$ in $L^1(0,1)$, where u is defined by (4.32), as $n \to \infty$.

To prove (4.50), we rewrite $H_{1,n}^\ell(u_n)$ as

$$\begin{aligned} H_{1,n}^\ell(u_n) =& \frac{1}{2} J_1 \left(\frac{u_n^1 - u_n^0}{\lambda_n} \right) + \sum_{i=0}^{\widehat{k}_0-1} \sigma_n^i + \sigma_n^{\widehat{k}_0} + \sigma_n^{\widehat{k}_0+1} + \sum_{i=\widehat{k}_0+2}^{k_n^1-1} \sigma_n^i + \sigma_n^{k_n^1} + \sum_{i=k_n^1+1}^{n-2} \sigma_n^i \\ &+ \frac{1}{2} J_1 \left(\frac{u_n^n - u_n^{n-1}}{\lambda_n} \right) - J_0(\gamma), \end{aligned} \tag{4.56}$$

where σ_n^i is defined in (4.9), and we use the definition of (u_n) above.

We start with the sum from $i = 0$ to $\widehat{k}_0 - 1$, and involve $\widehat{w}^j$ by introducing the new index $j = i - \widehat{k}_0 + 1$ and summing then from $j = -\widehat{k}_0 + 1$ up to 0, namely,

$$\sum_{i=0}^{\widehat{k}_0-1} \sigma_n^i = \sum_{j=-\widehat{k}_0+1}^{0} \left\{ J_2 \left(\frac{\widehat{w}^j - \widehat{w}^{j-2}}{2} \right) + \frac{1}{2} \left(J_1 \left(\widehat{w}^j - \widehat{w}^{j-1} \right) + J_1 \left(\widehat{w}^{j-1} - \widehat{w}^{j-2} \right) \right) - J_0(\gamma) \right\}. \tag{4.57}$$

We continue with the term $\sigma_n^{\widehat{k}_0}$ by observing that

$$\sigma_n^{\widehat{k}_0} = \frac{1}{2} J_1 \left(\widehat{w}^0 - \widehat{w}^{-1} \right) - J_0(\gamma) + \widehat{r}(n), \tag{4.58}$$

where $\widehat{r}(n)$ is defined by

$$\begin{aligned} \widehat{r}(n) =& J_2 \left(\frac{\ell}{2\lambda_n} + \frac{1}{2} \left(w^{k_n^1+1-n} - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)} - \widehat{w}^{-1} \right) \right) \\ &+ \frac{1}{2} J_1 \left(\frac{\ell}{\lambda_n} + w^{k_n^1+1-n} - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)} - \widehat{w}^0 \right) \end{aligned}$$

and converges to 0 as $n \to \infty$, since $J_2(+\infty) = J_1(+\infty) = 0$. Similarly,

$$\sigma_n^{\widehat{k}_0+1} = \frac{1}{2} J_1 \left(\widetilde{u}^1 - \widetilde{u}^0 \right) - J_0(\gamma) + r(n), \tag{4.59}$$

where

$$\begin{aligned} r(n) =& J_2 \left(\frac{\ell}{2\lambda_n} + \frac{1}{2} \left(w^{k_n^1+1-n} + \widetilde{u}^1 - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)} - \widehat{w}^0 \right) \right) \\ &+ \frac{1}{2} J_1 \left(\frac{\ell}{\lambda_n} + w^{k_n^1+1-n} - \widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)} - \widehat{w}^0 \right) \end{aligned}$$

converges to 0 as $n \to \infty$.

The sum from $i = \widehat{k}_0 + 2$ to $k_n^1 - 1$ can be rewritten in terms of $\widetilde{u}$ by introducing the new index $j = i - (\widehat{k}_0 + 2)$ ranging between 0 and $k_n^1 - 1 - (\widehat{k}_0 + 2)$. Actually, we can pass to an infinite sum, since the term for $j \geq \widetilde{N}$ gives zero contribution by (4.3) and, by (4.54), $k_n^1 - (\widehat{k}_0 + 2) \geq \widetilde{N}$. Thus we have

$$\sum_{i=\widehat{k}_0+2}^{k_n^1-1} \sigma_n^i = \sum_{j\geq 0} \left\{ J_2\left(\frac{\widetilde{u}^{j+2} - \widetilde{u}^j}{2}\right) + \frac{1}{2}\left(J_1\left(\widetilde{u}^{j+2} - \widetilde{u}^{j+1}\right) + J_1\left(\widetilde{u}^{j+1} - \widetilde{u}^j\right)\right) - J_0(\gamma)\right\}. \tag{4.60}$$

Next, we observe that

$$\sigma_n^{k_n^1} = 0. \tag{4.61}$$

Indeed, by (4.54),

$$\begin{aligned}\sigma_n^{k_n^1} =& J_2\left(\frac{(w^{k_n^1+2-n} - w^{k_n^1+1-n}) + (\widetilde{u}^{k_n^1+1-(\widehat{k}_0+2)} - \widetilde{u}^{k_n^1-(\widehat{k}_0+2)})}{2}\right) + J_1(\gamma) - J_0(\gamma) \\ =& J_2(\gamma) + J_1(\gamma) - J_0(\gamma) = 0.\end{aligned}$$

It remains to consider the sum from $i = k_n^1 + 1$ up to $n - 2$, which involves w by introducing the new index $j = i - n + 2$. Moreover, we can pass to the infinite sum for $j \leq 0$, since $k_n^1 - n + 2 \leq -N_2$ and the terms in the sum are 0 for $j \leq -N_2$. Therefore, we have

$$\sum_{i=k_n^1+1}^{n-2} \sigma_n^i = \sum_{j\leq 0} \left\{ J_2\left(\frac{w^j - w^{j-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w^j - w^{j-1}\right) + J_1\left(w^{j-1} - w^{j-2}\right)\right) - J_0(\gamma)\right\}. \tag{4.62}$$

In conclusion, by (4.56), (4.57)–(4.62) together with (4.51)–(4.53), we obtain

$$\begin{aligned} H_{1,n}^\ell(u_n) =& \frac{1}{2}J_1\left(u_0^{(1)}\right) - 3J_0(\gamma) + \widehat{r}(n) + r(n) + \frac{1}{2}J_1\left(\widehat{w}^0 - \widehat{w}^{-1}\right) \\ &+ \sum_{i=-\widehat{k}_0+1}^{0} \left\{ J_2\left(\frac{\widehat{w}^i - \widehat{w}^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(\widehat{w}^i - \widehat{w}^{i-1}\right) + J_1\left(\widehat{w}^{i-1} - \widehat{w}^{i-2}\right)\right) - J_0(\gamma)\right\} \\ &+ \frac{1}{2}J_1\left(\widetilde{u}^1 - \widetilde{u}^0\right) + \sum_{i\geq 0} \left\{ J_2\left(\frac{\widetilde{u}^{i+2} - \widetilde{u}^i}{2}\right) + \frac{1}{2}\left(J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^{i+1}\right) + J_1\left(\widetilde{u}^{i+1} - \widetilde{u}^i\right)\right) - J_0(\gamma)\right\} \\ &+ \frac{1}{2}J_1(w^0 - w^{-1}) + \sum_{i\leq 0} \left\{ J_2\left(\frac{w^i - w^{i-2}}{2}\right) + \frac{1}{2}\left(J_1\left(w^i - w^{i-1}\right) + J_1\left(w^{i-1} - w^{i-2}\right)\right) - J_0(\gamma)\right\} \\ \leq& \frac{1}{2}J_1\left(u_0^{(1)}\right) - 3J_0(\gamma) + B_b\left(u_0^{(1)}\right) + B(\gamma) + B\left(u_1^{(1)}, \gamma\right) + 3\eta + \widehat{r}(n) + r(n). \end{aligned}$$

Hence, (4.50) follows.

Internal jump. Without loss of generality we assume that $S_u = \left\{\frac{1}{2}\right\}$ where u is given by (4.41). We have to prove that there exists a sequence (u_n) converging to u in $L^1(0,1)$, satisfying (2.2) and such that

$$\limsup_n H_{1,n}^\ell(u_n) \leq B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) + 2B(\gamma) - 2J_0(\gamma). \tag{4.63}$$

Let us fix $\eta > 0$. By the definition of $B\left(u_0^{(1)}, \gamma\right)$ we can find $v : \mathbb{N} \to \mathbb{R}$ and $N_1 \in \mathbb{N}$ with $v^0 = 0$, $v^1 - v^0 = v^1 = u_0^{(1)}$, $v^{i+1} - v^i = \gamma$ if $i \geq N_1$, such that

$$\begin{aligned}&\frac{1}{2}J_1(v^1 - v^0) + \sum_{i\geq 0}\left\{J_2\left(\frac{v^{i+2} - v^i}{2}\right) + \frac{1}{2}\left(J_1\left(v^{i+2} - v^{i+1}\right) + J_1\left(v^{i+1} - v^i\right)\right) - J_0(\gamma)\right\}\\ &\leq B\left(u_0^{(1)}, \gamma\right) + \eta.\end{aligned} \tag{4.64}$$

Moreover, by the definition of $B(\gamma)$ there exist $\widetilde{u} : \mathbb{N} \to \mathbb{R}$ and $\widetilde{N} \in \mathbb{N}$ satisfying (4.51). Finally, by the definition of $B\left(u_1^{(1)}, \gamma\right)$ there exist $w : -\mathbb{N} \to \mathbb{R}$ and $N_2 \in \mathbb{N}$ as in (4.52).

Let k_n^0, k_n^1, h_n be sequences of integers with $\lambda_n k_n^0 \to \frac{1}{4}$, $\lambda_n k_n^1 \to \frac{3}{4}$, $\lambda_n h_n \to \frac{1}{2}$ as $n \to \infty$, such that

$$k_n^0 \geq N_1 + 1 \quad \text{and} \quad k_n^1 - n + 2 \leq -N_2 \tag{4.65}$$

$$\widetilde{N} \leq \min\{h_n - k_n^0 - 1, k_n^1 - h_n - 1\} \quad \text{for all } n \in \mathbb{N}. \tag{4.66}$$

We construct now the sequence (u_n) by means of the functions $v, \widetilde{u}$ and w:

$$u_n^i = \begin{cases}\lambda_n v^i & \text{if } 0 \leq i \leq k_n^0,\\ \lambda_n\left(v^{k_n^0} - \widetilde{u}^{h_n - i} + \widetilde{u}^{h_n - k_n^0}\right) & \text{if } k_n^0 \leq i \leq h_n,\\ \ell + \lambda_n\left(w^{k_n^1 + 1 - n} + \widetilde{u}^{i-(h_n+1)} - \widetilde{u}^{k_n^1 - h_n}\right) & \text{if } h_n + 1 \leq i \leq k_n^1 + 1,\\ \ell + \lambda_n w^{i-n} & \text{if } k_n^1 + 1 \leq i \leq n.\end{cases}$$

We observe that the sequence (u_n) satisfies the boundary conditions

$$u_n^0 = \lambda_n v^0 = 0,\ u_n^1 = \lambda_n v^1 = \lambda_n u_0^{(1)},\ u_n^n = \ell + \lambda_n w^0 = \ell,\ u_n^n - u_n^{n-1} = \lambda_n(w^0 - w^{-1}) = \lambda_n u_1^{(1)},$$

moreover, $u_n^{i+1} - u_n^i = \gamma$ for $N_1 \leq i \leq h_n - \widetilde{N}$ and for $\widetilde{N} + h_n + 1 \leq i \leq n - N_2$. We also have that

$$u_n^{h_n+1} - u_n^{h_n} \longrightarrow \ell - \gamma. \tag{4.67}$$

Indeed, by using the facts that $v^{i+1} - v^i = \gamma$ for $i \geq N_1$, $\widetilde{u}^{i+1} - \widetilde{u}^i = \gamma$ for $i \geq \widetilde{N}$ and $w^i - w^{i-1} = \gamma$ for $i \leq -N_2$, we have:

$$\begin{aligned}u_n^{h_n+1} - u_n^{h_n} &= \ell + \lambda_n\left(w^{k_n^1+1-n} + \widetilde{u}^0 - \widetilde{u}^{k_n^1 - h_n} - v^{k_n^0} + \widetilde{u}^0 - \widetilde{u}^{h_n - k_n^0}\right)\\ &= \ell + 2\lambda_n\widetilde{u}^0 - \lambda_n\left(\gamma(k_n^0 - N_1 + k_n^1 - h_n - \widetilde{N}) + v^{N_1} + \widetilde{u}^{\widetilde{N}}\right)\\ &\quad + \lambda_n\left(\gamma(k_n^1 - n + 1 + N_2 + k_n^0 - h_n + \widetilde{N}) + w^{-N_2} - \widetilde{u}^{\widetilde{N}}\right)\\ &= \ell + 2\lambda_n\widetilde{u}^0 - \gamma n\lambda_n + \lambda_n\left(\gamma(N_1 + 2\widetilde{N} + N_2 + 1) - v^{N_1} - 2\widetilde{u}^{\widetilde{N}} + w^{-N_2}\right).\end{aligned}$$

Therefore (4.67) holds. In conclusion, $u_n \to u$ in $L^1(0,1)$ as $n \to \infty$. We compute now $H_{1,n}^\ell(u_n)$, which turns out to be useful to write as follows.

$$\begin{aligned}H_{1,n}^\ell(u_n) = \frac{1}{2}J_1\left(\frac{u_n^1 - u_n^0}{\lambda_n}\right) &+ \sum_{i=0}^{k_n^0 - 2}\sigma_n^i + \sigma_n^{k_n^0 - 1} + \sum_{i=k_n^0}^{h_n - 2}\sigma_n^i + \sigma_n^{h_n - 1} + \sigma_n^{h_n} + \sum_{i=h_n+1}^{k_n^1 - 1}\sigma_n^i\\ &+ \sigma_n^{k_n^1} + \sum_{i=k_n^1+1}^{n-2}\sigma_n^i + \frac{1}{2}J_1\left(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\right) - J_0(\gamma),\end{aligned} \tag{4.68}$$

where σ_n^i is defined in (4.9). We observe that

$$\sigma_n^{k_n^0-1} = 0 \tag{4.69}$$

since, by (4.65),

$$J_2\left(\frac{v^{k_n^0} - \widetilde{u}^{h_n-k_n^0-1} + \widetilde{u}^{h_n-k_n^0} - v^{k_n^0-1}}{2}\right) + \frac{1}{2}\left(J_1(\widetilde{u}^{h_n-k_n^0} - \widetilde{u}^{h_n-k_n^0-1}) + J_1(v^{k_n^0} - v^{k_n^0-1})\right)$$
$$= J_2(\gamma) + J_1(\gamma)$$

which equals $J_0(\gamma)$ by (4.3). Similarly,

$$\sigma_n^{k_n^1} = 0 \tag{4.70}$$

because, by (4.66),

$$J_2\left(\frac{w^{k_n^1+2-n} - w^{k_n^1+1-n} - \widetilde{u}^{k_n^1-(h_n+1)} + \widetilde{u}^{k_n^1-h_n}}{2}\right) + \frac{1}{2}J_1(w^{k_n^1+2-n} - w^{k_n^1+1-n})$$
$$+ \frac{1}{2}J_1(\widetilde{u}^{k_n^1-h_n} - \widetilde{u}^{k_n^1-(h_n+1)})$$
$$= J_2(\gamma) + J_1(\gamma) = J_0(\gamma).$$

By (4.68)–(4.70), (4.64), (4.51) and (4.52), and computations analogous as in the case of the boundary jumps, we finally get

$$\limsup_n H_{1,n}^\ell(u_n) \leq B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - 3J_0(\gamma) + 2B(\gamma) + 4\eta,$$

which yields (4.63). □

5 Properties of boundary layer energies and location of fracture

In the previous sections we derived the energy contributions due to the boundary layers which occur in several different cases, see Theorems 4.3 and 4.8. Here we derive some properties of the boundary layer energies and look for the location of fracture, at which we proceed in the spirit of [BC07, Theorem 5.2].

First of all we establish some relations among the three different types of boundary layer energies that we used, namely $B(\gamma)$ as recalled in (4.28), $B(\theta, \gamma)$ as defined in (4.29) and $B_b(\theta)$ as defined in (4.27).

Lemma 5.1. *Let $[H1] - [H4]$ be satisfied. Then the following estimates hold true:*

(1) $\frac{1}{2}J_1(\delta_1) \leq B(\gamma) \leq \frac{1}{2}J_1(\gamma)$;

(2) $B(\gamma) = B_b(\gamma)$;

(3) $B(\gamma, \gamma) = \frac{1}{2}J_1(\gamma)$;

(4) $B(\theta, \gamma) \geq \frac{1}{2} J_1(\theta)$ *for all* $\theta > 0$*;*

(5) $B(\gamma) = \inf_{\theta>0} B(\theta, \gamma)$*;*

(6) $B_b(\theta) \geq \frac{1}{2} J_1(\delta_1)$ *for all* $\theta > 0$*;*

(7) $B_b(\delta_1) = \frac{1}{2} J_1(\delta_1)$*.*

Proof. (1) The infinite sum in the definition (4.28) of $B(\gamma)$ is non-negative since γ is the minimum point of J_0. Hence

$$B(\gamma) \geq \frac{1}{2} \min J_1 = \frac{1}{2} J_1(\delta_1).$$

On the other hand, since the function $u^i = \gamma i$ is a competitor in the minimum problem defining $B(\gamma)$, we have that

$$B(\gamma) \leq \frac{1}{2} J_1(\gamma) + \sum_{i \geq 0} \{J_2(\gamma) + J_1(\gamma) - J_0(\gamma)\} = \frac{1}{2} J_1(\gamma),$$

where we again apply (4.3).

(2) For $\theta = \gamma$, the definition of $B_b(\theta)$ in (4.27) reduces to that of $B(\gamma)$ in (4.28).

(3) See the derivation of (4.26).

(4) It is an immediate consequence of the definition of the boundary layer energy in (4.29), since the infinite sum is non-negative because γ is the minimum point of J_0.

(5) This follows directly comparing the definitions (4.28) and (4.29).

(6) Here we again apply that γ is the minimum point of J_0, which makes the terms in the sum defining the boundary layer energy (4.27) non-negative. Moreover recall that δ_1 is the minimum point of J_1.

(7) From (4.27) we notice that $(\widehat{v}^i, k) = (\delta_1(i-1), 0)$ is a competitor which gives the reverse inequality in *(6)*, therefore we have equality. □

Remark 5.2. From the proof of Lemma 5.1 we deduce that, if $\theta = \delta_1$, then $B_b(\delta_1) = \frac{1}{2} J_1(\delta_1)$ is attained for $k = 0$.

Next we present our result which asserts the location of fracture. More precisely we compare the costs for fracture in the interior and at the boundary in the continuum setting. At the end of this paper we discuss this issue by taking into account also an intermediate scale.

Theorem 5.3. *Suppose that hypotheses* $[H1] - [H4]$ *hold. Let* $\ell > \gamma$*. For* $u_0^{(1)} = u_1^{(1)} = \gamma$*, the fracture can appear indifferently inside or at the boundary of* $[0, 1]$*. If instead* $u_0^{(1)}$ *or* $u_1^{(1)}$ *is equal to* δ_1 *and* $\delta_1 \neq \gamma$*, then a boundary jump is more convenient than an internal jump, in terms of the energy.*

Proof. Since $\ell > \gamma$, we obtain by Theorem 4.8, in the case of bounded energy, that

$$\begin{aligned} H_1^\ell(u) = & B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) + \#\left(S_u \cap \{0\}\right)\left(B_{BJ}\left(u_0^{(1)}\right) - B\left(u_0^{(1)}, \gamma\right)\right) \\ & + \#(S_u \cap \{1\})\left(B_{BJ}\left(u_1^{(1)}\right) - B\left(u_1^{(1)}, \gamma\right)\right) + \#(S_u \cap (0,1)) B_{IJ}, \end{aligned}$$

where $B_{BJ}(\theta)$ and B_{IJ} are defined in (4.30) and (4.31), respectively.

Notice that if $u_0^{(1)}$ or $u_1^{(1)}$ is equal to γ, then by Lemma 5.1 *(2)* and *(3)* we obtain

$$\begin{aligned} B_{BJ}(\gamma) - B(\gamma,\gamma) &= \frac{1}{2}J_1(\gamma) + B_b(\gamma) + B(\gamma) - 2J_0(\gamma) - B(\gamma,\gamma) \\ &= 2B(\gamma) - 2J_0(\gamma) = B_{IJ}. \end{aligned}$$

Hence a jump in the interior of $[0,1]$ costs as much energy as a jump at the boundary.

Now assume that $u_0^{(1)}$ or $u_1^{(1)}$ is equal to δ_1. We show that $B_{BJ}(\delta_1) - B(\delta_1,\gamma) < B_{IJ}$. This is equivalent to proving

$$\frac{1}{2}J_1\big(\delta_1\big) + B_b\big(\delta_1\big) - B(\delta_1,\gamma) < B(\gamma),$$

which follows by Lemma 5.1 *(1)*, *(4)* and *(7)* and the observation that the first inequality in *(1)* of Lemma 5.1 is strict if $\delta_1 \neq \gamma$. □

In the remaining part of this section we show properties of the boundary layer energies in the case of a certain class of interaction potentials, namely the classical Lennard-Jones potentials J_1 and J_2 defined in Remark 4.1.

First we show that the second inequality in *(1)* of Lemma 5.1 is strict. This observation is applied in Remark 4.5, where we discuss that the first-order Γ-limit for $\ell = \gamma$ depends on whether the second and last but one atoms of the chain are prescribed.

Proposition 5.4. *Let J_1 and J_2 be Lennard-Jones potentials as defined in* (4.4). *Then*

$$B(\gamma) < \frac{1}{2}J_1(\gamma). \tag{5.1}$$

Moreover, there exists an $a > 1$ such that $B(a\gamma,\gamma) < B(\gamma,\gamma)$.

Proof. Due to property *(5)* in Lemma 5.1, it is sufficient to show that there exists $\theta > 0$ such that $B(\theta,\gamma) < \frac{1}{2}J_1(\gamma)$. We set $\theta = a\gamma$, $a > 0$. Therefore our claim reduces to proving the existence of $a > 0$ such that $B(a\gamma,\gamma) < \frac{1}{2}J_1(\gamma)$.

Our strategy consists in exhibiting a competitor for the minimum problem defining $B(a\gamma,\gamma)$ and in proving that, for some $a > 0$, its energy is strictly smaller than $\frac{1}{2}J_1(\gamma)$.

Since the function $u : \mathbb{N} \to \mathbb{R}$ defined as

$$u^i = \begin{cases} 0 & \text{if } i = 0, \\ a\gamma & \text{if } i = 1, \\ \gamma i & \text{if } i \geq 2, \end{cases}$$

is an admissible competitor for $B(a\gamma,\gamma)$, we have that

$$B(a\gamma,\gamma) \leq J_1(a\gamma) + J_1\big((2-a)\gamma\big) + \frac{1}{2}J_1(\gamma) + J_1(2\gamma) + J_1\big((3-a)\gamma\big) - 2J_0(\gamma).$$

Therefore our claim reduces to showing that there exists an $a > 0$ such that

$$J_1(a\gamma) + J_1\big((2-a)\gamma\big) + \frac{1}{2}J_1(\gamma) + J_1(2\gamma) + J_1\big((3-a)\gamma\big) - 2J_0(\gamma) < \frac{1}{2}J_1(\gamma), \tag{5.2}$$

that is, equivalently, to showing that there exists an $a > 0$ such that the function $f : \mathbb{R} \to \mathbb{R}$, defined as

$$f(a) := J_1(a\gamma) + J_1\big((2-a)\gamma\big) + J_1\big((3-a)\gamma\big) - J_1(2\gamma) - 2J_1(\gamma), \tag{5.3}$$

is strictly negative. Computing its derivative with respect to a we have, using the explicit expression of J_1 given in (4.4),

$$f'(a) = -\frac{12k_1\gamma}{(a\gamma)^{13}} + \frac{12k_1\gamma}{((2-a)\gamma)^{13}} + \frac{12k_1\gamma}{((3-a)\gamma)^{13}} + \frac{6k_2\gamma}{(a\gamma)^7} - \frac{6k_2\gamma}{((2-a)\gamma)^7} - \frac{6k_2\gamma}{((3-a)\gamma)^7}.$$

In particular, choosing $a = 1$ in the previous formula leads to

$$f'(1) = \frac{12k_1\gamma}{(2\gamma)^{13}} - \frac{6k_2\gamma}{(2\gamma)^7} = \frac{6\gamma k_2}{(2\gamma)^7}\left(\frac{1}{2^6}\frac{2k_1}{k_2\gamma^6} - 1\right) = \frac{6\gamma k_2}{(2\gamma)^7}\left(\frac{1+2^{-6}}{2^6+2^{-6}} - 1\right) < 0.$$

Therefore, since $f(1) = 0$ and $f'(1) < 0$, we have that the function f is strictly negative in a right neighbourhood of 1, i.e., there exists an $a > 1$ such that $f(a) < 0$. This proves (5.1). In particular we deduce that it is more convenient to have an initial slope strictly bigger than γ, which implies the second part of the assertion. □

Next we discuss the "depth" of boundary layers and the occurrence of cracks on the microscopic scale.

Proposition 5.5. *Let J_1 and J_2 be Lennard-Jones potentials as defined in* (4.4). *Then the infimum in $B(\gamma)$ is obtained for $N \to \infty$.*

Proof. For any $N \in \mathbb{N}$ we define A_N such that $B(\gamma) = \inf_{N\in\mathbb{N}} A_N$, that is, using also (4.4),

$$A_N = \min\Bigg\{\frac{1}{2}J_1\left(\widetilde{u}^1 - \widetilde{u}^0\right) + \sum_{i\geq 0}\Bigg\{J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^i\right) + \frac{1}{2}\left(J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^{i+1}\right) + J_1\left(\widetilde{u}^{i+1} - \widetilde{u}^i\right)\right)$$
$$- J_0(\gamma)\Bigg\} :\ \widetilde{u} : \mathbb{N} \to \mathbb{R}, \widetilde{u}^0 = 0, \widetilde{u}^{i+1} - \widetilde{u}^i = \gamma \text{ if } i \geq N\Bigg\}.$$

We note that if (u^i_N) is a minimiser for A_N, then it is an admissible competitor for A_{N+1}, since $u^{i+1}_N - u^i_N = \gamma$ for $i \geq N+1$. Therefore $A_N \geq A_{N+1}$ for all $N \geq 0$ and the sequence $N \mapsto A_N$ is non-increasing.

Let $\widetilde{N}$ be the smallest integer such that $B(\gamma) = A_{\widetilde{N}}$, and assume for contradiction that $\widetilde{N} < +\infty$. Hence we have that

$$A_{\widetilde{N}} = A_N \quad \text{for all } N \geq \widetilde{N}. \tag{5.4}$$

Notice that $\widetilde{N} \geq 1$, since the optimal deformation has the initial slope different from γ, by Proposition 5.4. Let us denote by $(\widetilde{u}^i)$ a minimiser of $A_{\widetilde{N}}$, then

$$\widetilde{u}^i = \begin{cases} \widetilde{u}^i & \text{if } i \leq \widetilde{N}, \\ \widetilde{u}^{\widetilde{N}} + \gamma(i - \widetilde{N}) & \text{if } i \geq \widetilde{N}. \end{cases}$$

Again by γ not being the slope of the optimal deformation, there exists $j \in \{1, \dots, \widetilde{N}\}$ with $\widetilde{u}^j - \widetilde{u}^{j-1} \neq \gamma$. By our previous assumptions, we may take $j = \widetilde{N}$.

We are going to prove that $A_{\widetilde{N}} > A_{\widetilde{N}+2}$, so that (5.4) will give the contradiction. More precisely, starting with $(\widetilde{u}^i)$ we construct a sequence $(\widetilde{v}^i)$ which is an admissible competitor for the minimum problem $A_{\widetilde{N}+2}$, and whose energy, denoted by $A_{\widetilde{N}+2}(\widetilde{v})$, is strictly smaller than $A_{\widetilde{N}}$. The idea is that the forces due to next-to-nearest neighbour interactions acting on atom $\widetilde{N}+1$ in the sequence $(\widetilde{u}^i)$ are asymmetric, whereas the forces due to nearest neighbour interactions cancel since the distance from atom $\widetilde{N}+1$ to atom $\widetilde{N}$ is the same as the distance to atom $\widetilde{N}+2$, namely γ. Because of the asymmetry of the forces on atom $\widetilde{N}+1$ due to next-to-nearest neighbour interactions we expect that this atom is moved to a different position in equilibrium. Therefore, for some $\delta \neq 0$, specified later, we set

$$\widetilde{v}^i = \begin{cases} \widetilde{u}^i & \text{if } i \neq \widetilde{N}+1, \\ \widetilde{u}^{\widetilde{N}+1} + \delta & \text{if } i = \widetilde{N}+1. \end{cases}$$

We show that shifting the position of atom $\widetilde{N}+1$ by an amount δ reduces the energy, i.e., $A_{\widetilde{N}+2}(\widetilde{v}) < A_{\widetilde{N}}$. Indeed we have

$$\begin{aligned} A_{\widetilde{N}} - A_{\widetilde{N}+2}(\widetilde{v}) = \sum_{i=\widetilde{N}-1}^{\widetilde{N}+1} \Bigg(&\left\{ J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^i\right) + \frac{1}{2}\left(J_1\left(\widetilde{u}^{i+2} - \widetilde{u}^{i+1}\right) + J_1\left(\widetilde{u}^{i+1} - \widetilde{u}^i\right)\right) - J_0(\gamma) \right\} \\ &- \left\{ J_1\left(\widetilde{v}^{i+2} - \widetilde{v}^i\right) + \frac{1}{2}\left(J_1\left(\widetilde{v}^{i+2} - \widetilde{v}^{i+1}\right) + J_1\left(\widetilde{v}^{i+1} - \widetilde{v}^i\right)\right) - J_0(\gamma) \right\} \Bigg) \\ = J_1\Big((\widetilde{u}^{\widetilde{N}} - \widetilde{u}^{\widetilde{N}-1}) + \gamma\Big) &- J_1\Big((\widetilde{u}^{\widetilde{N}} - \widetilde{u}^{\widetilde{N}-1}) + \gamma + \delta\Big) - J_1(2\gamma) \\ - J_1(\gamma - \delta) &- J_1(\gamma + \delta) - J_1(2\gamma - \delta) + 2J_0(\gamma). \end{aligned}$$

For the minimising sequence $(\widetilde{u}^i)$ we set $\widetilde{u}^{\widetilde{N}} - \widetilde{u}^{\widetilde{N}-1} = a\gamma$. We know from the non-interpenetration of atoms that $a > 0$, and from the choice of $\widetilde{N}$ that $a \neq 1$ (we specify further properties of a below). Then, we continue the computations above and we obtain by using also the equality $J_0(\gamma) = J_1(\gamma) + J_1(2\gamma)$

$$\begin{aligned} A_{\widetilde{N}} - A_{\widetilde{N}+2}(\widetilde{v}) &= J_1((a+1)\gamma) - J_1((a+1)\gamma + \delta) - J_1(\gamma - \delta) - J_1(\gamma + \delta) \\ &\quad - J_1(2\gamma - \delta) + 2J_1(\gamma) + J_1(2\gamma) \\ &=: f(\delta). \end{aligned} \tag{5.5}$$

We show below that there exists a $\delta \neq 0$ such that $f(\delta) > 0$, or equivalently $A_{\widetilde{N}} - A_{\widetilde{N}+2}(\widetilde{v}) > 0$, in contradiction to our assumption $B(\gamma) = A_{\widetilde{N}}$ with finite $\widetilde{N}$.

Next we elaborate on further properties of the parameter a. We will deduce that we can exclude a being close to zero by exhibiting a competitor having strictly smaller energy.

For the moment we assume $\widetilde{N} \geq 2$. Let $b > 0$ be such that $\widetilde{u}^{\widetilde{N}-1} - \widetilde{u}^{\widetilde{N}-2} = b\gamma$ and consider the competitor $\widetilde{w} : \mathbb{N} \to \mathbb{R}$ defined as

$$\widetilde{w}^i = \begin{cases} \widetilde{u}^i & \text{if } i \leq \widetilde{N}-1, \\ \widetilde{u}^{\widetilde{N}-1} + \gamma(i - \widetilde{N} + 1) & \text{if } i \geq \widetilde{N}-1. \end{cases}$$

Let us denote by $A_{\widetilde{N}-1}(\widetilde{w})$ the energy associated to $\widetilde{w}$. Then

$$A_{\widetilde{N}} - A_{\widetilde{N}-1}(\widetilde{w}) = J_1\left((a+b)\gamma\right) + J_1(a\gamma) + J_1((a+1)\gamma) - J_1((1+b)\gamma) - J_1(\gamma) - J_1(2\gamma).$$

Note that $J_1(\gamma) = \frac{k_1 k_2}{\gamma^6} \frac{1+2^{-6}-2(1+2^{-12})}{2k_1(1+2^{-12})} < 0$. Furthermore, by the assumptions on the potential J_1, there holds $J_1(z) \leq 0$ for every $z \geq \gamma$. Hence we have in particular that $J_1((1+b)\gamma) < 0$ and $J_1(2\gamma) < 0$. Moreover, $J_1(z) \geq J_1(\delta_1) = -\frac{k_2}{2\delta_1^6}$ for every z. Thus

$$A_{\widetilde{N}} - A_{\widetilde{N}-1}(\widetilde{w}) \geq J_1(a\gamma) + 2J_1(\delta_1) - J_1(2\gamma) - J_1(\gamma) > J_1(a\gamma) - \frac{k_2}{\delta_1^6}. \tag{5.6}$$

Since $J_1(z) \to +\infty$ as $z \to 0^+$, we have that if a is close to zero, then $A_{\widetilde{N}} - A_{\widetilde{N}-1}(\widetilde{w}) > 0$, in contradiction to the minimality of $\widetilde{u}^i$. We actually have more: since $J_1(a\gamma) > \frac{k_2}{\delta_1^6}$ for all $a < a_1$ with

$$a_1 := \left(\frac{\sqrt{3}-1}{2} \frac{1+2^{-6}}{1+2^{-12}} \right)^{\frac{1}{6}},$$

we have that $\widetilde{w}^i$ has an energy strictly smaller than $A_{\widetilde{N}}$ at least for all $a < a_1$. Therefore we can assume that $a \geq a_1$ in the case $\widetilde{N} \geq 2$.

Now, if $\widetilde{N} = 1$, the minimising sequence $(\widetilde{u}^i)$ reads

$$\widetilde{u}^i = \begin{cases} 0 & \text{if } i = 0, \\ a\gamma + \gamma(i-1) & \text{if } i \geq 1, \end{cases}$$

whose energy is denoted by A_1. We consider the competitor $\widetilde{w} : \mathbb{N} \to \mathbb{R}$ defined as $\widetilde{w}^i = \gamma i$ and denote its energy by $A_0(\widetilde{w})$. Then

$$A_1 - A_0(\widetilde{w}) = J_1(a\gamma) + J_1((a+1)\gamma) - J_1(\gamma) - J_1(2\gamma) J_1(a\gamma) - \frac{k_2}{2\delta_1^6}, \tag{5.7}$$

where the inequality follows by a similar reasoning as above. Since estimate (5.7) implies estimate (5.6), the properties deduced from the latter also hold for $\widetilde{N} = 1$. Thus $a \geq a_1$ for all $\widetilde{N} \geq 1$.

Summarising, we can restrict to the case of slope $a\gamma$ for $a \geq a_1$ and $a \neq 1$. We finally prove that the function $f(\delta)$ defined in (5.5) is strictly positive for some $\delta \neq 0$. In order to show this we observe that $f(0) = 0$ and then show that $f'(0) \neq 0$ for every admissible a. As in the proof of Proposition 5.4 this allows to deduce that there exists a δ close to 0 but different from 0, such that $f(\delta) > 0$ and hence the assertion. Since

$$f'(\delta) = -J_1'((a+1)\gamma + \delta) + J_1'(\gamma - \delta) - J_1'(\gamma + \delta) + J_1'(2\gamma - \delta),$$

we have $f'(0) = -J_1'((a+1)\gamma) + J_1'(2\gamma) =: g(a)$. Therefore the claim reduces to describing the zero-set of the function g and proving that it does not intersect the set of admissible a's. Observe that $g'(a) = -\gamma J_1''((a+1)\gamma)$ is positive if and only if $a > \left(\frac{13}{7} \frac{1+2^{-6}}{1+2^{-12}}\right)^{\frac{1}{6}} - 1 := a_0$. Therefore, since $a_0 < a_1$, the function g is strictly increasing for $a \geq a_1$. Since $a_1 < 1$ and $g(1) = 0$, we deduce that $a = 1$ is the only zero of g in the interval $a \geq a_1$. Hence g does not have any zeros which are admissible. Thus the assertion follows. □

By Lemma 5.1 *(2)* we know $B_b(\gamma) = B(\gamma)$. Hence if J_1 and J_2 are Lennard-Jones potentials as defined in (4.4), then the infimum in $B_b(\gamma)$ is obtained for $k \to \infty$. On the contrary, as noted in Remark 5.2, $B_b(\delta_1)$ is attained for $k = 0$. Furthermore, recall that for the boundary layer energy related to the elastic behaviour at the boundary, cf. (4.29), we show in the derivation of (4.26) that: If $\theta = \gamma$, then $B(\gamma, \gamma) = \frac{1}{2} J_1(\gamma)$ is attained for $N = 0$.

Finally we discuss the "depth" of boundary layers and the occurrence of cracks on a mesoscopic scale. Here, this is a rather abstract scale between the atomistic and the continuum scale. To illustrate this, we consider the following situation: imagine there are two bodies being in contact on the continuum scale, but being a distance apart on the atomistic scale. Now, if we let the microscopic distance between the bodies tend to infinity while keeping the bodies in contact on the macroscopic scale, we speak about the mesoscopic scale. This setting is analysed extensively in the context of magnetic bodies in [SS09] and led to a thorough understanding of some formulae describing magnetic forces.
In the context of this paper a similar situation occurs in the following sense: in Proposition 5.5 we prove that the infimum in $B(\gamma)$ is obtained for $N \to \infty$ in the case of Lennard-Jones potentials. That is, the slope of the optimal test function is constantly γ only for $N \to \infty$. On the other hand we know by the compactness result, Proposition 4.2, that the slope of the deformation u is γ almost everywhere in the continuum limit, i.e., on the macroscopic scale. Consider for instance Figure 5 on the macroscopic scale: the slope of the deformation equals γ everywhere except at the jump point, while it takes infinitely many atoms away from the crack until the deformation reaches its equilibrium slope in the microscopic/mesoscopic scale.
As outlined above, a similar situation occurs for the boundary layer energies at the boundaries of $[0, 1]$. Let us for instance consider the situation of Figure 4 with $u_0^{(1)} = \gamma$. Then the infimum in $B_b(\gamma)$ is obtained for $k \to \infty$, i.e., the crack in the atomistic setting is not close to zero but infinitely far apart though the jump in the continuum setting is at 0. This allows for the following interpretation: though macroscopically the crack is at the boundary, the crack occurs in the interior on a mesoscopic scale. Further discussions of this will be the topic of future research.

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