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TOWARDS UNIFORMLY Γ-EQUIVALENT THEORIES FOR NONCONVEX DISCRETE SYSTEMS

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Abstract. In this paper we consider a one-dimensional chain of atoms which interact through nearest and next-to-nearest neighbour interactions of Lennard-Jones type. We impose four Dirichlet boundary conditions, in the sense that we prescribe the deformations of the first two atoms and of the last two ones. We are interested in a good approximation of the energy functional of this system for a large number of atoms. We show that the canonical Γ-development does not provide an accurate description close to the threshold between the elastic regime and fracture. To overcome this drawback, we perform some preliminary analysis which helps to construct a uniformly Γ-equivalent approximation as introduced by Braides and Truskinovsky. More precisely, we provide a Γ-convergence result for some rescaled energy. This yields an example of a uniformly Γ-equivalent approximation at first order.

1. **Introduction.** With this paper we want to contribute to finding a good mathematical model for the behaviour of a brittle body subject to a boundary deformation. The starting point of our analysis is a discrete model, which we regard as the exact model. Since the discrete model fails to be applicable when the number of atoms in the system is too large, we seek for a suitable approximation of the discrete model by performing a continuum limit. We will focus on the Γ-convergence approach, which provides a rigorous way of performing this discrete-to-continuum derivation (see [6] and [8] for a comprehensive introduction on the topic).

The standard way in which the limiting process is performed is to get rid of the discrete parameter describing the interatomic distance by letting it vanish. This corresponds to an increasing number of interacting particles, for which a continuum model is expected to be a good approximation. This is indeed true for some systems, as for instance in a purely linearly elastic material, for which the Γ-limit provides a sufficiently rich model. Unfortunately this is not always the case:

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There are effects like crack opening, where the scale separation is broken and better approximations are needed, cf. e.g. [2], [3], [4], [9], [12], [13], as the Γ-limit fails to capture the main features of the discrete model.

In this paper we provide some preliminary steps for the derivation of so-called *uniformly Γ-equivalent theories* as introduced by Braides and Truskinvosky [7]. In the quoted paper they apply their method to a series of examples coming from different fields and in particular in the context of a one-dimensional chain of atoms with Lennard-Jones interactions between nearest neighbours, cf. [7, Example 8.5]. Here we generalize that one-dimensional model to incorporate also boundary layer effects, which are present in fracture mechanics. We started to study this model in [11].

We consider a one-dimensional chain of $n+1$ atoms subject to nearest and next-to-nearest neighbour interactions modeled by the Lennard-Jones type potentials J_1 and J_2, see Section 2. We impose four Dirichlet boundary conditions, in the sense that we prescribe the deformation u from the reference configuration of the first two atoms and of the last two ones of the chain. Accordingly, the energy in the atomistic setting is given by

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

where $\lambda_n = \frac{1}{n}$ denotes the interatomic distance in the reference configuration, and $\ell > 0$ is the deformation of the last atom of the chain. We notice that the discrete functionals H_n^ℓ depend on two parameters: the discrete parameter λ_n and the continuum parameter ℓ, which describes the relative elongation of the chain.

It has been already observed in the context of fracture mechanics [13] that a physically meaningful model (in the continuum setting) must keep the presence of the small parameter λ_n in order to ensure that a crack opens at finite (and not infinitesimal) tension. Hence a natural idea is to consider a Γ-development [1] of the discrete functionals H_n^ℓ. In [11] we computed the Γ-limit and the first order Γ-limit recalled in Section 3 below. These limits represent the bulk part and the surface part of the energy in the continuum model, respectively, where some boundary layer energy terms show up due to the imposition of the first and last slope in the discrete setting.

If we consider the Γ-expansion of the discrete functional up to first order in λ_n and we regard it as a function of the parameter ℓ, we notice though that it exhibits a discontinuity for a special value of the parameter ℓ, namely $\ell = \gamma$, where γ is the minimum point of the Γ-limit of H_n^ℓ (see Section 4 for details). More precisely, $\ell = \gamma$ represents a threshold between the elastic regime ($\ell < \gamma$), and the regime $\ell > \gamma$ in which the chain experiences the opening of a crack. Therefore, according to [7] we aim to construct a uniformly Γ-equivalent approximation, overcoming the drawback of the Γ-development formal approach near γ, see Section 5.

The new idea developed in [7] is to construct a functional which matches the asymptotic expansion for $\ell < \gamma$ with the asymptotic expansion for $\ell > \gamma$ along a curve in the plane (ℓ_n, λ_n), sufficiently close to γ. This is achieved by performing a suitable change of variables in the discrete functional providing the first order Γ-limit and then computing the Γ-limit of this discrete functional in the new variables. The change of variables is chosen in such a way that the separation of scales between bulk and surface contributions to the energy drops. The relevant change of variables is $u = \gamma t + \sqrt{\lambda_n} v$ and was already identified in [13]. Braides, Lew and Ortiz [5] computed the Γ-limit of the functional in the new variables for periodic boundary conditions. As it becomes evident below, it is not possible to apply directly their result in the present model due to the additional boundary conditions we impose.
In Section 6 we compute the Γ-limit in the new variables for our boundary conditions, which provides an elastic integral contribution as in [5] and boundary layer energies as in [11]. This Γ-limit, after pulling back the variable, also represents a good approximation of the discrete functional near γ. This allows us to construct a uniform Γ-equivalent functional by matching the Γ-expansion near γ with the regular Γ-expansions outside this point, cf. Section 5.

2. **Setting of the problem.**

The setting of the problem is as in our paper [11]. We recall here the notation as well as those results which we will apply in the following sections.

We consider a one-dimensional chain of $n+1$ atoms in $[0, 1]$, cf. Figure 1. Later we will let n tend to ∞. We denote the distance between two consecutive atoms by $\lambda_n = \frac{1}{n}$ and the deformation from the reference configuration $\lambda_n\mathbb{Z} \cap [0, 1]$ by a function $u : \lambda_n\mathbb{Z} \cap [0, 1] \to \mathbb{R}$. We write u^i as short for $u(i\lambda_n)$. Note that we similarly write $v^i = v(i)$ for a function $v : \mathbb{Z} \to \mathbb{R}$.

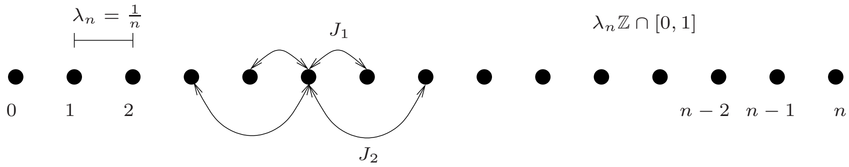

FIGURE 1. A chain of $n+1$ atoms.

Furthermore we identify the functions $u : \lambda_n\mathbb{Z}\cap[0,1] \to \mathbb{R}$ with their piecewise affine interpolations and set

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

As in [11] we impose the following boundary conditions for given ℓ, $u_0^{(1)}$, $u_1^{(1)} > 0$

$$\begin{aligned} &u(0) = u^0 = 0, && u(1) = u^n = \ell,\\ &u(\lambda_n) = u^1 = \lambda_n u_0^{(1)}, && u(1-\lambda_n) = u^{n-1} = \ell - \lambda_n u_1^{(1)}. \end{aligned} \tag{2.1}$$

Next we list all the mathematical assumptions needed in this work. We assume that the nearest neighbours as well as the next-to-nearest neighbours interact through potentials of Lennard-Jones type defined below. Let $J_1, J_2 : \mathbb{R} \to (-\infty, +\infty]$ be functions. The effective potential is defined as

$$J_0(z) = J_2(z) + \frac{1}{2}\inf\{J_1(z_1) + J_1(z_2) : z_1 + z_2 = 2z\}, \qquad z \in \mathbb{R}. \tag{2.2}$$

We say that J_1, J_2 are *Lennard-Jones type potentials* if the following conditions are satisfied:
[$H1$] Strict convexity of J_0 in its convexity points;
[$H2$] Uniqueness of minimal energy configurations at convexity points of J_0, i.e.,

$$J_0(z) = J_1(z) + J_2(z) \quad \text{for every } z \in \mathbb{R} \text{ such that } J_0(z) = J_0^{**}(z); \tag{2.3}$$

[$H3$] Regularity and behaviour at $+\infty$. $J_1, J_2 : \mathbb{R} \to (-\infty, +\infty]$ be C^2 on their domains, i.e., on $\{z \in \mathbb{R} \ : \ J_j(z) < +\infty\}$, $j = 1, 2$, and such that $J_0 \in C^2$ 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.

(a) There exist a convex function $\Psi : \mathbb{R} \to [0, +\infty]$, superlinear at $-\infty$, and constants $c_1^j, c_2^j > 0$ for $j = 1, 2$ such that

$$c_1^j(\Psi(z) - 1) \le J_j(z) \le c_2^j \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}, \quad j = 1, 2. \tag{2.4}$$

(b) 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 denoted by γ.

(c) $J_0(+\infty) > J_0(\gamma)$.

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

For instance the assumptions [$H1$]–[$H5$] are satisfied by the classical Lennard-Jones potentials as well as the so-called Morse-potentials, see [11, Remark 4.1] for details. We remark that in the results from [11] quoted below we used the weaker assumption J_1, J_2 in $C^{1,\alpha}$, $0 < \alpha \le 1$, on their domains, and such that $J_0 \in C^1$ on its domain.

In order to define the discrete energy, we choose the space of admissible deformations. To incorporate the boundary conditions in the energy functional, we define for given ℓ, $u_0^{(1)}$, $u_1^{(1)} > 0$, the following subspace of $\mathcal{A}_n(0,1)$:

$$\mathcal{A}_n^\ell(0,1) := \big\{u \in \mathcal{A}_n(0,1) : u^0 = 0, u^1 = \lambda_n u_0^{(1)}, u^{n-1} = \ell - \lambda_n u_1^{(1)}, u^n = \ell\big\}. \tag{2.5}$$

Given all this, the energy of the discrete system reads as

$$H_n^\ell(u) = \begin{cases} H_n(u) & \text{if } u \in \mathcal{A}_n^\ell(0,1),\\ +\infty & \text{else in } \mathcal{A}_n(0,1), \end{cases} \tag{2.6}$$

where

$$H_n(u) = \sum_{i=0}^{n-1} \lambda_n J_1\left(\frac{u^{i+1} - u^i}{\lambda_n}\right) + \sum_{i=0}^{n-2} \lambda_n J_2\left(\frac{u^{i+2} - u^i}{2\lambda_n}\right). \tag{2.7}$$

Finally we define the function space $BV^\ell(0,1)$ for given $\ell > 0$ as the space of functions u in $BV_{\mathrm{loc}}(\mathbb{R})$ such that $u = 0$ on $(-\infty, 0)$ and $u = \ell$ on $(1, +\infty)$. Similarly we define the space of special functions with bounded variation $SBV^\ell(0,1)$. Moreover, we denote by S_u the jump set of $u \in BV^\ell(0,1)$ and for $t \in S_u$ we set $[u(t)] = u(t^+) - u(t^-)$. In the case $\ell > \gamma$ we also use the notation

$$SBV_c^\ell(0,1) = \left\{u \in SBV^\ell(0,1) : 0 < \#S_u < +\infty;\ [u] > 0 \text{ on } S_u;\ u' = \gamma \text{ a.e.}\right\}.$$

3. **The Γ-limit and the first order Γ-limit of the discrete energy.** For later reference we recall the Γ-limit and the first order Γ-limits of the discrete energy, which we derived in [11]. The Γ-limit yields the effective bulk energy of the system.

Theorem 3.1 ([11, Theorem 3.1]). *Let $J_1, J_2 : \mathbb{R} \to (-\infty, +\infty]$ be Borel functions bounded from below such that $[H4](a)$ is satisfied and 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*

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

on $L^1(0,1)$, where J_0^{**} denotes the convexification of the effective potential J_0 defined in (2.2).

Moreover by Jensen's inequality

$$\min_u H^\ell(u) = J_0^{**}(\ell) = \begin{cases} J_0(\ell) & \text{if } \ell \le \gamma, \\ J_0(\gamma) & \text{if } \ell > \gamma. \end{cases} \tag{3.1}$$

By definition, the first order Γ-limit of H_n^ℓ is the Γ-limit of the functional $H_{1,n}^\ell$ given by

$$H_{1,n}^\ell(u) = \frac{H_n^\ell(u) - \min_u H^\ell(u)}{\lambda_n}. \tag{3.2}$$

The first order Γ-limit involves some boundary layer energies due to the imposed Dirichlet boundary conditions and due to the opening of a crack, at the boundary of the newly created surface.

In the parameter range $0 < \ell \le \gamma$ the chain does not experience the formation of a fracture and only elastic boundary layers are present in the first order Γ-limit. The elastic boundary layer energy is defined in [11, Eqn. (4.13)], for any $0 < \ell \le \gamma$ and $\theta > 0$, by

$$\begin{aligned} B(\theta, \ell) = \inf_{N \in \mathbb{N}} \min \Bigg\{ & \frac{1}{2} J_1\left(w^1 - w^0\right) + \sum_{i \ge 0} \Bigg\{ J_2\left(\frac{w^{i+2} - w^i}{2}\right) \\ & + \frac{1}{2}\left(J_1\left(w^{i+2} - w^{i+1}\right) + J_1\left(w^{i+1} - w^i\right)\right) - J_0(\ell) - J_0'(\ell)\left(\frac{w^{i+2} - w^i}{2} - \ell\right)\Bigg\} : \\ & w : \mathbb{N} \to \mathbb{R}, w^0 = 0, w^1 - w^0 = w^1 = \theta, w^{i+1} - w^i = \ell \text{ if } i \ge N \Bigg\}. \end{aligned} \tag{3.3}$$

Here the parameter θ is a microscopic parameter; it will be related to the boundary conditions $u_0^{(1)}$ and $u_1^{(1)}$ on the second and last but one atoms.

Theorem 3.2 ([11, Theorem 4.3]). *Suppose that hypotheses $[H1] - [H5]$ hold and let $0 < \ell \le \gamma$ and $u_0^{(1)}$, $u_1^{(1)} > 0$. Then $H_{1,n}^\ell$ Γ-converges with respect to the L^∞-topology to the functional H_1^ℓ 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 the parameter range $\ell > \gamma$ the chain of atoms experiences the opening of a crack, which can be located in the interior or at the boundary of the chain.

In the case of an internal jump, the following boundary layer energy occurs on both sides of the newly created free surface, see [2] and also [11, Eqn. (4.28)],

$$\begin{aligned} B(\gamma) = \inf_{N\in\mathbb{N}} \min \Bigg\{ \frac{1}{2} J_1\left(\widetilde{w}^1 - \widetilde{w}^0\right) + \sum_{i\geq 0} \Bigg\{ J_2\left(\frac{\widetilde{w}^{i+2}-\widetilde{w}^i}{2}\right) \\ + \frac{1}{2}\left(J_1\left(\widetilde{w}^{i+2}-\widetilde{w}^{i+1}\right) + J_1\left(\widetilde{w}^{i+1}-\widetilde{w}^i\right)\right) - J_0(\gamma)\Bigg\} : \\ \widetilde{w}:\mathbb{N}\to\mathbb{R}, \widetilde{w}^0 = 0, \widetilde{w}^{i+1}-\widetilde{w}^i = \gamma \text{ if } i \geq N\Bigg\}. \end{aligned} \tag{3.4}$$

If the jump occurs at the boundary of the chain, then the boundary layer energy on the two sides of the crack is different, due to the Dirichlet boundary conditions. More precisely, the boundary layer energy at the free surface is exactly $B(\gamma)$ defined in (3.4); on the side of the crack where the boundary condition is imposed, the boundary layer energy is defined as (see [11, Eqn. (4.27)])

$$\begin{aligned} B_b(\theta) = \inf_{k\in\mathbb{N}} \min \Bigg\{ \frac{1}{2} J_1\left(\widehat{w}^1 - \widehat{w}^0\right) + \sum_{i=0}^{k-1} \Bigg\{ J_2\left(\frac{\widehat{w}^{i+2}-\widehat{w}^i}{2}\right) \\ + \frac{1}{2}\left(J_1\left(\widehat{w}^{i+2}-\widehat{w}^{i+1}\right) + J_1\left(\widehat{w}^{i+1}-\widehat{w}^i\right)\right) - J_0(\gamma)\Bigg\} : \\ \widehat{w}:\mathbb{N}\to\mathbb{R}, \widehat{w}^{k+1} = 0, \widehat{w}^{k+1}-\widehat{w}^k = -\widehat{w}^k = \theta\Bigg\}. \end{aligned} \tag{3.5}$$

Furthermore, the elastic boundary layer energies at those ends of the chain where there is no crack are defined as follows (see [11, Eqn. (4.29)]). For $\theta > 0$,

$$\begin{aligned} B(\theta,\gamma) = \inf_{N\in\mathbb{N}} \min \Bigg\{ \frac{1}{2} J_1\left(w^1 - w^0\right) + \sum_{i\geq 0} \Bigg\{ J_2\left(\frac{w^{i+2}-w^i}{2}\right) \\ + \frac{1}{2}\left(J_1\left(w^{i+2}-w^{i+1}\right) + J_1\left(w^{i+1}-w^i\right)\right) - J_0(\gamma)\Bigg\} : \\ w:\mathbb{N}\to\mathbb{R}, w^0 = 0, w^1 - w^0 = w^1 = \theta, w^{i+1}-w^i = \gamma \text{ if } i \geq N\Bigg\}. \end{aligned} \tag{3.6}$$

Note that (3.6) equals (3.3) at $\ell = \gamma$.

The first order Γ-limit for $\ell > \gamma$ reads as follows:

Theorem 3.3 ([11, 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*

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

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

$$B_{BJ}(\theta) = \frac{1}{2}J_1(\theta) + B_b(\theta) + B(\gamma) - 2J_0(\gamma) \tag{3.7}$$

and

$$B_{IJ} = 2B(\gamma) - 2J_0(\gamma). \tag{3.8}$$

4. **Non-accuracy of the expansion.** In the present section we discuss the continuity of the minima of the Γ-limit and of the first order Γ-limit of the discrete functional H_n^ℓ with respect to the dependence on the parameter ℓ.

We recall that the minimum of the Γ-limit H^ℓ is $m^{(0)}(\ell) := \min H^\ell = J_0^{**}(\ell)$, see (3.1). We remark that for $\ell \leq \gamma$ the only minimizer of H^ℓ is the continuous function $u_\ell(t) = \ell t$, $t \in [0,1]$, while for $\ell > \gamma$ all the functions $u \in SBV_c^\ell(0,1)$ are admissible minimizers of H^ℓ.

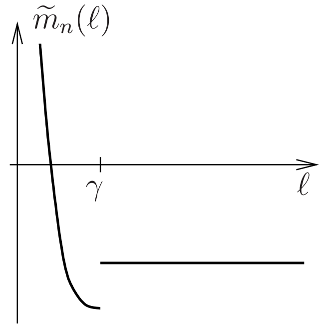

FIGURE 2. Discontinuity of the minimum values $\widetilde{m}_n(\ell) := m^{(0)}(\ell) + \lambda_n m^{(1)}(\ell)$.

By Theorems 3.2 and 3.3, the minimum of the first order Γ-limit H_1^ℓ is

$$m^{(1)}(\ell) := \min H_1^\ell = \begin{cases} B\left(u_0^{(1)}, \ell\right) + B\left(u_1^{(1)}, \ell\right) - J_0(\ell) - J_0'(\ell)\left(\frac{u_0^{(1)}+u_1^{(1)}}{2} - \ell\right) & \text{if } \ell \le \gamma, \\ B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) + \beta_{\min} & \text{if } \ell > \gamma, \end{cases}$$

where

$$\beta_{\min} := \min\{\beta_0, \beta_1, \beta_{\text{int}}\} \tag{4.1}$$

with

$$\beta_0 := B_{BJ}\left(u_0^{(1)}\right) - B\left(u_0^{(1)}, \gamma\right), \quad \beta_1 := B_{BJ}\left(u_0^{(1)}\right) - B\left(u_1^{(1)}, \gamma\right), \quad \text{and} \quad \beta_{\text{int}} := B_{IJ}. \tag{4.2}$$

Also for the first order Γ-limit the only minimizer of H_1^ℓ for $\ell \le \gamma$ is the continuous function $u_\ell(t) = \ell t$, $t \in [0,1]$. For $\ell > \gamma$ the minimizers of H_1^ℓ have only one jump point. The location of the jump depends on $\beta_{\min}$: The jump is at $t = 0$ if $\beta_{\min} = \beta_0$, at $t = 1$ if $\beta_{\min} = \beta_1$ and at some $t \in]0,1[$ if $\beta_{\min} = \beta_{\text{int}}$; see [11, Theorem 5.3] for a discussion concerning the location of fracture.

The approximation of the minimum value $m_n(\ell)$ of the functional H_n^ℓ up to the first order in terms of $m^{(0)}(\ell)$ and $m^{(1)}(\ell)$ is given by

$$m_n(\ell) \simeq m^{(0)}(\ell) + \lambda_n m^{(1)}(\ell).$$

It is immediate to notice that, while the left-hand side is continuous with respect to ℓ, the right-hand side exhibits a discontinuity at the point $\ell = \gamma$, cf. Figure 2. Indeed,

$$m^{(0)}(\gamma^-) + \lambda_n m^{(1)}(\gamma^-) = J_0(\gamma) + \lambda_n\left(B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma)\right),$$
$$m^{(0)}(\gamma^+) + \lambda_n m^{(1)}(\gamma^+) = J_0(\gamma) + \lambda_n\left(B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) + \beta_{\min}\right),$$

so that we have for the jump of $m^{(0)} + \lambda_n m^{(1)}$ at γ

$$\left[m^{(0)} + \lambda_n m^{(1)}\right](\gamma) = \lambda_n \beta_{\min}. \tag{4.3}$$

As equation (4.3) shows, close to γ, the error in the approximation of $m_n(\ell)$ via the asymptotic expansion (up to first order in λ_n) is of the same order as the approximation itself. This proves the non-accuracy of the canonical Γ-development close to the point $\ell = \gamma$. The physical reason for this is that at $\ell = \gamma$ a crack is opened. Such a crack is of the order of λ_n and thus breaks the separation of scales needed for a correct Γ-development. In the next section we overcome this drawback by introducing a uniformly Γ-equivalent functional.

5. **Uniformly Γ-equivalent energy functionals.** Following the method presented by Braides and Truskinovsky in [7], we aim to construct an approximation of the discrete functional H_n^ℓ which is uniformly equivalent to H_n^ℓ in the sense of Γ-convergence. This then implies in particular that the minima are continuous with respect to ℓ, i.e., also at $\ell = \gamma$. More precisely we define, as in [7, Definition 6.3],

Definition 5.1. Two families of functionals H_n^ℓ and G_n^ℓ are *uniformly* Γ*-equivalent at order* λ_n^p *(for* $p \geq 0$*) at* $\ell_0 > 0$ if there exist translations m_n^ℓ such that for all $\lambda_{n_j} \xrightarrow{j\to\infty} 0$ and all $\ell_j \xrightarrow{j\to\infty} \ell_0$ the following equation holds upon extraction of a subsequence

$$\Gamma - \lim_{j\to\infty} \frac{H_{n_j}^{\ell_j} - m_{n_j}^{\ell_j}}{\lambda_{n_j}^p} = \Gamma - \lim_{j\to\infty} \frac{G_{n_j}^{\ell_j} - m_{n_j}^{\ell_j}}{\lambda_{n_j}^p},$$

and these Γ-limits are not trivial. We call two families H_n^ℓ and G_n^ℓ *uniformly* Γ*-equivalent at order* λ_n^p (or uniformly Γ-equivalent *at p-th order*) if they are uniformly Γ-equivalent at order λ_n^p at ℓ_0 for all $\ell_0 > 0$.

In what follows we will consider the case $p = 1$, and we will construct a functional Γ-equivalent to H_n^ℓ at first order. In future work we intend to derive an equivalent theory both at zeroth order (i.e. at order $\lambda_n^0 = 1$, which means that the Γ-limits of the functionals are the same) and at first order. By [7, Theorem 6.4], if H_n^ℓ and G_n^ℓ are uniformly coercive and uniformly Γ-equivalent at order λ_n, there holds that

$$\sup_{\ell>0} \left| \inf_u G_n^\ell(u) - \inf_u H_n^\ell(u) \right| = o(\lambda_n).$$

According to the theory developed in [7] the points $\ell \neq \gamma$ are *regular* points for the functional H_n^ℓ at order $\lambda_n^0 = 1$ and order λ_n. Further, γ is a regular point at order $\lambda_n^0 = 1$, while γ is a *singular* point at order λ_n, since the function $\ell \mapsto m^{(0)}(\ell) + \lambda_n m^{(1)}(\ell)$ is discontinuous at $\ell = \gamma$.

Following [7, Definition 8.3], the *table* of first order Γ-limits of H_n^ℓ at γ is given by all the sequences ℓ_n with $\ell_n \to \gamma$ and the functionals

$$H^{(1)}_{(\lambda_n,\ell_n)} := \Gamma - \lim_{n\to\infty} \frac{H_n^{\ell_n} - \min_u H^\gamma(u)}{\lambda_n} = \Gamma - \lim_{n\to\infty} \frac{H_n^{\ell_n} - J_0(\gamma)}{\lambda_n}. \tag{5.1}$$

This gives a list of different limiting behaviours of the energy functional in the vicinity of $\ell = \gamma$ depending on the rate at which the sequence ℓ_n converges to γ. Notice that $H^{(1)}_{(\lambda_n,\ell_n)}(u)$ does not depend on n; the notation indicates the chosen sequences.

Since the discontinuity appears when a crack opens, we focus on the fracture regime, that is we consider $\ell_n > \gamma$. Moreover, we will perform a blow-up analysis for the functional close to the singular point γ by considering a suitable change of variables in $H^{(1)}_{(\lambda_n,\ell_n)}$ and by computing the Γ-limit of the functional in the new variables (see Theorem 6.1). More precisely, we will consider the change of variables

$$v^i := \frac{u^i - \lambda_n \gamma i}{\sqrt{\lambda_n}}, \quad i = 1, \dots, n,$$

which follows by scaling the bulk and surface energies in the same way, cf. [13] and see also Section 6 below. For another motivation, related to some renormalization group arguments, we refer to [5, 10]. Then, by (5.1), (2.7) and applying the convergence of the minima implied by Γ-convergence (see e.g. [6, Theorem 1.21]),

$$\begin{aligned}
\min_u H^{(1)}_{(\lambda_n,\ell_n)}(u) &= \lim_{n\to\infty} \min \left\{ \frac{H_n^{\ell_n}(u) - J_0(\gamma)}{\lambda_n} : u \in \mathcal{A}_n^{\ell_n} \right\} \\
&= \lim_{n\to\infty} \min_u \left\{ \sum_{i=0}^{n-1} J_1\left(\frac{u^{i+1} - u^i}{\lambda_n}\right) + \sum_{i=0}^{n-2} J_2\left(\frac{u^{i+2} - u^i}{2\lambda_n}\right) - \frac{J_0(\gamma)}{\lambda_n} : u \in \mathcal{A}_n^{\ell_n} \right\} \\
&= \lim_{n\to\infty} \min_v \left\{ \sum_{i=0}^{n-1} J_1\left(\frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \gamma\right) + \sum_{i=0}^{n-2} J_2\left(\frac{v^{i+2} - v^i}{2\sqrt{\lambda_n}} + \gamma\right) - \frac{J_0(\gamma)}{\lambda_n} : \right. \\
&\qquad \left. v^0 = 0,\, v^1 = \sqrt{\lambda_n}\left(u_0^{(1)} - \gamma\right),\, v^{n-1} = \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} - \sqrt{\lambda_n}\left(u_1^{(1)} - \gamma\right),\, v^n = \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} \right\}.
\end{aligned}$$

Next consider $\ell_n > \gamma$ with $\ell_n \to \gamma$ and such that $\frac{\ell_n - \gamma}{\sqrt{\lambda_n}}$ converges to some value $\delta \geq 0$. Then, by using the notation in (6.3), $\min_u H^{(1)}_{(\lambda_n,\ell_n)}(u) = \lim_{n\to\infty} \min_v E_n(v)$. At this point we apply our Γ-convergence result for E_n in the rescaled variable v and we obtain a limiting functional E_0

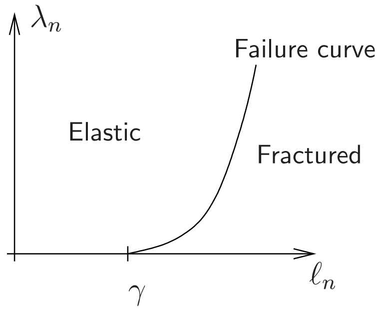

FIGURE 3. The threshold between elastic behaviour and fracture.

(see Theorem 6.1). This yields, by the convergence of the minima for Γ-converging functionals,

$$\begin{aligned}\min_u H^{(1)}_{(\lambda_n,\ell_n)}(u) &= \min_v \{E_0(v) : v(0)=0, v(1)=\delta\}\\ &= \min\left\{\alpha\delta^2,\, \beta_{\min}\right\} + B\left(u_0^{(1)},\gamma\right) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma)\\ &= \lim_{n\to\infty}\min\left\{\alpha\,\frac{(\ell_n-\gamma)^2}{\lambda_n},\, \beta_{\min}\right\} + B\left(u_0^{(1)},\gamma\right) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma)\end{aligned}$$

with $\alpha := \frac{1}{2}J_0''(\gamma)$ and $\beta_{\min}$ as in (4.1). We notice that via the functional E_0 we obtained the required matching property close to γ. Indeed, if

$$\min\left\{\alpha\,\frac{(\ell_n-\gamma)^2}{\lambda_n},\, \beta_{\min}\right\} = \alpha\,\frac{(\ell_n-\gamma)^2}{\lambda_n}$$

then we are in the regime of *elasticity*, i.e., the minimizer is the continuous function $v(t) = \frac{\ell_n-\gamma}{\sqrt{\lambda_n}}t$, while if

$$\min\left\{\alpha\,\frac{(\ell_n-\gamma)^2}{\lambda_n},\, \beta_{\min}\right\} = \beta_{\min}$$

we are in the regime of *fracture*, i.e., the minimizers have one jump point. Therefore, the transition between *elasticity* and *fracture* depends on the rate of convergence of ℓ_n to γ with respect to λ_n. The border between these two regions is given by a curve in the (ℓ_n,λ_n)-plane for $\ell_n > \gamma$, see Figure 3. This suggests that the matching between the approximations for $\ell < \gamma$ and $\ell > \gamma$ should be done along the curve $\ell_n = \gamma + \sqrt{\lambda_n\frac{\beta_{\min}}{\alpha}}$. Moreover, the functional providing such a matching will be E_0, computed in the u-variables. To this end we need to *pull-back* the variables, which we do via the change of variables in the continuum $u(t) = \gamma t + \sqrt{\lambda_n}v(t)$; note that this corresponds to the change of variables $v^i := \frac{u^i-\lambda_n\gamma i}{\sqrt{\lambda_n}}$ in the discrete, that we performed before. In the variables u, the functional $E_0(v)$ in Theorem 6.1 reads

$$\begin{aligned}\widetilde{E}_0(u) := E_0(v(u)) =& \frac{\alpha}{\lambda_n}\int_0^1 |u'-\gamma|^2 dt + B\big(u_0^{(1)},\gamma\big) + B\big(u_1^{(1)},\gamma\big) - J_0(\gamma)\\ &+ \beta_0\#(S_u\cap\{0\}) + \beta_1\#(S_u\cap\{1\}) + \beta_{\mathrm{int}}\#(S_u\cap(0,1)).\end{aligned}\tag{5.2}$$

Knowing this, we are in a position to define a functional G_n^ℓ which is a uniformly Γ-equivalent functional at order λ_n to H_n^ℓ. Since we are only interested in the equivalence at first order, the functional G_n^ℓ will be defined on the domain of the functional H_1^ℓ.

For $\ell \le \gamma$ we define G_n^ℓ as

$$G_n^\ell(u) = \begin{cases} J_0(\ell) + \lambda_n\Big(B\big(u_0^{(1)},\ell\big) + B\big(u_1^{(1)},\ell\big) - J_0(\ell)\Big) & \\ -\lambda_n J_0'(\ell)\Big(\frac{u_0^{(1)}+u_1^{(1)}}{2} - \ell\Big) & \text{if } u = \ell t\\ +\infty & \text{else.}\end{cases}$$

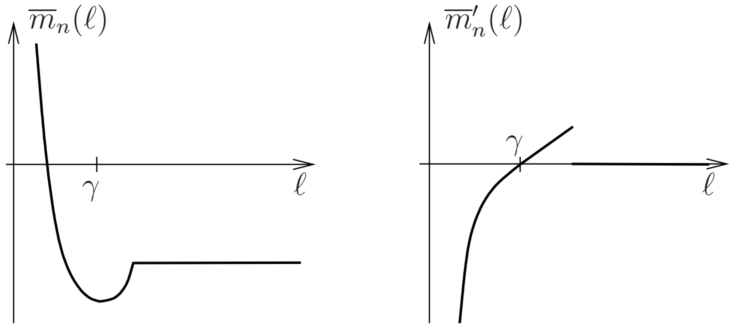

FIGURE 4. Continuity of the minimum values $\overline{m}_n(\ell) = \min_u G_n^\ell(u)$ of the uniformly Γ-equivalent theory G_n^ℓ.

For $\ell > \gamma$, taking into account (5.2), we define G_n^ℓ as

$$G_n^\ell(u) = \begin{cases} J_0(\gamma) + \alpha \displaystyle\int_0^1 |u' - \gamma|^2 dt + \lambda_n \Big(B\big(u_0^{(1)}, \gamma\big) + B\big(u_1^{(1)}, \gamma\big) - J_0(\gamma)\Big) & \text{if } u = \ell t \\ +\lambda_n \left(\beta_0 \#(S_u \cap \{0\}) + \beta_1 \#(S_u \cap \{1\}) + \beta_{\text{int}} \#(S_u \cap (0,1))\right) & \text{or } u \in SBV_c^\ell(0,1) \\ +\infty & \text{else.} \end{cases}$$

To show Γ-equivalence we choose $m_n^\ell = \min_u H^\ell(u)$, cf. Definition 5.1. If $\ell \le \gamma$,

$$\frac{G_n^\ell(u) - J_0(\ell)}{\lambda_n} = B\big(u_0^{(1)}, \ell\big) + B\big(u_1^{(1)}, \ell\big) - J_0(\ell) - J_0'(\ell)\left(\frac{u_0^{(1)} + u_1^{(1)}}{2} - \ell\right)$$

if $u = \ell t$ and it is infinity otherwise. This is independent of n and is exactly $H_1^\ell(u)$ for $\ell \le \gamma$ (see Theorem 3.2). Hence the equivalence of G_n^ℓ and H_n^ℓ at first order follows trivially in the case $\ell \le \gamma$. If $\ell > \gamma$ and u is in the domain of G_n^ℓ we have

$$\begin{aligned} \frac{G_n^\ell(u) - J_0(\gamma)}{\lambda_n} &= \frac{\alpha}{\lambda_n} \int_0^1 (u' - \gamma)^2 \, dt + B\big(u_0^{(1)}, \gamma\big) + B\big(u_1^{(1)}, \gamma\big) - J_0(\gamma) \\ &\quad + \beta_0 \#(S_u \cap \{0\}) + \beta_1 \#(S_u \cap \{1\}) + \beta_{\text{int}} \#(S_u \cap (0,1)). \end{aligned}$$

Note that the Γ-limit of this expression is finite only if $u \in SBV_c^\ell(0,1)$ and it equals H_1^ℓ, see Theorem 3.3. This shows that G_n^ℓ is uniformly Γ-equivalent to H_n^ℓ at first order.

Next we prove that $\ell \mapsto \min_u G_n^\ell(u)$ is continuous. If $\ell \le \gamma$,

$$\begin{aligned} \min_u G_n^\ell(u) &= G_n^\ell(u_\ell) \\ &= J_0(\ell) + \lambda_n \left(B\big(u_0^{(1)}, \ell\big) + B\big(u_1^{(1)}, \ell\big) - J_0(\ell) - J_0'(\ell)\left(\frac{u_0^{(1)} + u_1^{(1)}}{2} - \ell\right)\right) \end{aligned}$$

with $u_\ell(t) = \ell t$. If $\ell > \gamma$,

$$\begin{aligned} \min_u G_n^\ell(u) &= \min\left\{ G_n^\ell(u_\ell), \min_{u \in SBV_c^\ell(0,1)} G_n^\ell(u) \right\} \\ &= \min\left\{\alpha(\ell - \gamma)^2, \lambda_n \beta_{\min}\right\} + J_0(\gamma) + \lambda_n \Big(B\big(u_0^{(1)}, \gamma\big) + B\big(u_1^{(1)}, \gamma\big) - J_0(\gamma)\Big). \end{aligned}$$

This gives the continuity of the minimum values, cf. also Figure 4.

We notice that the functional G_n^ℓ provides a *correction* of the asymptotic expansion close to the singular value γ which allows to recover the continuity of the minima. In summary, the functional G_n^ℓ yields an approximation of the system under consideration which illustrates the non-separability of scales in the case of an occuring crack, as indicated by the presence of the parameter λ_n in the model. Furthermore, the model shows crack initiation at finite tension, which is shown in the right plot in Figure 4. Hence the uniformly Γ-equivalent theory G_n^ℓ is a good candidate for an approximation of the original energy of the nonconvex discrete system.

In future work, we intend to provide uniformly Γ-equivalent approximations in the continuum setting, both at zeroth order and first order.

6. **Γ-limit of a rescaled functional.** In the present section we focus on the behaviour of the functional $H_{1,n}^\ell$ defined in (3.2); instead of a fixed ℓ we now study the behaviour for a particular sequence ℓ_n converging to γ at a given rate. According to this rate of convergence we will define a rescaled displacement v obtained from u via a change of variables, and compute the Γ-limit of the functional $H_{1,n}^\ell(u)$ in the v-variable. Clearly, this limiting behaviour will give us information about the first order Γ-limit of the discrete sequence H_n^ℓ close to the critical threshold γ.

More precisely, we now introduce a sequence (ℓ_n) converging to γ such that $\ell_n > \gamma$ and

$$\delta_n := \frac{\ell_n - \gamma}{\sqrt{\lambda_n}} \to \delta \geq 0. \tag{6.1}$$

For fixed $u_0^{(1)}, u_1^{(1)} > 0$, and for $u \in \mathcal{A}_n^{\ell_n}(0,1)$ (see (2.5)), we set $v^i := \frac{u^i - \lambda_n \gamma i}{\sqrt{\lambda_n}}$, for all $i \in \mathbb{N}$. The newly defined functions v belong to the space

$$\hat{\mathcal{A}}_n^{\delta_n}(0,1) := \left\{ v \in \mathcal{A}_n(0,1) : v^0 = 0, v^1 = \sqrt{\lambda_n}(u_0^{(1)} - \gamma), v^{n-1} = \delta_n - \sqrt{\lambda_n}(u_1^{(1)} - \gamma), v^n = \delta_n \right\}. \tag{6.2}$$

We express the functional $H_{1,n}^{\ell_n}$ in terms of the new displacements v and set

$$E_n^{\delta_n}(v) = H_{1,n}^{\ell_n}(u).$$

Moreover, as $E_n^{\delta_n}(v)$ is identically $+\infty$ if $v \notin \hat{\mathcal{A}}_n^{\delta_n}(0,1)$, we can write

$$E_n^{\delta_n}(v) = \begin{cases} E_n(v) & \text{if } v \in \hat{\mathcal{A}}_n^{\delta_n}(0,1), \\ +\infty & \text{else in } \mathcal{A}_n(0,1), \end{cases} \tag{6.3}$$

where, using that $J_0^{**}(\ell_n) = J_0(\gamma)$,

$$E_n(v) := \sum_{i=0}^{n-1} J_1\left(\frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \gamma\right) + \sum_{i=0}^{n-2} J_2\left(\frac{v^{i+2} - v^i}{2\sqrt{\lambda_n}} + \gamma\right) - \frac{1}{\lambda_n} J_0(\gamma). \tag{6.4}$$

We are now in a position to state the main theorem of this paper. This theorem is closely related to Theorem 4 in [5], where periodic and thus different boundary conditions are imposed at the endpoints of the atomic chain. Our Dirichlet boundary conditions yield additional boundary layer contributions at the end points of the chain, which can be dealt with using the methods developed in [11]. However, the elastic integral that shows up in the Γ-limit is the same as in [5] and is derived with analogous methods.

Theorem 6.1. *Assume [H1]–[H4]. Let $u_0^{(1)}, u_1^{(1)} > 0$, $\ell_n > \gamma$, with $\ell_n \to \gamma$ such that formula (6.1) defining δ_n and δ is satisfied. Let $\alpha = \frac{1}{2}J_0''(\gamma)$, and β_0, β_1, $\beta_{\rm int}$ and $\beta_{\min}$ as in (4.2) and (4.1), respectively. Then E_n Γ-converges with respect to the L^1-topology to the functional E_0 defined on piecewise H^1-functions v such that $v(0) = 0$ and $v(1) = \delta$, by*

$$E_0(v) := \begin{cases} \alpha \displaystyle\int_0^1 |v'|^2\, dt + B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) \\ +\beta_0 \#(S_v \cap \{0\}) + \beta_1 \#(S_v \cap \{1\}) + \beta_{\rm int} \#(S_v \cap (0,1)) & \text{if } [v] > 0 \text{ on } S_v, \\ +\infty & \text{else.} \end{cases}$$

Moreover, if $\delta > 0$, the minimum values of E_n converge to

$$\min_v E_0(v) = \min\left\{\alpha\delta^2, \beta_{\min}\right\} + B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma). \tag{6.5}$$

Proof. **Compactness.** Let (v_n) be a sequence with equibounded energy E_n. It is useful to rearrange the terms of the energy $E_n(v_n)$ as follows:

$$E_n(v_n) = \sum_{i=0}^{n-2} \varsigma_n^i + \frac{1}{2} J_1\left(\frac{v_n^1 - v_n^0}{\sqrt{\lambda_n}} + \gamma\right) + \frac{1}{2} J_1\left(\frac{v_n^n - v_n^{n-1}}{\sqrt{\lambda_n}} + \gamma\right) - J_0(\gamma), \tag{6.6}$$

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

$$\varsigma_n^i := J_2\left(\frac{v_n^{i+2} - v_n^i}{2\sqrt{\lambda_n}} + \gamma\right) + \frac{1}{2}J_1\left(\frac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}} + \gamma\right) + \frac{1}{2}J_1\left(\frac{v_n^{i+2} - v_n^{i+1}}{\sqrt{\lambda_n}} + \gamma\right) - J_0(\gamma). \quad (6.7)$$

By assumptions $[H1]$–$[H4]$, as also noticed in [5, Remark 3], the so-called uniform Cauchy-Born hypothesis near the ground state holds. In particular this implies that there exist $\eta > 0$ and $C > 0$ such that

$$\frac{1}{2}J_1(z_1) + \frac{1}{2}J_1(z_2) \geq J_1(z) + C\big(|z_1 - z|^2 + |z_2 - z|^2\big) \quad (6.8)$$

whenever $z_1 + z_2 = 2z$ and $|z_1 - z| + |z_2 - z| + |z - \gamma| < \eta$. Then, by [5, Remark 4], there exist constants K_1, $K_2 > 0$ such that

$$\begin{aligned} \varsigma_n^i &\geq K_1\left\{\left(\tfrac{v_n^{i+2} - v_n^{i+1}}{\sqrt{\lambda_n}}\right)^2 + \left(\tfrac{v_n^{i+1} - v_n^i}{\sqrt{\lambda_n}}\right)^2\right\} \wedge K_2 \\ &\geq \lambda_n K_1 \left(\tfrac{v_n^{i+1} - v_n^i}{\lambda_n}\right)^2 \wedge K_2, \end{aligned} \quad (6.9)$$

where $a \wedge b$ is shorthand for $\min\{a, b\}$. Since J_1 is bounded from below by its (finite) minimum value $J_1(\delta_1)$ and $J_0(\gamma) < +\infty$, we derive that there exists a constant K_3 such that

$$E_n(v_n) \geq \sum_{i=0}^{n-2}\left(\lambda_n K_1 \left(\frac{v_n^{i+1} - v_n^i}{\lambda_n}\right)^2 \wedge K_2\right) + K_3.$$

Therefore the sequence (v_n) is in particular bounded in $L^1(0,1)$, and using also the fact that $\sup_n E_n(v_n) < +\infty$ it follows that, upon a finite set $S \subset [0,1]$, there exists a subsequence of (v_n) weakly converging in $H^1((0,1) \setminus S)$ (cf., e.g., [6, Section 8.3]).

Liminf inequality. Without loss of generality we can assume that there is only one jump point, i.e., $\#S_v = 1$. 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 are similar due to symmetry, we only treat the boundary jump at 0.

Jump at 0. Assume that $S_v = \{0\}$ and let (v_n) be a sequence converging to v in L^1 such that $\sup_n E_n(v_n) < +\infty$. We prove that

$$\liminf_{n\to\infty} E_n(v_n) \geq \alpha \int_0^1 |v'|^2\, dt + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) + B_{BJ}\left(u_0^{(1)}\right), \quad (6.10)$$

where we recall that $B_{BJ}\left(u_0^{(1)}\right) = \frac{1}{2}J_1\left(u_0^{(1)}\right) + B_b\left(u_0^{(1)}\right) + B(\gamma) - 2J_0(\gamma)$, cf. (3.7).

Let S be a finite set such that the sequence (v_n) converges weakly in $H^1((0,1) \setminus S)$ to v, compare the compactness result above. Fix $\varrho > 0$ small (at least $\varrho < \frac{1}{2}$) such that $S \cap [0, \varrho) = \{0\}$. Then in particular the L^2-norm of (v_n') in the interval $(\frac{\varrho}{2}, \varrho)$ is uniformly bounded, and similarly we may assume that $S \cap (1-\varrho, 1-\frac{\varrho}{2}) = \emptyset$ so that the L^2-norm of (v_n') is uniformly bounded in $(1-\varrho, 1-\frac{\varrho}{2})$. A proof by contradiction then yields that there exist $j_n^\varrho, k_n^\varrho \in \mathbb{N}$ such that $\frac{\varrho}{2} \leq \lambda_n(j_n^\varrho + 1) \leq \lambda_n(j_n^\varrho + 2) \leq \varrho$, $\lambda_n j_n^\varrho \to \varrho$, $1 - \varrho \leq \lambda_n(k_n^\varrho + 1) \leq \lambda_n(k_n^\varrho + 2) \leq 1 - \frac{\varrho}{2}$, $\lambda_n k_n^\varrho \to 1 - \varrho$ and

$$\lim_{n\to\infty} \frac{v_n^{j_n^\varrho+2} - v_n^{j_n^\varrho+1}}{\sqrt{\lambda_n}} = 0, \qquad \lim_{n\to\infty} \frac{v_n^{k_n^\varrho+2} - v_n^{k_n^\varrho+1}}{\sqrt{\lambda_n}} = 0. \quad (6.11)$$

Since, by assumption, $v_n \to v$ in L^1 and $S_v = \{0\}$, arguing as in [5, Proof of Theorem 4], we have that there exists $h_n \in \mathbb{N}$ with $\lambda_n h_n \to 0$ such that

$$\lim_{n\to\infty} \frac{v_n^{h_n+1} - v_n^{h_n}}{\sqrt{\lambda_n}} = +\infty. \quad (6.12)$$

We then split the energy $E_n(v_n)$, starting from (6.6), as follows

$$\begin{aligned} &E_n(v_n) \\ &= \frac{1}{2}J_1\left(\frac{v_n^1 - v_n^0}{\sqrt{\lambda_n}} + \gamma\right) + \sum_{i=0}^{j_n^\varrho} \varsigma_n^i + \sum_{i=j_n^\varrho+1}^{k_n^\varrho} \varsigma_n^i + \sum_{i=k_n^\varrho+1}^{n-2} \varsigma_n^i + \frac{1}{2}J_1\left(\frac{v_n^n - v_n^{n-1}}{\sqrt{\lambda_n}} + \gamma\right) - J_0(\gamma), \end{aligned} \quad (6.13)$$

and proceed as in [11, Theorem 4.8]. First of all we can write

$$\sum_{i=0}^{j_n^\varrho} \varsigma_n^i = \sum_{i=0}^{h_n-2} \varsigma_n^i + \frac{1}{2} J_1 \left(\frac{v_n^{h_n} - v_n^{h_n-1}}{\sqrt{\lambda_n}} + \gamma \right) + \frac{1}{2} J_1 \left(\frac{v_n^{h_n+2} - v_n^{h_n+1}}{\sqrt{\lambda_n}} + \gamma \right) + \sum_{i=h_n+1}^{j_n^\varrho} \varsigma_n^i - 2J_0(\gamma) + r_1(n), \tag{6.14}$$

where

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

and is infinitesimal as $n \to \infty$, since $J_1(+\infty) = J_2(+\infty) = 0$. We show that

$$\frac{1}{2} J_1 \left(\frac{v_n^{h_n} - v_n^{h_n-1}}{\sqrt{\lambda_n}} + \gamma \right) + \sum_{i=0}^{h_n-2} \varsigma_n^i \geq B_b \left(u_0^{(1)} \right), \tag{6.15}$$

$$\frac{1}{2} J_1 \left(\frac{v_n^{h_n+2} - v_n^{h_n+1}}{\sqrt{\lambda_n}} + \gamma \right) + \sum_{i=h_n+1}^{j_n^\varrho} \varsigma_n^i \geq B(\gamma) - r_2(n), \tag{6.16}$$

with $r_2(n) \to 0$ as $n \to \infty$, see below for details. Let us start by proving the inequality in (6.15). We define for $j = 0, \dots, h_n - 2$

$$\widehat{w}_n^j := -\frac{v_n^{h_n-j}}{\sqrt{\lambda_n}} - (h_n - j)\gamma.$$

Then

$$\frac{1}{2} J_1 \left(\frac{v_n^{h_n} - v_n^{h_n-1}}{\sqrt{\lambda_n}} + \gamma \right) + \sum_{i=0}^{h_n-2} \varsigma_n^i = \frac{1}{2} J_1 \left(\widehat{w}_n^1 - \widehat{w}_n^0 \right) + \sum_{j=0}^{h_n-2} \left\{ J_2 \left(\frac{\widehat{w}_n^{j+2} - \widehat{w}_n^j}{2} \right) + \frac{1}{2} \left(J_1 \left(\widehat{w}_n^{j+2} - \widehat{w}_n^{j+1} \right) + J_1 \left(\widehat{w}_n^{j+1} - \widehat{w}_n^j \right) \right) - J_0(\gamma) \right\}$$

and, moreover, $\widehat{w}_n^{h_n} = 0$, $\widehat{w}_n^{h_n} - \widehat{w}_n^{h_n-1} = u_0^{(1)}$, which means that $\widehat{w}_n$ is an admissible test for $B_b \left(u_0^{(1)} \right)$ with $h_n - 1$ playing the rôle of k, cf. (3.5). Thus (6.15) holds true.

To prove (6.16) we define for $j \in \mathbb{N}$

$$\widetilde{u}_n^j := \begin{cases} \gamma j + \dfrac{v_n^{h_n+1+j} - v_n^{h_n+1}}{\sqrt{\lambda_n}} & \text{if } j \leq j_n^\varrho - h_n + 1, \\ \gamma j + \dfrac{v_n^{j_n^\varrho+2} - v_n^{h_n+1}}{\sqrt{\lambda_n}} & \text{if } j \geq j_n^\varrho - h_n + 1. \end{cases}$$

Therefore we find

$$\frac{1}{2} J_1 \left(\frac{v_n^{h_n+2} - v_n^{h_n+1}}{\sqrt{\lambda_n}} + \gamma \right) + \sum_{i=h_n+1}^{j_n^\varrho} \varsigma_n^i = \frac{1}{2} J_1 \left(\widetilde{u}_n^1 - \widetilde{u}_n^0 \right) + \sum_{j \geq 0} \left\{ J_2 \left(\frac{\widetilde{u}_n^{j+2} - \widetilde{u}_n^j}{2} \right) + \frac{1}{2} \left(J_1 \left(\widetilde{u}_n^{j+2} - \widetilde{u}_n^{j+1} \right) + J_1 \left(\widetilde{u}_n^{j+1} - \widetilde{u}_n^j \right) \right) - J_0(\gamma) \right\} - r_2(n),$$

where $r_2(n)$ corresponds to the term $j = j_n^\varrho - h_n$ and converges to 0 as $n \to \infty$ by (6.11) and (2.3). We can consider an infinite sum since the terms for $j \geq j_n^\varrho - h_n + 1$ are identically 0. Note that $\widetilde{u}_n^0 = 0$, $\widetilde{u}_n^{j+1} - \widetilde{u}_n^j = \gamma$ for all $j \geq j_n^\varrho - h_n + 1$. According to the definition of $B(\gamma)$ recalled in (3.4), we thus obtain (6.16).

In order to estimate the part $\frac{1}{2} J_1 \left(\frac{v_n^n - v_n^{n-1}}{\sqrt{\lambda_n}} + \gamma \right) + \sum_{i=k_n^\varrho+1}^{n-2} \varsigma_n^i$ in (6.13), we argue in a similar way as above and use the fact that the function $w_n : \mathbb{N} \to \mathbb{R}$ defined as

$$w_n^j := \begin{cases} \gamma j - \frac{v_n^{n-j} - \delta_n}{\sqrt{\lambda_n}} & \text{if } 0 \leq j \leq n - k_n^\varrho - 1, \\ \gamma j - \frac{v_n^{k_n^\varrho+1} - \delta_n}{\sqrt{\lambda_n}} & \text{if } j \geq n - k_n^\varrho - 1 \end{cases} \tag{6.17}$$

satisfies $w_n^0 = -\frac{v_n^n - \delta_n}{\sqrt{\lambda_n}} = 0$, $w_n^1 - w_n^0 = \frac{v_n^n - v_n^{n-1}}{\sqrt{\lambda_n}} + \gamma = u_1^{(1)}$, $w_n^{j+1} - w_n^j = \gamma$ for $j \geq n - k_n^\varrho - 1$, and therefore is a competitor for the minimization problem defining $B\left(u_1^{(1)}, \gamma\right)$, cf. (3.6). Hence

$$\begin{aligned}\frac{1}{2}J_1\left(\frac{v_n^n - v_n^{n-1}}{\sqrt{\lambda_n}} + \gamma\right) + \sum_{i=k_n^\varrho+1}^{n-2} \varsigma_n^i &= \frac{1}{2}J_1\left(w_n^1 - w_n^0\right) + \sum_{j\geq 0}\Bigg\{J_2\left(\frac{w_n^{j+2} - w_n^j}{2}\right) \\ &\quad + \frac{1}{2}\left(J_1\left(w_n^{j+2} - w_n^{j+1}\right) + J_1\left(w_n^{j+1} - w_n^j\right)\right) - J_0(\gamma)\Bigg\} - \omega(n) \\ &\geq B\left(u_1^{(1)}, \gamma\right) - \omega(n), \end{aligned} \tag{6.18}$$

with $\omega(n) \to 0$ as $n \to \infty$.

Finally, we discuss the sum from $j_n^\varrho + 1$ to k_n^ϱ, which yields the integral term in the Γ-limit. Note that (6.7) and (2.2) and a Taylor expansion of J_0 around γ yield

$$\begin{aligned}\sum_{i=j_n^\varrho+1}^{k_n^\varrho} \varsigma_n^i &\geq \sum_{i=j_n^\varrho+1}^{k_n^\varrho}\left\{J_0\left(\frac{v_n^{i+2} - v_n^i}{2\sqrt{\lambda_n}} + \gamma\right) - J_0(\gamma)\right\} \\ &= \sum_{i=j_n^\varrho+1}^{k_n^\varrho} \frac{\alpha}{2}\left(\frac{v_n^{i+2} - v_n^i}{2\lambda_n}\right)^2 2\lambda_n + o(1) \\ &\geq \sum_{\substack{i=j_n^\varrho+2 \\ i \text{ even}}}^{k_n^\varrho-1} \alpha\left(\frac{v_n^{i+2} - v_n^i}{2\lambda_n}\right)^2 2\lambda_n + o(1).\end{aligned}$$

In the spirit of Section 8.3 in [6] we define

$$I_n := \left\{i \ : \ \left(v_n^{i+2} - v_n^i\right)^2 > 2\lambda_n\right\}$$

and a piecewise $W^{1,\infty}(0,1)$-function $\tilde{v}_n$ with $S(\tilde{v}_n) = I_n$ such that, for i being even, $\left(\tilde{v}_n^i\right)^+ - \left(\tilde{v}_n^i\right)^- = v_n^{i+2} - v_n^i$ if $i \in I_n$ and

$$\tilde{v}_n'(t) = \begin{cases} \frac{v_n^{i+2} - v_n^i}{2\lambda_n} & \text{if } t \in (i\lambda_n, (i+2)\lambda_n), i \notin I_n, \\ 0 & \text{if } t \in (i\lambda_n, (i+2)\lambda_n), i \in I_n. \end{cases}$$

We observe that $(\tilde{v}_n)$, like (v_n), converges weakly to v in $H^1((0,1) \setminus S)$. Then, since the terms of the sum are non-negative,

$$\sum_{i=j_n^\varrho+1}^{k_n^\varrho} \varsigma_n^i \geq \int_{(j_n^\varrho+2)\lambda_n}^{(k_n^\varrho-1)\lambda_n} \alpha|\tilde{v}_n'(t)|^2\, dt + o(1).$$

Hence, by lower semicontinuity,

$$\liminf_{n\to\infty} \sum_{i=j_n^\varrho+1}^{k_n^\varrho} \varsigma_n^i \geq \alpha \int_\varrho^{1-\varrho} |v'|^2\, dt. \tag{6.19}$$

In summary, from (6.13)–(6.16), (6.18) and (6.19), together with the arbitrariness of ϱ, we obtain the desired liminf inequality (6.10).

Internal jump. Assume that $S_v = \{\bar{t}\}$, where $\bar{t} \in (0,1)$. Without loss of generality we consider $\bar{t} = \frac{1}{2}$. Let (v_n) be a sequence converging to v in L^1 such that $\sup_n E_n(v_n) < +\infty$. We prove

$$\liminf_{n\to\infty} E_n(v_n) \geq \alpha \int_0^1 |v'|^2\, dt + B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - 3J_0(\gamma) + 2B(\gamma). \tag{6.20}$$

Let $\varrho > 0$ be small enough (at least $\varrho < \frac{1}{4}$) such that $S \cap (\frac{1}{2} - \varrho, \frac{1}{2} + \varrho) = \{\frac{1}{2}\}$, where S is a finite set such that v_n converges weakly in $H^1((0,1) \setminus S)$ as in the compactness result above. Furthermore let $k_n^0, j_n^\varrho, h_n, k_n^\varrho, k_n^1$ be integers with $\lambda_n(k_n^0 + 2) \leq \varrho$ and $\lambda_n k_n^0 \to \varrho$, $\frac{1}{2} - \varrho \leq \lambda_n(j_n^\varrho + 1) \leq$

$\lambda_n(j_n^\varrho+2)<\frac{1}{2}$ and $\lambda_n j_n^\varrho \to \frac{1}{2}-\varrho$, $\frac{1}{2}<\lambda_n(k_n^\varrho+1)\le\lambda_n(k_n^\varrho+2)\le\frac{1}{2}+\varrho$ and $\lambda_n k_n^\varrho\to\frac{1}{2}+\varrho$, $\lambda_n(k_n^1+1)\ge 1-\varrho$ and $\lambda_n k_n^1\to 1-\varrho$, $\lambda_n h_n\le\frac{1}{2}$ and $\lambda_n h_n\to\frac{1}{2}$ such that

$$\begin{aligned}&\frac{v_n^{k_n^0+2}-v_n^{k_n^0+1}}{\sqrt{\lambda_n}}\to 0,\ \frac{v_n^{k_n^1+2}-v_n^{k_n^1+1}}{\sqrt{\lambda_n}}\to 0,\ \frac{v_n^{h_n+1}-v_n^{h_n}}{\sqrt{\lambda_n}}\to+\infty\\&\frac{v_n^{j_n^\varrho+2}-v_n^{j_n^\varrho+1}}{\sqrt{\lambda_n}}\to 0,\ \frac{v_n^{k_n^\varrho+2}-v_n^{k_n^\varrho+1}}{\sqrt{\lambda_n}}\to 0,\quad \text{as } n\to\infty.\end{aligned}\tag{6.21}$$

We then decompose the energy $E_n(v_n)$, starting from (6.6), as follows:

$$\begin{aligned}E_n(v_n)=&\frac{1}{2}J_1\left(\frac{v_n^1-v_n^0}{\sqrt{\lambda_n}}+\gamma\right)+\sum_{i=0}^{k_n^0}\varsigma_n^i+\sum_{i=k_n^0+1}^{j_n^\varrho}\varsigma_n^i+\sum_{i=j_n^\varrho+1}^{k_n^\varrho}\varsigma_n^i\\&+\sum_{i=k_n^\varrho+1}^{k_n^1}\varsigma_n^i+\sum_{i=k_n^1+1}^{n-2}\varsigma_n^i+\frac{1}{2}J_1\left(\frac{v_n^n-v_n^{n-1}}{\sqrt{\lambda_n}}+\gamma\right)-J_0(\gamma).\end{aligned}\tag{6.22}$$

Arguing as in (6.18) we have

$$\frac{1}{2}J_1\left(\frac{v_n^n-v_n^{n-1}}{\sqrt{\lambda_n}}+\gamma\right)+\sum_{i=k_n^1+1}^{n-2}\varsigma_n^i\ge B\left(u_1^{(1)},\gamma\right)-\omega(n),\tag{6.23}$$

and in a similar way we get

$$\frac{1}{2}J_1\left(\frac{v_n^1-v_n^0}{\sqrt{\lambda_n}}+\gamma\right)+\sum_{i=0}^{k_n^0}\varsigma_n^i\ge B\left(u_0^{(1)},\gamma\right)-\omega(n),\tag{6.24}$$

for some (in general different) functions $\omega(n)$, converging to 0 as $n\to\infty$. Moreover, as in (6.19)

$$\liminf_{n\to\infty}\sum_{i=k_n^0+1}^{j_n^\varrho}\varsigma_n^i\ge\alpha\int_\varrho^{\frac{1}{2}-\varrho}|v'|^2\,dt\tag{6.25}$$

and

$$\liminf_{n\to\infty}\sum_{i=k_n^\varrho+1}^{k_n^1}\varsigma_n^i\ge\alpha\int_{\frac{1}{2}+\varrho}^{1-\varrho}|v'|^2\,dt.\tag{6.26}$$

It remains to estimate the sum from $j_n^\varrho+1$ to k_n^ϱ in (6.22). We can write

$$\begin{aligned}\sum_{i=j_n^\varrho+1}^{k_n^\varrho}\varsigma_n^i=&\frac{1}{2}J_1\left(\frac{v_n^{h_n}-v_n^{h_n-1}}{\sqrt{\lambda_n}}+\gamma\right)+\sum_{i=j_n^\varrho+1}^{h_n-2}\varsigma_n^i+\frac{1}{2}J_1\left(\frac{v_n^{h_n+2}-v_n^{h_n+1}}{\sqrt{\lambda_n}}+\gamma\right)\\&+\sum_{i=h_n+1}^{k_n^\varrho}\varsigma_n^i-2J_0(\gamma)+\omega(n),\end{aligned}\tag{6.27}$$

where

$$\omega(n):=J_2\left(\frac{v_n^{h_n+1}-v_n^{h_n-1}}{2\sqrt{\lambda_n}}+\gamma\right)+J_1\left(\frac{v_n^{h_n+1}-v_n^{h_n}}{\sqrt{\lambda_n}}+\gamma\right)+J_2\left(\frac{v_n^{h_n+2}-v_n^{h_n}}{2\sqrt{\lambda_n}}+\gamma\right),$$

which is infinitesimal as $n\to\infty$ by (6.21). Similarly to the proof of Theorem 4.8 in [11] there follows

$$\frac{1}{2}J_1\left(\frac{v_n^{h_n}-v_n^{h_n-1}}{\sqrt{\lambda_n}}+\gamma\right)+\sum_{i=j_n^\varrho+1}^{h_n-2}\varsigma_n^i\ge B(\gamma)+r_1(n),\tag{6.28}$$

$$\frac{1}{2}J_1\left(\frac{v_n^{h_n+2}-v_n^{h_n+1}}{\sqrt{\lambda_n}}+\gamma\right)+\sum_{i=h_n+1}^{k_n^\varrho}\varsigma_n^i\ge B(\gamma)+r_2(n),\tag{6.29}$$

with $r_i(n)\to 0$, for $i=1,2$, as $n\to\infty$.

This concludes the proof of the liminf inequality, since (6.28)–(6.29) together with (6.22)–(6.27) and the arbitrariness of ϱ give (6.20).

Limsup inequality. As before we distinguish between the case of having a jump at the boundary or in the interior. We consider first the case of a jump at 0.

Jump at 0. Let v be a piecewise H^1-function with $S_v = \{0\}$. By a density argument, see, e.g., [6, Remark 1.29], we can assume that $v \in C^2(0,1)$ and that there exists a small $\varrho > 0$ such that $v = v(0^+)$ on $(0, \varrho)$ and $v = v(1) = \delta$ on $(1-\varrho, 1]$.

We prove that there is a sequence (v_n) converging to v in $L^1(0,1)$ such that

$$\limsup_n E_n(v_n) \leq \alpha \int_0^1 |v'|^2\,dt + B\left(u_1^{(1)}, \gamma\right) - J_0(\gamma) + B_{BJ}\left(u_0^{(1)}\right), \tag{6.30}$$

where $B_{BJ}\left(u_0^{(1)}\right) = \frac{1}{2}J_1\left(u_0^{(1)}\right) + B_b\left(u_0^{(1)}\right) + B(\gamma) - 2J_0(\gamma)$, cf. (3.7).

Let us fix $\eta > 0$. Then by the definition of the boundary layer energy (3.5) we can find $\widehat{w} : \mathbb{N} \to \mathbb{R}$ and $\widehat{k}_0 \in \mathbb{N}$ such that $\widehat{w}^{\widehat{k}_0+1} = 0$, $\widehat{w}^{\widehat{k}_0} = -u_0^{(1)}$ and

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

Similarly, by (3.4) there exist $\widetilde{w} : \mathbb{N} \to \mathbb{R}$ and $\widetilde{N} \in \mathbb{N}$ such that $\widetilde{w}^0 = 0$, $\widetilde{w}^{i+1} - \widetilde{w}^i = \gamma$ if $i \geq \widetilde{N}$ and

$$\frac{1}{2}J_1\left(\widetilde{w}^1 - \widetilde{w}^0\right) + \sum_{i\geq 0}\left\{J_2\left(\frac{\widetilde{w}^{i+2} - \widetilde{w}^i}{2}\right) + \frac{1}{2}\left(J_1\left(\widetilde{w}^{i+2} - \widetilde{w}^{i+1}\right) + J_1\left(\widetilde{w}^{i+1} - \widetilde{w}^i\right)\right) - J_0(\gamma)\right\}$$
$$\leq B(\gamma) + \eta. \tag{6.31}$$

Moreover, by (3.6) there exist $w : \mathbb{N} \to \mathbb{R}$ and $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^1 = u_1^{(1)}$, $w^{i+1} - w^i = \gamma$ if $i \geq N_2$ such that

$$\frac{1}{2}J_1\left(w^1 - w^0\right) + \sum_{i\geq 0}\left\{J_2\left(\frac{w^{i+2} - w^i}{2}\right) + \frac{1}{2}\left(J_1\left(w^{i+2} - w^{i+1}\right) + J_1\left(w^{i+1} - w^i\right)\right) - J_0(\gamma)\right\}$$
$$\leq B\left(u_1^{(1)}, \gamma\right) + \eta. \tag{6.32}$$

The idea is to construct a recovery sequence which yields the elastic contribution $\alpha\int_0^1 |v'|^2$ in $[\frac{\varrho}{2}, 1-\frac{\varrho}{2}]$, the boundary layer energy $B\left(u_1^{(1)}, \gamma\right)$ in $(1-\frac{\varrho}{2}, 1]$, and the two boundary layer energies $B_b\left(u_0^{(1)}\right)$ and $B(\gamma)$ about the jump point in $[0, \frac{\varrho}{2})$, cf. Figure 5.

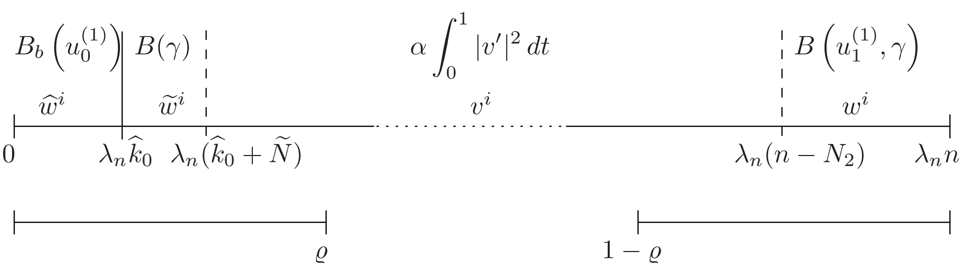

FIGURE 5. Related to the construction of the recovery sequence.

Let (k_n^0) be a sequence of integers with $\lambda_n k_n^0 \to \frac{\varrho}{2}$ as $n \to \infty$, and let (k_n^1) be a sequence of integers with $\lambda_n k_n^1 \to 1 - \frac{\varrho}{2}$ as $n \to \infty$ such that for any $n \in \mathbb{N}$

$$\widehat{k}_0 + \widetilde{N} + 3 \leq k_n^0 \leq \frac{\varrho}{\lambda_n} - 2 \qquad \text{and} \qquad \frac{1-\varrho}{\lambda_n} \leq k_n^1 \leq n - N_2 - 2.$$

We define a sequence (v_n) by means of the functions v, $\widetilde{w}$, w and $\widehat{w}$ as follows and then show that this serves as a recovery sequence. For any $i \in \mathbb{N}$ we set

$$v_n^i = \begin{cases} -\sqrt{\lambda_n}\left(\widehat{w}^{\widehat{k}_0+1-i} + \gamma i\right) & \text{if } 0 \le i \le \widehat{k}_0 + 1, \\ v(0^+) + \delta_n - \delta + \sqrt{\lambda_n}\left(\widetilde{w}^{i-\widehat{k}_0-2} - \widetilde{w}^{\widetilde{N}} - w^{N_2+1}\right) & \\ \qquad\qquad -\sqrt{\lambda_n}\gamma\left(i - \widehat{k}_0 - 3 - \widetilde{N} - N_2\right) & \text{if } \widehat{k}_0 + 2 \le i \le k_n^0 + 1, \\ v^i + \delta_n - \delta + \sqrt{\lambda_n}\left(-w^{N_2+1} + \gamma(N_2+1)\right) & \text{if } k_n^0 + 1 \le i \le k_n^1 + 1, \\ \delta_n + \sqrt{\lambda_n}\left(-w^{n-i} + \gamma(n-i)\right) & \text{if } k_n^1 + 1 \le i \le n. \end{cases}$$

Observe that the four boundary conditions are satisfied since $\widehat{w}^{\widehat{k}_0+1} = 0$, $\widehat{w}^{\widehat{k}_0} = -u_0^{(1)}$ and $w^0 = 0$, $w^1 = u_1^{(1)}$. Next we show that the sequence (v_n) is uniquely defined in $i = k_n^0 + 1$. Indeed,

$$\begin{aligned} & v^{k_n^0+1} + \delta_n - \delta + \sqrt{\lambda_n}\left(-w^{N_2+1} + \gamma(N_2+1)\right) - \Big[v(0^+) + \delta_n - \delta \\ & + \sqrt{\lambda_n}\left(\widetilde{w}^{k_n^0+1-\widehat{k}_0-2} - \widetilde{w}^{\widetilde{N}} - w^{N_2+1} - \gamma\left(k_n^0 + 1 - \widehat{k}_0 - 3 - \widetilde{N} - N_2\right)\right)\Big] \\ & = v^{k_n^0+1} - v(0^+) - \sqrt{\lambda_n}\left(\widetilde{w}^{k_n^0-1-\widehat{k}_0} - \widetilde{w}^{\widetilde{N}} - \gamma\left(k_n^0 - 1 - \widehat{k}_0 - \widetilde{N}\right)\right) = 0 \end{aligned}$$

since $v^{k_n^0+1} = v(0^+)$ by construction and since $\widetilde{w}^{i+1} - \widetilde{w}^i = \gamma$ if $i \ge \widetilde{N}$ (notice that $k_n^0 - 2 - \widehat{k}_0 \ge \widetilde{N}$). Similarly we have that (v_n) is uniquely defined in $i = k_n^1 + 1$.

Furthermore v_n converges to v in $L^1(0,1)$. Indeed, let us discuss the convergence in the subset $(1 - \frac{\varrho}{2}, 1)$, since then with similar arguments the convergence in the remaining subintervals $(0, \frac{\varrho}{2})$ and $[\frac{\varrho}{2}, 1 - \frac{\varrho}{2}]$ can be derived. Note that $v^i = v(\lambda_n i) = \delta$ for every $i \in \{k_n^1 + 1, \dots, n\}$ by construction. We claim that for the corresponding Riemann sums

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=k_n^1+1}^{n} \left|v_n^i - \delta\right| = 0.$$

Indeed, since $v_n^i = \delta_n + \sqrt{\lambda_n}\left(\gamma(N_2+1) - w^{N_2+1}\right)$ for $k_n^1 + 1 \le i \le n - N_2$, we have

$$\begin{aligned} \frac{1}{n} \sum_{i=k_n^1+1}^{n} \left|v_n^i - \delta\right| &= \frac{1}{n} \sum_{i=k_n^1+1}^{n-N_2} \left|\delta_n + \sqrt{\lambda_n}\left(\gamma(N_2+1) - w^{N_2+1}\right) - \delta\right| + \frac{1}{n} \sum_{i=n-N_2+1}^{n} \left|v_n^i - \delta\right| \\ &\le \left|\delta_n - \delta + \sqrt{\lambda_n}\left(\gamma(N_2+1) - w^{N_2+1}\right)\right| \left(1 - \frac{N_2}{n} - \frac{k_n^1}{n}\right) \\ &\quad + \frac{N_2}{n} \max_{n-N_2+1 \le i \le n} |v_n^i - \delta|, \end{aligned}$$

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

Moreover, for later reference, notice that $\frac{v_n^{\widehat{k}_0+2} - v_n^{\widehat{k}_0+1}}{\sqrt{\lambda_n}}$, $\frac{v_n^{\widehat{k}_0+2} - v_n^{\widehat{k}_0}}{2\sqrt{\lambda_n}}$ and $\frac{v_n^{\widehat{k}_0+3} - v_n^{\widehat{k}_0+1}}{2\sqrt{\lambda_n}}$ converge to ∞ as $n \to \infty$, by the definition of v_n.

We are now in a position to discuss the upper limit of the energy $E_n(v_n)$ as $n \to \infty$. Starting from (6.6), we split the sum as follows

$$\sum_{i=0}^{n-2} \varsigma_n^i = \sum_{i=0}^{\widehat{k}_0-1} \varsigma_n^i + \varsigma_n^{\widehat{k}_0} + \varsigma_n^{\widehat{k}_0+1} + \sum_{i=\widehat{k}_0+2}^{k_n^0-1} \varsigma_n^i + \varsigma_n^{k_n^0} + \sum_{i=k_n^0+1}^{k_n^1-1} \varsigma_n^i + \varsigma_n^{k_n^1} + \sum_{i=k_n^1+1}^{n-2} \varsigma_n^i,$$

where ς_n^i is defined in (6.7). Proceeding as in Theorem 4.8 of [11], we first observe that

$$\sum_{i=0}^{\widehat{k}_0-1} \varsigma_n^i + \varsigma_n^{\widehat{k}_0} \le B_b\left(u_0^{(1)}\right) + \eta + r(n) - J_0(\gamma)$$

with $\lim_{n\to\infty} r(n) = J_2(+\infty) + \frac{1}{2}J_1(+\infty) = 0$. Similarly we obtain

$$\varsigma_n^{\widehat{k}_0+1} + \sum_{i=\widehat{k}_0+2}^{k_n^0-1} \varsigma_n^i \le B(\gamma) + \eta + r(n) - J_0(\gamma), \tag{6.33}$$

where $r(n)$ is a function with the same limiting properties as the one above.

Since $v^{k_n^0+1} = v^{k_n^0+2} = v\left(0^+\right)$ by construction and since $\widetilde{w}^{k_n^0-\widehat{k}_0-2} - \widetilde{w}^{\widetilde{N}} = \gamma(k_n^0 - \widehat{k}_0 - 2 - \widetilde{N})$ and $\widetilde{w}^{k_n^0-\widehat{k}_0-1} - \widetilde{w}^{k_n^0-\widehat{k}_0-2} = \gamma$ by $k_n^0 - \widehat{k}_0 - 3 \geq \widetilde{N}$, we have $\varsigma_n^{k_n^0} = J_2(\gamma) + J_1(\gamma) - J_0(\gamma) = 0$. Similarly, $\varsigma_n^{k_n^1} = 0$.

Next we consider the sum from $i = k_n^1 + 1$ to $n - 2$. By writing the sum in terms of j with $j = n - i - 2$ and by observing that we can pass to an infinite sum for $j \geq 0$ as $n - k_n^1 - 2 \geq N_2$ by construction, we obtain

$$\sum_{i=k_n^1+1}^{n-2} \varsigma_n^i \leq B\left(u_1^{(1)}, \gamma\right) - \frac{1}{2} J_1\left(w^1 - w^0\right) + \eta.$$

It remains to estimate the sum from $i = k_n^0+1$ up to $k_n^1 - 1$, which will yield the elastic integral. By identifying v with its piecewise affine interpolation we can speak about the derivative of v and use the identity

$$\frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} = \sqrt{\lambda_n}\frac{v\left((i+1)\lambda_n\right) - v\left(i\lambda_n\right)}{\lambda_n} = \sqrt{\lambda_n} v'(i\lambda_n)$$

to rewrite ς_n^i defined in (6.7). We have

$$\begin{aligned} \varsigma_n^i = &J_2\left(\frac{\sqrt{\lambda_n}}{2}\left(v'(i\lambda_n) + v'((i+1)\lambda_n)\right) + \gamma\right) + \frac{1}{2} J_1\left(\sqrt{\lambda_n} v'(i\lambda_n) + \gamma\right) \\ &+ \frac{1}{2} J_1\left(\sqrt{\lambda_n} v'((i+1)\lambda_n) + \gamma\right) - J_0(\gamma). \end{aligned} \tag{6.34}$$

Moreover, Taylor expansions of J_1 and J_2 around γ up to the second order in λ yield

$$\begin{aligned} \varsigma_n^i &= \frac{\lambda_n}{4}\left\{J_1''(\gamma)\left(v'(i\lambda_n)^2 + v'((i+1)\lambda_n)^2\right) + \frac{1}{2} J_2''(\gamma)\left(v'(i\lambda_n) + v'((i+1)\lambda_n)\right)^2 + o(1)\right\} \\ &= \frac{\lambda_n}{8}\left\{J_1''(\gamma)\left(v'(i\lambda_n) - v'((i+1)\lambda_n)\right)^2 + J_0''(\gamma)\left(v'(i\lambda_n) + v'((i+1)\lambda_n)\right)^2 + o(1)\right\}, \end{aligned} \tag{6.35}$$

where we also used the assumptions $J_1(\gamma) + J_2(\gamma) = J_0(\gamma)$, $J_1'(\gamma) + J_2'(\gamma) = J_0'(\gamma) = 0$ and $J_2''(\gamma) = J_0''(\gamma) - J_1''(\gamma)$.

Recall that v' is continuous by assumption. Thus $(v'(i\lambda_n) - v'((i+1)\lambda_n))^2$ is of order $o(1)$. Moreover, since $J_0''(\gamma) > 0$, we obtain by using (6.35) and the definition $\alpha = \frac{1}{2} J_0''(\gamma)$

$$\begin{aligned} \sum_{i=k_n^0+1}^{k_n^1-1} \varsigma_n^i &\leq \sum_{i=k_n^0+1}^{k_n^1-1} \frac{\lambda_n}{4}\left\{J_0''(\gamma)\left(v'(i\lambda_n)^2 + v'((i+1)\lambda_n)^2\right) + o(1)\right\} \\ &\leq \frac{1}{2}\alpha\left(\sum_{i=k_n^0+1}^{k_n^1-1} v'(i\lambda_n)^2\lambda_n + \sum_{i=k_n^0+1}^{k_n^1-1} v'((i+1)\lambda_n)^2\lambda_n\right) + o(1) \\ &\leq \alpha\int_0^1 |v'|^2\, dt + o(1). \end{aligned} \tag{6.36}$$

We summarize all estimates and obtain from the splitting of the energy in (6.6)

$$\begin{aligned} \limsup_{n\to\infty} E_n(v_n) &= \limsup_{n\to\infty} \sum_{i=0}^{n-2} \varsigma_n^i + \frac{1}{2} J_1\left(u_0^{(1)}\right) + \frac{1}{2} J_1\left(u_1^{(1)}\right) - J_0(\gamma) \\ &\leq B_b\left(u_0^{(1)}\right) + B(\gamma) + B\left(u_1^{(1)}, \gamma\right) + \alpha\int_0^1 |v'|^2\, dt - 3J_0(\gamma) + \frac{1}{2} J_1\left(u_0^{(1)}\right) + 3\eta, \end{aligned}$$

which gives (6.30) since $\eta > 0$ can be chosen arbitrarily small.

Internal jump. Without loss of generality we assume that $S_v = \left\{\frac{1}{2}\right\}$ where $v \in C^2([0,1] \setminus \{\frac{1}{2}\})$, with $v(0) = 0$ and $v(1) = \delta$. Moreover, as in the case of the jump at 0, we note that it is not restrictive to assume that $v = v(0)$ on $[0, \varrho)$, $v = v(\frac{1}{2}^-)$ on $(\frac{1}{2} - \varrho, \frac{1}{2})$, $v = v(\frac{1}{2}^+)$ on $(\frac{1}{2}, \frac{1}{2} + \varrho)$, and $v = v(1) = \delta$ on $(1 - \varrho, 1]$ for some $\varrho > 0$ small enough.

We prove that there exists a sequence (v_n) converging to v in $L^1(0,1)$ such that

$$\limsup_{n\to\infty} E_n(v_n) \leq \alpha\int_0^1 |v'|^2\, dt + B\left(u_0^{(1)}, \gamma\right) + B\left(u_1^{(1)}, \gamma\right) - 3J_0(\gamma) + 2B(\gamma). \tag{6.37}$$

Let us fix $\eta > 0$. Then by the definitions of the boundary layer energies we can find $\widehat{v} : \mathbb{N} \to \mathbb{R}$ and $N_1 \in \mathbb{N}$ such that $\widehat{v}^0 = 0$, $\widehat{v}^1 - \widehat{v}^0 = \widehat{v}^1 = u_0^{(1)}$, $\widehat{v}^{i+1} - \widehat{v}^i = \gamma$ if $i \geq N_1$ and

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

Similarly, there exist $w : \mathbb{N} \to \mathbb{R}$ and $N_2 \in \mathbb{N}$ with $w^0 = 0$, $w^1 = u_1^{(1)}$, $w^{i+1} - w^i = \gamma$ if $i \geq N_2$ such that (6.32) is satisfied. Moreover, by the definition of $B(\gamma)$ there exist $\widetilde{w} : \mathbb{N} \to \mathbb{R}$ and $\widetilde{N} \in \mathbb{N}$ such that $\widetilde{w}^0 = 0$, $\widetilde{w}^{i+1} - \widetilde{w}^i = \gamma$ if $i \geq \widetilde{N}$ and (6.31) holds.

The idea is to construct a recovery sequence which yields the elastic contribution $\alpha \int_0^1 |v'|^2$ in $[\frac{\varrho}{2}, \frac{1}{2} - \frac{\varrho}{2}] \cup [\frac{1}{2} + \frac{\varrho}{2}, 1 - \frac{\varrho}{2}]$, the boundary layer energy $B\left(u_0^{(1)}, \gamma\right)$ in $[0, \frac{\varrho}{2})$, the boundary layer energy $B\left(u_1^{(1)}, \gamma\right)$ in $(1 - \frac{\varrho}{2}, 1]$ and $2B(\gamma)$ about the jump point in $(\frac{1}{2} - \frac{\varrho}{2}, \frac{1}{2} + \frac{\varrho}{2})$.

Let $k_n^0, j_n^\varrho, h_n, k_n^\varrho, k_n^1$ be integers with $\lambda_n k_n^0 \to \frac{\varrho}{2}$, $\lambda_n j_n^\varrho \to \frac{1}{2} - \frac{\varrho}{2}$, $\lambda_n h_n \to \frac{1}{2}$, $\lambda_n k_n^\varrho \to \frac{1}{2} + \frac{\varrho}{2}$, $\lambda_n k_n^1 \to 1 - \frac{\varrho}{2}$, as $n \to \infty$ such that for any $n \in \mathbb{N}$

$$N_1 + 2 \leq k_n^0 \leq \frac{\varrho}{\lambda_n} - 2, \quad \frac{1}{2\lambda_n} - \frac{\varrho}{\lambda_n} \leq j_n^\varrho \leq \frac{1}{2\lambda_n}, \quad \frac{1}{2\lambda_n} \leq k_n^\varrho + 1 \leq \frac{1}{2\lambda_n} + \frac{\varrho}{\lambda_n},$$
$$\frac{1-\varrho}{\lambda_n} \leq k_n^1 \leq n - N_2 - 2, \quad \widetilde{N} \leq \min\left\{h_n - j_n^\varrho - 2, k_n^\varrho - h_n - 2\right\}. \tag{6.38}$$

We define a sequence (v_n) with the help of the functions $\widehat{v}$, $\widetilde{w}$ and w as follows and then show that this serves as a recovery sequence. For any $i \in \mathbb{N}$ we set

$$v_n^i = \begin{cases} \sqrt{\lambda_n}(\widehat{v}^i - \gamma i) & \text{if } 0 \leq i \leq k_n^0, \\ v^i + \sqrt{\lambda_n}(\widehat{v}^{N_1} - \gamma N_1) & \text{if } k_n^0 \leq i \leq j_n^\varrho, \\ v\left(\frac{1}{2}^-\right) + \sqrt{\lambda_n}(-\widetilde{w}^{h_n - i} + \widetilde{w}^{\widetilde{N}} + \widehat{v}^{N_1} & \\ \qquad -\gamma(i - h_n + \widetilde{N} + N_1)) & \text{if } j_n^\varrho \leq i \leq h_n, \\ v\left(\frac{1}{2}^+\right) + \delta_n - \delta + \sqrt{\lambda_n}(\widetilde{w}^{i-(h_n+1)} - \widetilde{w}^{\widetilde{N}} - w^{N_2+1} & \\ \qquad -\gamma(i - h_n - 2 - \widetilde{N} - N_2)) & \text{if } h_n + 1 \leq i \leq k_n^\varrho + 1, \\ v^i + \delta_n - \delta + \sqrt{\lambda_n}\left(-w^{N_2+1} + \gamma(N_2+1)\right) & \text{if } k_n^\varrho + 1 \leq i \leq k_n^1 + 1, \\ \delta_n - \sqrt{\lambda_n}\left(w^{n-i} - \gamma(n-i)\right) & \text{if } k_n^1 + 1 \leq i \leq n. \end{cases}$$

Observe that the four boundary conditions are satisfied since $\widehat{v}^0 = 0$, $\widehat{v}^1 = u_0^{(1)}$ and $w^0 = 0$, $w^1 = u_1^{(1)}$. By the definitions of the functions $\widehat{v}$, w and $\widetilde{w}$ and the relations (6.38), the sequence v_n^i is uniquely defined in $i = k_n^0$, $i = j_n^\varrho$, $i = k_n^\varrho + 1$ and $i = k_n^1 + 1$.

Furthermore v_n converges to v in $L^1(0,1)$, which can be proved similarly as for the case of a jump at 0. Moreover, for later reference, notice that $\frac{v_n^{h_n+2} - v_n^{h_n}}{2\sqrt{\lambda_n}}$, $\frac{v_n^{h_n+1} - v_n^{h_n}}{\sqrt{\lambda_n}}$ and $\frac{v_n^{h_n+1} - v_n^{h_n-1}}{2\sqrt{\lambda_n}}$ converge to ∞ as $n \to \infty$.

We are now in a position to discuss the upper limit of the energy $E_n(v_n)$ as $n \to \infty$. We start from (6.6) and now split the sum as follows

$$\sum_{i=0}^{n-2} \varsigma_n^i = \sum_{i=0}^{k_n^0 - 2} \varsigma_n^i + \varsigma_n^{k_n^0 - 1} + \sum_{i=k_n^0}^{j_n^\varrho - 2} \varsigma_n^i + \varsigma_n^{j_n^\varrho - 1} + \sum_{i=j_n^\varrho}^{h_n - 2} \varsigma_n^i + \varsigma_n^{h_n - 1} + \varsigma_n^{h_n} + \sum_{i=h_n+1}^{k_n^\varrho - 1} \varsigma_n^i$$
$$+ \varsigma_n^{k_n^\varrho} + \sum_{i=k_n^\varrho + 1}^{k_n^1 - 1} \varsigma_n^i + \varsigma_n^{k_n^1} + \sum_{i=k_n^1+1}^{n-2} \varsigma_n^i, \tag{6.39}$$

where ς_n^i is defined in (6.7). We observe that

$$\sum_{i=0}^{k_n^0-2} \varsigma_n^i \le B\left(u_0^{(1)},\gamma\right) - \frac{1}{2}J_1\left(\widehat{v}^1 - \widehat{v}^0\right) + \eta; \qquad \sum_{i=j_n^\varrho}^{h_n-2} \varsigma_n^i + \varsigma_n^{h_n-1} \le B(\gamma) + \eta + r(n) - J_0(\gamma)$$

$$\sum_{i=k_n^1+1}^{n-2} \varsigma_n^i \le B\left(u_1^{(1)},\gamma\right) - \frac{1}{2}J_1\left(w^1 - w^0\right) + \eta; \qquad \varsigma_n^{h_n} + \sum_{i=h_n+1}^{k_n^\varrho-1} \varsigma_n^i \le B(\gamma) + \eta + r(n) - J_0(\gamma), \tag{6.40}$$

where $r(n)$ denotes as usual some infinitesimal function for $n \to \infty$.

From the definitions of the functions $\widehat{v}$, w and $\widetilde{w}$ and the relations (6.38) it follows that $\varsigma_n^{k_n^0-1} = \varsigma_n^{j_n^\varrho-1} = \varsigma_n^{k_n^\varrho} = \varsigma_n^{k_n^1} = 0$.

The sum from $i = k_n^\varrho + 1$ to $i = k_n^1 - 1$ in (6.39) can be treated as the corresponding sum for the case of a jump at 0 in (6.36) and we obtain

$$\sum_{i=k_n^\varrho+1}^{k_n^1-1} \varsigma_n^i \le \sum_{i=k_n^\varrho+1}^{k_n^1-1} \frac{\lambda_n}{4}\left\{J_0''(\gamma)\left(v'(i\lambda_n)^2 + v'((i+1)\lambda_n)^2\right) + o(1)\right\}$$
$$\le \alpha \int_{\frac{1}{2}}^{1} |v'|^2\,dt + o(1).$$

Similarly, for the sum from $i = k_n^0$ to $i = j_n^\varrho - 2$ in (6.39) we have

$$\sum_{i=k_n^0}^{j_n^\varrho-2} \varsigma_n^i \le \alpha \int_0^{\frac{1}{2}} |v'|^2\,dt + o(1).$$

We summarize all estimates and obtain from the splitting of the energy in (6.39)

$$\limsup_{n\to\infty} E_n(v_n) = \limsup_{n\to\infty} \sum_{i=0}^{n-2} \varsigma_n^i + \frac{1}{2}J_1\left(u_0^{(1)}\right) + \frac{1}{2}J_1\left(u_1^{(1)}\right) - J_0(\gamma)$$
$$\le B\left(u_0^{(1)},\gamma\right) + 2B(\gamma) + \alpha\int_0^1 |v'|^2\,dt + B\left(u_1^{(1)},\gamma\right) - 3J_0(\gamma) + 4\eta,$$

which is the asserted upper bound on the energy since $\eta > 0$ can be chosen arbitrarily small.

Convergence of minimization problems. The convergence of minimum values follows from the Γ-convergence of the functionals. To verify (6.5) we first observe that for $\delta > 0$

$$\min_v E_0(v) = B\left(u_0^{(1)},\gamma\right) + B\left(u_1^{(1)},\gamma\right) - J_0(\gamma)$$
$$+ \min\Big\{\alpha\int_0^1 |v'|^2\,dt + \beta_0\#\left(S_v\cap\{0\}\right) + \beta_1\#\left(S_v\cap\{1\}\right) + \beta_{\text{int}}\#(S_v\cap(0,1)) \;:\; v(0)=0, v(1)=\delta,\ [v]>0 \text{ on } S_v\Big\}.$$

Let $\delta > 0$ be fixed and let v satisfy the two boundary conditions $v(0) = 0$ and $v(1) = \delta$, and such that $[v] > 0$ on S_v. If $S_v = \emptyset$, then we have to minimize

$$\alpha\int_0^1 |v'|^2\,dt,$$

and the minimizer is $v(t) = \delta t$ with energy $\alpha\delta^2$. If $S_v = \{\overline{t}\}$, then the minimizer is the piecewise constant function

$$v(t) := \begin{cases} 0 & \text{if } t \in [0,\overline{t}), \\ \delta & \text{if } t \in (\overline{t},1] \end{cases}$$

with energy $\beta_{\min}$. □

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